Molecule recommendations for TMC-1

Lee *et al.*

2021-07-28

Foreword

The following molecules were identified to be of astrochemical interest towards the dark molecular cloud TMC-1 using the unsupervised machine learning methodology described in:

Lee *et al.*, "Unsupervised Machine Learning of Interstellar Chemical Inventories" (2021)

This PDF presents preliminary data for 1510 molecules that are of interest to the chemical inventory of TMC-1, as identified with machine learning. The molecules are identified based on a Euclidean distance cutoff, providing up to 100 of the closest molecules to those already seen in TMC-1. Structures were generated from their SMILES strings using `OpenBabel` and `rdkit`, and geometry optimization carried out using the geomeTRIC program:

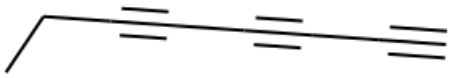
> Wang, L.-P.; Song, C.C. (2016), *J. Chem, Phys.* 144, 214108. http://dx.doi.org/10.1063/1.4952956

Electronic structure calculations were performed using `psi4`, with both geometry optimization and dipole moments calculated at at the ωB97X-D/6-31+G(d) level of theory. Equilibrium dipole moments and rotational constants are reported in unsigned debye and MHz respectively; for the latter, we provide effective scaled parameters as well that empirically correct for vibration-rotation interactions. Please refer to "Lee, K. L. K. and McCarthy, M. 2020, *J Phys Chem A*, 5, 898" for information regarding their uncertainties. For molecules where SCF/geometry optimizations failed to converge, we provide their dipole moments based on the molecular mechanics structures. These molecules will be indicated by "Is DFT optimized?: False".

The predicted column densities and uncertainties are given with a simple Gaussian Process with rational quadratic and white noise kernels. Simply put, the predicted column densities of unseen molecules are given as functions of distance in chemical space that decays naturally to zero for infinite distance from other data points. The reader is encouraged to look at the distances between recommendations and TMC-1 molecules to develop an intuition for how the predicted column density behaves roughly with distance, and interpret them with the uncertainties accordingly: as a guide but not to rule out molecules specifically. Molecules with particularly large uncertainties are likely to be impactful in constraining the chemistry of the source, even if we provide just an upper limit.

Finally, there is no real ordering of which the molecules are given. This is quasi-random, although there are pockets of similar molecules based on how similar the TMC-1 molecules are between searches.

geom1



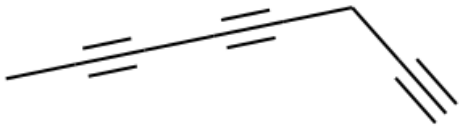
SMILES: C#CC#CC#CCC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (2.63)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	octa-1,3,5-triyne
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	19617.4923, 555.7001, 544.0459
A_s, B_s, C_s	19560.6016, 554.0885, 542.4682
Charge, Multiplicity	0, 1
Predicted log column density	10.648±2.875
Electronic energy	-308.16417

geom2



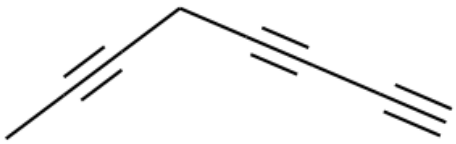
SMILES: C#CCC#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (2.70)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	octa-1,4,6-triyne
$\mu_{a,b,c}$	0.8, 0.3, 0.0
A, B, C	9363.2737, 614.5400, 580.8564
A_s, B_s, C_s	9336.1202, 612.7578, 579.1719
Charge, Multiplicity	0, 1
Predicted log column density	11.594±2.193
Electronic energy	-308.15466

geom3



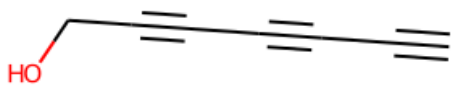
SMILES: C#CC#CCC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (3.01)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	octa-1,3,6-triyne
$\mu_{a,b,c}$	1.2, 0.1, 0.0
A, B, C	5807.9407, 688.5945, 620.3514
A_s, B_s, C_s	5791.0976, 686.5976, 618.5523
Charge, Multiplicity	0, 1
Predicted log column density	10.268±2.782
Electronic energy	-308.15341

geom4



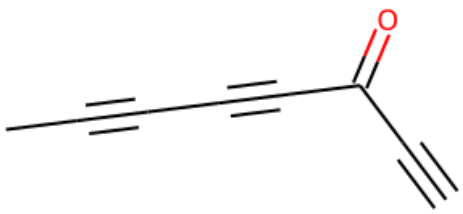
SMILES: C#CC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#C (3.55)

Is DFT optimized?: True

Property	Value
Formula	C7H4O
Molecular weight	104.108
IUPAC name	hepta-2,4,6-triyn-1-ol
$\mu_{a,b,c}$	0.6, 0.5, 1.3
A, B, C	23657.8452, 544.7921, 534.8793
A_s, B_s, C_s	23589.2374, 543.2122, 533.3282
Charge, Multiplicity	0, 1
Predicted log column density	10.602±3.211
Electronic energy	-344.04470

geom5



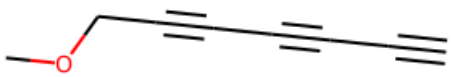
SMILES: C#CC(=O)C#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (3.90)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	3.7, 3.4, 0.0
A, B, C	4972.8925, 553.6091, 499.7139
A_s, B_s, C_s	4958.4711, 552.0036, 498.2647
Charge, Multiplicity	0, 1
Predicted log column density	10.488±3.824
Electronic energy	-382.13559

geom6



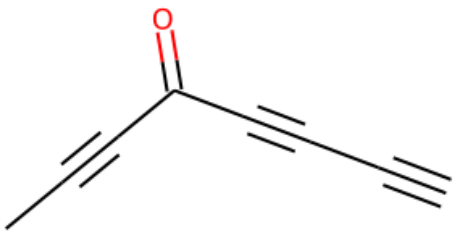
SMILES: C#CC#CC#CCOC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.08)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	7-methoxyhepta-1,3,5-triyne
$\mu_{a,b,c}$	1.7, 1.3, 0.0
A, B, C	18724.8080, 395.0020, 388.7497
A_s, B_s, C_s	18670.5061, 393.8565, 387.6223
Charge, Multiplicity	0, 1
Predicted log column density	12.613±3.753
Electronic energy	-383.33617

geom7



SMILES: C#CC#CC(=O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.14)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	0.3, 4.5, 0.0
A, B, C	2899.3262, 688.5331, 558.3437
A_s, B_s, C_s	2890.9182, 686.5363, 556.7245
Charge, Multiplicity	0, 1
Predicted log column density	9.600±3.891
Electronic energy	-382.13585

geom8

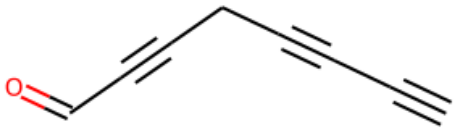
SMILES: CC#CC#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.19)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	octa-2,4,6-triyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	79645.3866, 494.2492, 494.2490
A_s, B_s, C_s	79414.4150, 492.8159, 492.8157
Charge, Multiplicity	0, 1
Predicted log column density	12.556±1.798
Electronic energy	-308.17643

geom9



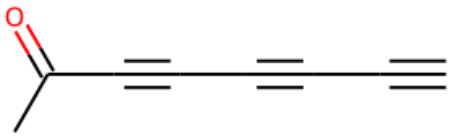
SMILES: C#CC#CCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.24)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	3.2, 0.4, 0.7
A, B, C	5828.8588, 475.5916, 442.0603
A_s, B_s, C_s	5811.9551, 474.2124, 440.7783
Charge, Multiplicity	0, 1
Predicted log column density	8.326±3.175
Electronic energy	-382.12589

geom10



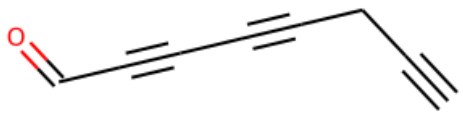
SMILES: C#CC#CC#CC(C)=O

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.24)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	octa-3,5,7-triyn-2-one
$\mu_{a,b,c}$	2.1, 2.8, 0.0
A, B, C	10252.3413, 459.4953, 440.9920
A_s, B_s, C_s	10222.6095, 458.1628, 439.7131
Charge, Multiplicity	0, 1
Predicted log column density	9.688±3.741
Electronic energy	-382.14572

geom11



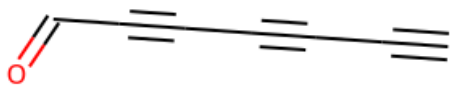
SMILES: C#CCC#CC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.30)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	3.4, 2.8, 0.2
A, B, C	6803.4930, 451.0968, 424.3095
A_s, B_s, C_s	6783.7629, 449.7886, 423.0790
Charge, Multiplicity	0, 1
Predicted log column density	9.653±2.420
Electronic energy	-382.12559

geom12



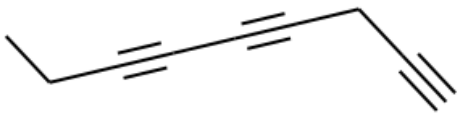
SMILES: C#CC#CC#CC=O

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (4.11)

Is DFT optimized?: True

Property	Value
Formula	C7H2O
Molecular weight	102.092
IUPAC name	hepta-2,4,6-triynal
$\mu_{a,b,c}$	3.3, 1.9, 0.0
A, B, C	46806.0187, 556.1260, 549.5960
A_s, B_s, C_s	46670.2812, 554.5132, 548.0021
Charge, Multiplicity	0, 1
Predicted log column density	10.453±1.995
Electronic energy	-342.83000

geom13



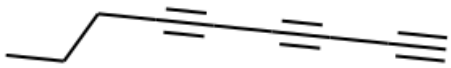
SMILES: C#CCC#CC#CCC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.47)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.3, 0.0
A, B, C	7938.7142, 431.8641, 412.7271
A_s, B_s, C_s	7915.6919, 430.6117, 411.5302
Charge, Multiplicity	0, 1
Predicted log column density	9.820±3.700
Electronic energy	-347.45769

geom14



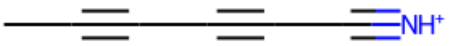
SMILES: C#CC#CC#CCCC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.49)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	nona-1,3,5-triyne
$\mu_{a,b,c}$	1.8, 0.0, 0.0
A, B, C	15783.6407, 388.6109, 381.9674
A_s, B_s, C_s	15737.8682, 387.4839, 380.8597
Charge, Multiplicity	0, 1
Predicted log column density	10.174±3.530
Electronic energy	-347.46817

geom15



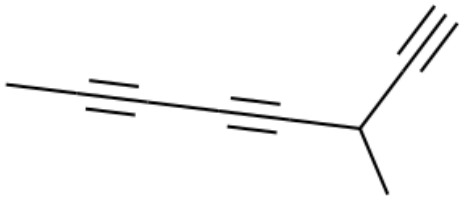
SMILES: CC#CC#CC#[NH+]

Nearest TMC-1 molecule (distance): CC#CC#CC#N (3.27)

Is DFT optimized?: True

Property	Value
Formula	C6H4N+
Molecular weight	90.105
IUPAC name	
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	157850.1296, 759.8642, 759.8629
A_s, B_s, C_s	157392.3643, 757.6606, 757.6593
Charge, Multiplicity	1, 1
Predicted log column density	11.499±1.638
Electronic energy	-285.26667

geom16



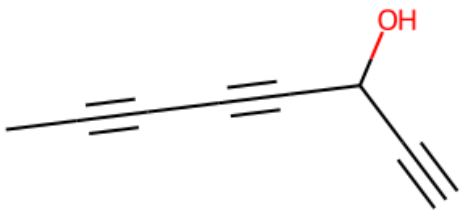
SMILES: C#CC(C)C#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.58)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	3-methylocta-1,4,6-triyne
$\mu_{a,b,c}$	0.7, 0.5, 0.1
A, B, C	4341.5451, 548.8777, 500.3494
A_s, B_s, C_s	4328.9546, 547.2860, 498.8983
Charge, Multiplicity	0, 1
Predicted log column density	10.221±4.211
Electronic energy	-347.45947

geom17



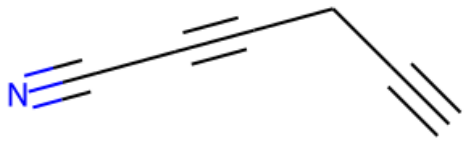
SMILES: C#CC(O)C#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.58)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	2.0, 1.4, 0.8
A, B, C	4460.2556, 548.0640, 499.7583
A_s, B_s, C_s	4447.3208, 546.4746, 498.3090
Charge, Multiplicity	0, 1
Predicted log column density	10.325±4.309
Electronic energy	-383.34149

geom18



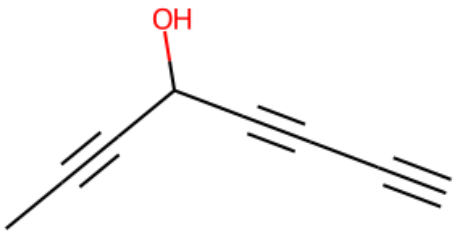
SMILES: C#CCC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (2.70)

Is DFT optimized?: True

Property	Value
Formula	C6H3N
Molecular weight	89.097
IUPAC name	
$\mu_{a,b,c}$	4.6, 1.6, 0.0
A, B, C	11286.8229, 1021.3060, 942.0095
A_s, B_s, C_s	11254.0911, 1018.3442, 939.2777
Charge, Multiplicity	0, 1
Predicted log column density	11.448±2.036
Electronic energy	-284.92718

geom19



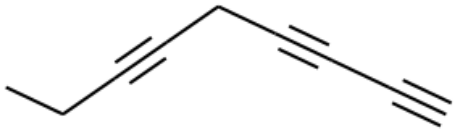
SMILES: C#CC#CC(O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.75)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	0.9, 2.1, 0.7
A, B, C	2633.3783, 694.4444, 565.4709
A_s, B_s, C_s	2625.7415, 692.4306, 563.8310
Charge, Multiplicity	0, 1
Predicted log column density	9.999±4.412
Electronic energy	-383.34079

geom20



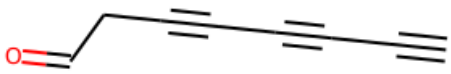
SMILES: C#CC#CCC#CCC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.75)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	1.1, 0.2, 0.0
A, B, C	2998.5204, 575.9950, 487.5546
A_s, B_s, C_s	2989.8247, 574.3246, 486.1406
Charge, Multiplicity	0, 1
Predicted log column density	8.494±4.183
Electronic energy	-347.45658

geom21



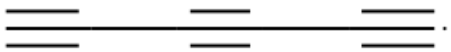
SMILES: C#CC#CC#CCC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.77)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	1.8, 0.8, 0.8
A, B, C	14818.0689, 407.4730, 398.4828
A_s, B_s, C_s	14775.0965, 406.2913, 397.3272
Charge, Multiplicity	0, 1
Predicted log column density	7.966±2.951
Electronic energy	-382.14011

geom22



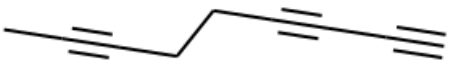
SMILES: [C]#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (2.54)

Is DFT optimized?: True

Property	Value
Formula	C6H
Molecular weight	73.074
IUPAC name	hexa-1,3,5-triyne
$\mu_{a,b,c}$	1.1, 0.0, 0.0
A, B, C	∞, 1384.9588, 1384.9588
A_s, B_s, C_s	∞, 1380.9424, 1380.9424
Charge, Multiplicity	0, 2
Predicted log column density	12.690±1.038
Electronic energy	-228.82093

geom23



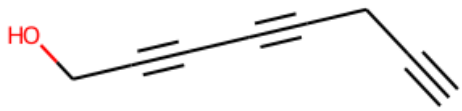
SMILES: C#CC#CCCC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.81)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	1.4, 0.2, 0.0
A, B, C	17292.6550, 406.9035, 400.5140
A_s, B_s, C_s	17242.5063, 405.7235, 399.3525
Charge, Multiplicity	0, 1
Predicted log column density	9.812±3.240
Electronic energy	-347.46331

geom24



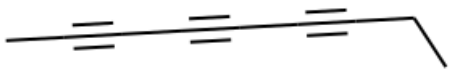
SMILES: C#CCC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.82)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	1.4, 0.1, 1.2
A, B, C	8360.1069, 423.1266, 405.1244
A_s, B_s, C_s	8335.8626, 421.8996, 403.9495
Charge, Multiplicity	0, 1
Predicted log column density	9.785±4.084
Electronic energy	-383.33898

geom25



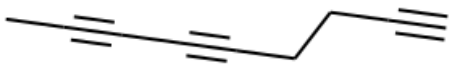
SMILES: CC#CC#CC#CCC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.83)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	nona-2,4,6-triyne
$\mu_{a,b,c}$	0.1, 0.1, 0.0
A, B, C	16960.1584, 367.1530, 361.8048
A_s, B_s, C_s	16910.9739, 366.0883, 360.7556
Charge, Multiplicity	0, 1
Predicted log column density	10.789±3.037
Electronic energy	-347.47954

geom26



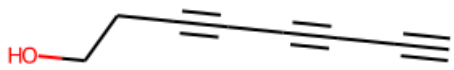
SMILES: C#CCCC#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.85)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.2, 0.0
A, B, C	15655.1350, 399.9903, 392.8786
A_s, B_s, C_s	15609.7351, 398.8304, 391.7392
Charge, Multiplicity	0, 1
Predicted log column density	11.133±2.775
Electronic energy	-347.46495

geom27



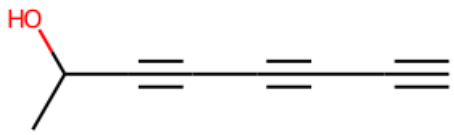
SMILES: C#CC#CC#CCCO

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.85)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	octa-3,5,7-triyn-1-ol
$\mu_{a,b,c}$	0.1, 1.0, 0.9
A, B, C	6799.0772, 463.4118, 440.1604
A_s, B_s, C_s	6779.3599, 462.0679, 438.8839
Charge, Multiplicity	0, 1
Predicted log column density	10.150±3.911
Electronic energy	-383.35517

geom28



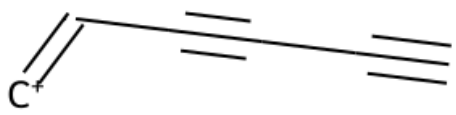
SMILES: C#CC#CC#CC(C)O

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.87)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	0.1, 1.1, 0.9
A, B, C	6792.3606, 463.7760, 440.4267
A_s, B_s, C_s	6772.6627, 462.4310, 439.1495
Charge, Multiplicity	0, 1
Predicted log column density	11.156±4.400
Electronic energy	-383.35517

geom29



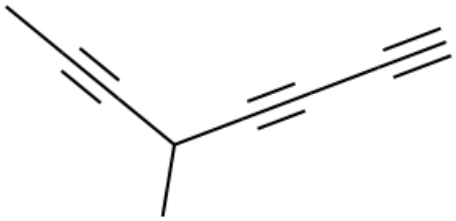
SMILES: C#CC#C[C]=[CH+]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (2.64)

Is DFT optimized?: True

Property	Value
Formula	C6H2+
Molecular weight	74.082
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	13479917354.5965, 1330.8549, 1330.8548
A_s, B_s, C_s	13440825594.2682, 1326.9954, 1326.9953
Charge, Multiplicity	1, 2
Predicted log column density	12.668±1.228
Electronic energy	-229.20873

geom30



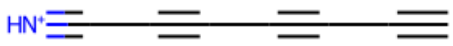
SMILES: C#CC#CC(C)C#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (4.89)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	1.3, 0.2, 0.1
A, B, C	2679.1916, 680.7736, 560.4167
A_s, B_s, C_s	2671.4219, 678.7994, 558.7915
Charge, Multiplicity	0, 1
Predicted log column density	9.887±4.393
Electronic energy	-347.45832

geom31



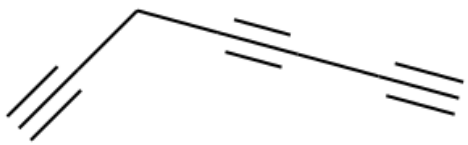
SMILES: C#CC#CC#CC#[NH+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (2.99)

Is DFT optimized?: True

Property	Value
Formula	C7H2N+
Molecular weight	100.100
IUPAC name	hepta-2,4,6-triynenitrilium
$\mu_{a,b,c}$	5.1, 0.0, 0.0
A, B, C	∞, 551.2034, 551.2034
A_s, B_s, C_s	∞, 549.6049, 549.6049
Charge, Multiplicity	1, 1
Predicted log column density	11.095±1.586
Electronic energy	-322.06700

geom32



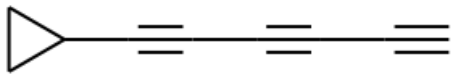
SMILES: C#CC#CCC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (2.70)

Is DFT optimized?: True

Property	Value
Formula	C7H4
Molecular weight	88.109
IUPAC name	hepta-1,3,6-triyne
$\mu_{a,b,c}$	0.5, 0.5, 0.0
A, B, C	11279.6487, 1016.6285, 937.9680
A_s, B_s, C_s	11246.9377, 1013.6803, 935.2479
Charge, Multiplicity	0, 1
Predicted log column density	11.387±2.096
Electronic energy	-268.83961

geom33



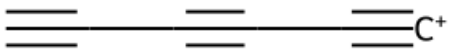
SMILES: C#CC#CC#CC1CC1

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.04)

Is DFT optimized?: True

Property	Value
Formula	C9H6
Molecular weight	114.147
IUPAC name	hexa-1,3,5-triynylcyclopropane
$\mu_{a,b,c}$	2.0, 0.0, 0.2
A, B, C	13208.1043, 451.5390, 450.9443
A_s, B_s, C_s	13169.8008, 450.2295, 449.6366
Charge, Multiplicity	0, 1
Predicted log column density	10.151±4.047
Electronic energy	-346.22468

geom34



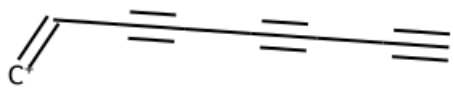
SMILES: [C+]#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (2.47)

Is DFT optimized?: True

Property	Value
Formula	C6H+
Molecular weight	73.074
IUPAC name	hexa-1,3,5-triyne
$\mu_{a,b,c}$	0.0, 5.2, 0.0
A, B, C	1624805222112.9878, 1381.7575, 1381.7575
A_s, B_s, C_s	1620093286968.8601, 1377.7504, 1377.7504
Charge, Multiplicity	1, 1
Predicted log column density	12.248±1.462
Electronic energy	-228.47256

geom35



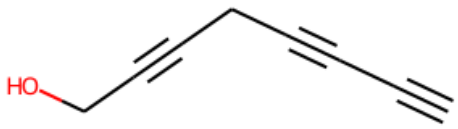
SMILES: C#CC#CC#C[C]=[CH+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (2.64)

Is DFT optimized?: True

Property	Value
Formula	C8H2+
Molecular weight	98.104
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	7318415085.5517, 569.0689, 569.0688
A_s, B_s, C_s	7297191681.8036, 567.4186, 567.4185
Charge, Multiplicity	1, 2
Predicted log column density	12.125±1.517
Electronic energy	-305.34908

geom36



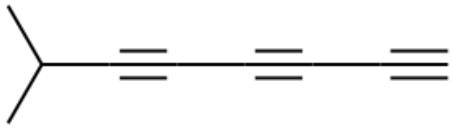
SMILES: C#CC#CCC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.07)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	1.0, 0.7, 0.9
A, B, C	3407.1471, 529.4789, 469.0443
A_s, B_s, C_s	3397.2663, 527.9434, 467.6841
Charge, Multiplicity	0, 1
Predicted log column density	8.463±4.642
Electronic energy	-383.33872

geom37



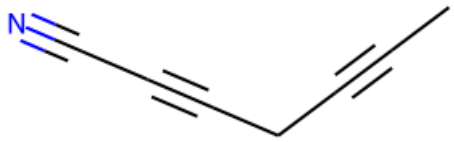
SMILES: C#CC#CC#CC(C)C

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.11)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	7-methylocta-1,3,5-triyne
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	7608.6066, 461.7012, 444.0118
A_s, B_s, C_s	7586.5416, 460.3623, 442.7242
Charge, Multiplicity	0, 1
Predicted log column density	11.306±4.425
Electronic energy	-347.46899

geom38



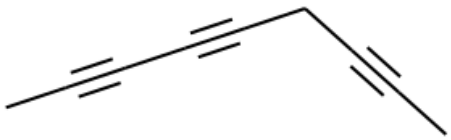
SMILES: CC#CCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (3.01)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	5.1, 1.9, 0.0
A, B, C	5721.2866, 693.6268, 623.4250
A_s, B_s, C_s	5704.6949, 691.6153, 621.6171
Charge, Multiplicity	0, 1
Predicted log column density	10.129±2.794
Electronic energy	-324.24178

geom39



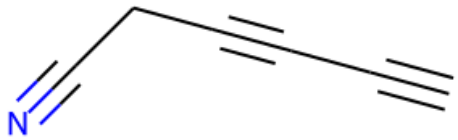
SMILES: CC#CC#CCC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.18)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	nona-2,4,7-triyne
$\mu_{a,b,c}$	0.1, 0.4, 0.0
A, B, C	4585.8174, 449.8680, 412.8401
A_s, B_s, C_s	4572.5186, 448.5633, 411.6429
Charge, Multiplicity	0, 1
Predicted log column density	10.438±3.101
Electronic energy	-347.46813

geom40



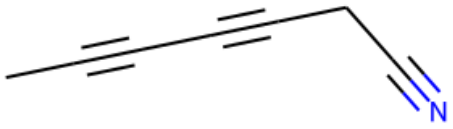
SMILES: C#CC#CCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (2.91)

Is DFT optimized?: True

Property	Value
Formula	C6H3N
Molecular weight	89.097
IUPAC name	hexa-3,5-diynenitrile
$\mu_{a,b,c}$	2.3, 3.0, 0.0
A, B, C	11983.2183, 1012.2355, 938.8252
A_s, B_s, C_s	11948.4670, 1009.3000, 936.1026
Charge, Multiplicity	0, 1
Predicted log column density	10.255±2.106
Electronic energy	-284.93275

geom41



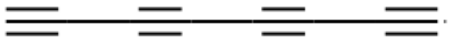
SMILES: CC#CC#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (2.91)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	hepta-3,5-diynenitrile
$\mu_{a,b,c}$	3.5, 2.9, 0.0
A, B, C	9850.7812, 611.3249, 579.7669
A_s, B_s, C_s	9822.2139, 609.5520, 578.0856
Charge, Multiplicity	0, 1
Predicted log column density	10.303±2.294
Electronic energy	-324.24866

geom42



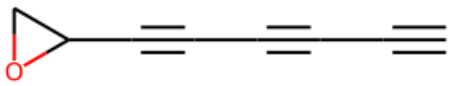
SMILES: [C]#CC#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (2.54)

Is DFT optimized?: True

Property	Value
Formula	C8H
Molecular weight	97.096
IUPAC name	octa-1,3,5,7-tetrayne
$\mu_{a,b,c}$	1.2, 0.0, 0.0
A, B, C	∞, 583.8458, 583.8458
A_s, B_s, C_s	∞, 582.1526, 582.1526
Charge, Multiplicity	0, 2
Predicted log column density	12.110±1.511
Electronic energy	-304.94540

geom43



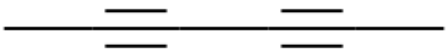
SMILES: C#CC#CC#CC1CO1

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.25)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	0.0, 1.4, 1.5
A, B, C	15457.7373, 445.7824, 445.3151
A_s, B_s, C_s	15412.9098, 444.4896, 444.0237
Charge, Multiplicity	0, 1
Predicted log column density	10.117±4.579
Electronic energy	-382.10353

geom44



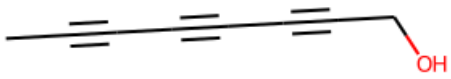
SMILES: CC#CC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.19)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	hexa-2,4-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	79730.7873, 1105.7669, 1105.7653
A_s, B_s, C_s	79499.5680, 1102.5602, 1102.5586
Charge, Multiplicity	0, 1
Predicted log column density	12.794±1.749
Electronic energy	-232.05086

geom45



SMILES: CC#CC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.33)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	octa-2,4,6-triyn-1-ol
$\mu_{a,b,c}$	2.3, 0.4, 1.2
A, B, C	19768.2840, 359.9032, 355.2866
A_s, B_s, C_s	19710.9560, 358.8595, 354.2562
Charge, Multiplicity	0, 1
Predicted log column density	10.776±3.356
Electronic energy	-383.36063

geom46

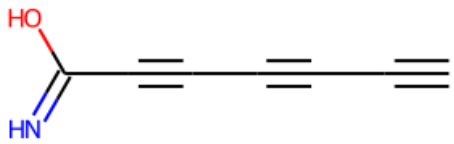
SMILES: C#CCC#CCC#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.52)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	nona-1,4,7-triyne
$\mu_{a,b,c}$	0.8, 0.4, 0.0
A, B, C	6787.0985, 466.6367, 440.1918
A_s, B_s, C_s	6767.4159, 465.2834, 438.9153
Charge, Multiplicity	0, 1
Predicted log column density	9.442±4.023
Electronic energy	-347.44805

geom47



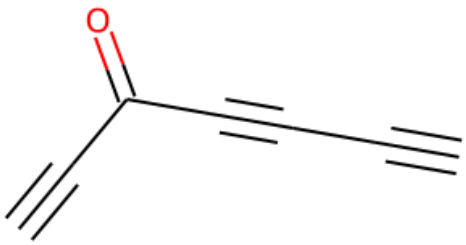
SMILES: C#CC#CC#CC(=N)O

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (5.01)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	4.9, 0.9, 0.0
A, B, C	11123.9162, 461.2651, 442.8998
A_s, B_s, C_s	11091.6569, 459.9274, 441.6154
Charge, Multiplicity	0, 1
Predicted log column density	11.059±3.846
Electronic energy	-398.17070

geom48



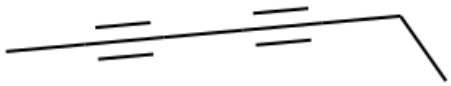
SMILES: C#CC#CC(=O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (3.90)

Is DFT optimized?: True

Property	Value
Formula	C7H2O
Molecular weight	102.092
IUPAC name	hepta-1,4,6-triyn-3-one
$\mu_{a,b,c}$	1.8, 3.4, 0.0
A, B, C	5254.1768, 937.6083, 795.6284
A_s, B_s, C_s	5238.9397, 934.8893, 793.3211
Charge, Multiplicity	0, 1
Predicted log column density	10.289±3.797
Electronic energy	-342.81852

geom49



SMILES: CC#CC#CCC

Nearest TMC-1 molecule (distance): CC#CC#C (4.83)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	hepta-2,4-diyne
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	18035.1313, 769.6282, 748.4531
A_s, B_s, C_s	17982.8294, 767.3963, 746.2826
Charge, Multiplicity	0, 1
Predicted log column density	11.031±3.015
Electronic energy	-271.35391

geom50

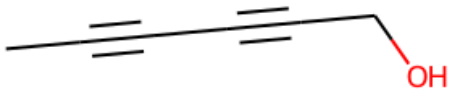
SMILES: C#CCCC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.85)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	4.7, 0.8, 0.0
A, B, C	19985.1629, 609.3180, 595.6466
A_s, B_s, C_s	19927.2060, 607.5509, 593.9192
Charge, Multiplicity	0, 1
Predicted log column density	10.883±2.592
Electronic energy	-324.23830

geom51



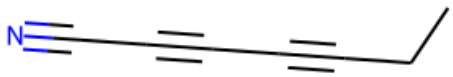
SMILES: CC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#C (5.33)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hexa-2,4-diyn-1-ol
$\mu_{a,b,c}$	2.2, 0.3, 1.2
A, B, C	21205.5778, 756.6610, 738.3390
A_s, B_s, C_s	21144.0816, 754.4667, 736.1978
Charge, Multiplicity	0, 1
Predicted log column density	11.005±3.322
Electronic energy	-307.23562

geom52



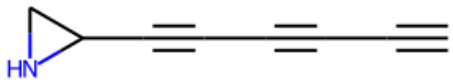
SMILES: CCC#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (2.63)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	6.6, 0.4, 0.0
A, B, C	19485.9650, 554.6716, 542.9619
A_s, B_s, C_s	19429.4557, 553.0631, 541.3873
Charge, Multiplicity	0, 1
Predicted log column density	10.485±2.887
Electronic energy	-324.25102

geom53



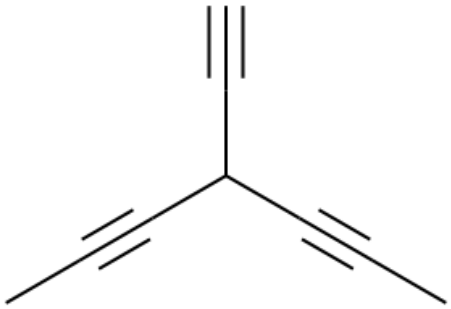
SMILES: C#CC#CC#CC1CN1

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (5.63)

Is DFT optimized?: True

Property	Value
Formula	C8H5N
Molecular weight	115.135
IUPAC name	
$\mu_{a,b,c}$	0.4, 0.7, 1.1
A, B, C	13815.4668, 451.7753, 451.5550
A_s, B_s, C_s	13775.4020, 450.4652, 450.2455
Charge, Multiplicity	0, 1
Predicted log column density	8.917±5.151
Electronic energy	-362.24493

geom54



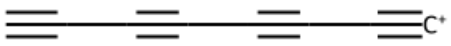
SMILES: C#CC(C#CC)C#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#C (5.75)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	0.0, 1.0, 0.1
A, B, C	1753.0865, 933.6988, 640.2738
A_s, B_s, C_s	1748.0026, 930.9911, 638.4170
Charge, Multiplicity	0, 1
Predicted log column density	9.483±4.613
Electronic energy	-347.44412

geom55



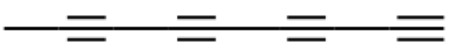
SMILES: [C+]#CC#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (2.47)

Is DFT optimized?: False

Property	Value
Formula	C8H+
Molecular weight	97.096
IUPAC name	octa-1,3,5,7-tetrayne
$\mu_{a,b,c}$	-, -, -
A, B, C	∞, 524.7169, 524.7169
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 1
Predicted log column density	11.844±1.609
Electronic energy	-

geom56



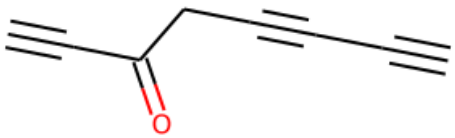
SMILES: C#CC#CC#CC#CC

Nearest TMC-1 molecule (distance): [C]#CC#CC#CC#C (4.19)

Is DFT optimized?: True

Property	Value
Formula	C9H4
Molecular weight	112.131
IUPAC name	nona-1,3,5,7-tetrayne
$\mu_{a,b,c}$	1.9, 0.0, 0.0
A, B, C	159168.6420, 375.0309, 375.0308
A_s, B_s, C_s	158707.0529, 373.9433, 373.9432
Charge, Multiplicity	0, 1
Predicted log column density	12.153±1.567
Electronic energy	-344.98589

geom57



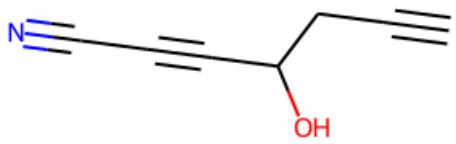
SMILES: C#CC#CCC(=O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (4.75)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	1.9, 1.4, 1.5
A, B, C	3303.1614, 791.6546, 665.9750
A_s, B_s, C_s	3293.5822, 789.3588, 664.0437
Charge, Multiplicity	0, 1
Predicted log column density	11.008±3.974
Electronic energy	-382.12914

geom58



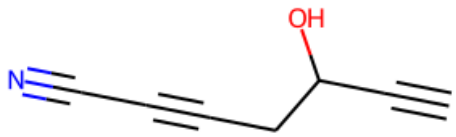
SMILES: C#CCC(O)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.64)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	4.2, 0.1, 1.1
A, B, C	2681.7666, 853.0643, 724.0629
A_s, B_s, C_s	2673.9894, 850.5904, 721.9631
Charge, Multiplicity	0, 1
Predicted log column density	10.957±4.492
Electronic energy	-399.42770

geom59



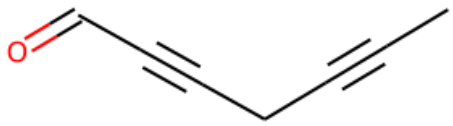
SMILES: C#CC(O)CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.61)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	6.0, 2.1, 1.3
A, B, C	6955.5933, 583.1129, 550.6241
A_s, B_s, C_s	6935.4220, 581.4219, 549.0273
Charge, Multiplicity	0, 1
Predicted log column density	9.950±4.798
Electronic energy	-399.42644

geom60



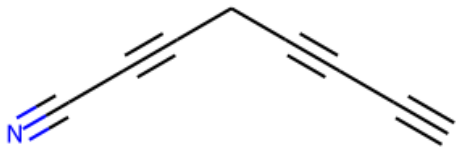
SMILES: CC#CCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.93)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	3.3, 1.7, 1.5
A, B, C	5084.3011, 682.9581, 618.5472
A_s, B_s, C_s	5069.5566, 680.9775, 616.7534
Charge, Multiplicity	0, 1
Predicted log column density	8.723±3.364
Electronic energy	-345.31672

geom61



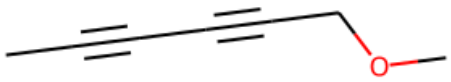
SMILES: C#CC#CCC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (3.01)

Is DFT optimized?: True

Property	Value
Formula	C8H3N
Molecular weight	113.119
IUPAC name	
$\mu_{a,b,c}$	3.9, 2.8, 0.0
A, B, C	4394.7272, 531.8641, 475.8413
A_s, B_s, C_s	4381.9825, 530.3217, 474.4614
Charge, Multiplicity	0, 1
Predicted log column density	9.748±2.612
Electronic energy	-361.04963

geom62



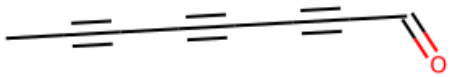
SMILES: CC#CC#CCOC

Nearest TMC-1 molecule (distance): CC#CC#C (5.70)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	0.1, 1.2, 0.0
A, B, C	17951.8849, 528.8082, 518.7290
A_s, B_s, C_s	17899.8244, 527.2746, 517.2246
Charge, Multiplicity	0, 1
Predicted log column density	13.006±3.817
Electronic energy	-346.52680

geom63



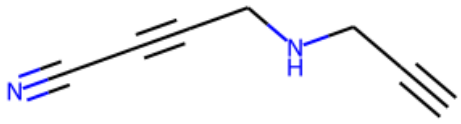
SMILES: CC#CC#CC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.38)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	octa-2,4,6-triynal
$\mu_{a,b,c}$	5.1, 1.8, 0.0
A, B, C	34757.7832, 367.2764, 364.2704
A_s, B_s, C_s	34656.9856, 366.2113, 363.2140
Charge, Multiplicity	0, 1
Predicted log column density	10.612±2.127
Electronic energy	-382.14710

geom64



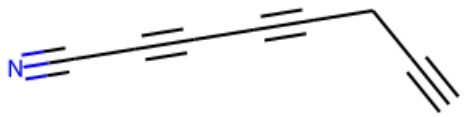
SMILES: C#CCNCC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.46)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	4.7, 2.4, 1.1
A, B, C	6425.7150, 480.9326, 450.4242
A_s, B_s, C_s	6407.0804, 479.5379, 449.1179
Charge, Multiplicity	0, 1
Predicted log column density	12.362±4.811
Electronic energy	-379.55441

geom65



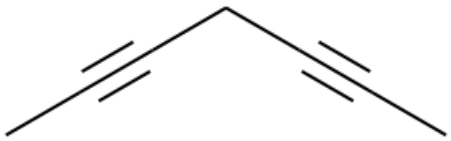
SMILES: C#CCC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (2.70)

Is DFT optimized?: True

Property	Value
Formula	C8H3N
Molecular weight	113.119
IUPAC name	
$\mu_{a,b,c}$	5.7, 1.2, 0.0
A, B, C	9228.4993, 452.0722, 432.1103
A_s, B_s, C_s	9201.7366, 450.7612, 430.8572
Charge, Multiplicity	0, 1
Predicted log column density	11.076±2.064
Electronic energy	-361.04989

geom66



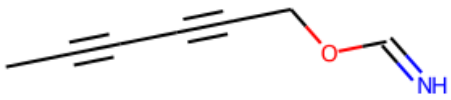
SMILES: CC#CCC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.18)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	hepta-2,5-diyne
$\mu_{a,b,c}$	0.0, 0.3, 0.0
A, B, C	6943.5563, 943.8026, 843.9609
A_s, B_s, C_s	6923.4200, 941.0655, 841.5134
Charge, Multiplicity	0, 1
Predicted log column density	10.654±3.086
Electronic energy	-271.34329

geom67



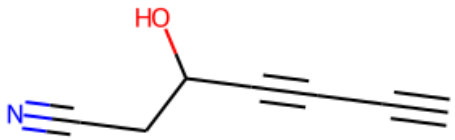
SMILES: CC#CC#CCOC=N

Nearest TMC-1 molecule (distance): CC#CC#CC#C (6.08)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	3.9, 1.6, 0.0
A, B, C	9818.9803, 413.0156, 398.3340
A_s, B_s, C_s	9790.5052, 411.8178, 397.1788
Charge, Multiplicity	0, 1
Predicted log column density	13.686±4.793
Electronic energy	-400.65086

geom68



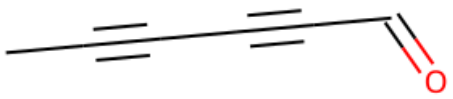
SMILES: C#CC#CC(O)CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.51)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	1.3, 2.7, 1.9
A, B, C	2214.8103, 914.9313, 668.1955
A_s, B_s, C_s	2208.3873, 912.2780, 666.2578
Charge, Multiplicity	0, 1
Predicted log column density	9.794±4.587
Electronic energy	-399.43271

geom69



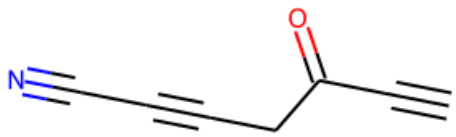
SMILES: CC#CC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#N (5.38)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	hexa-2,4-diynal
$\mu_{a,b,c}$	4.6, 1.8, 0.0
A, B, C	38363.2297, 770.7114, 759.1306
A_s, B_s, C_s	38251.9763, 768.4763, 756.9292
Charge, Multiplicity	0, 1
Predicted log column density	10.854±2.066
Electronic energy	-306.02307

geom70



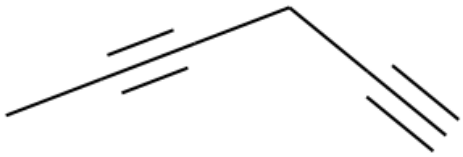
SMILES: C#CC(=O)CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.75)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	6.2, 3.8, 0.0
A, B, C	8624.3680, 589.5479, 553.7011
A_s, B_s, C_s	8599.3574, 587.8383, 552.0954
Charge, Multiplicity	0, 1
Predicted log column density	10.970±3.923
Electronic energy	-398.21577

geom71



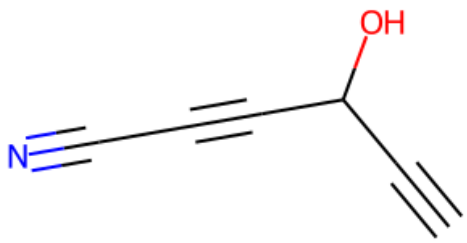
SMILES: C#CCC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (2.70)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	hexa-1,4-diyne
$\mu_{a,b,c}$	0.8, 0.2, 0.0
A, B, C	12258.0027, 1499.0501, 1358.2352
A_s, B_s, C_s	12222.4545, 1494.7028, 1354.2963
Charge, Multiplicity	0, 1
Predicted log column density	11.873±2.182
Electronic energy	-232.03002

geom72



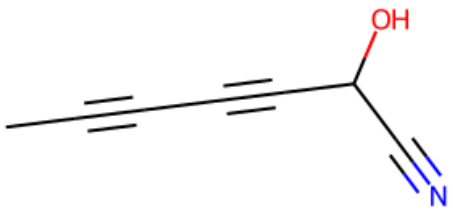
SMILES: C#CC(O)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.58)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO
Molecular weight	105.096
IUPAC name	
$\mu_{a,b,c}$	4.1, 0.8, 0.3
A, B, C	4670.8143, 930.4406, 799.7176
A_s, B_s, C_s	4657.2690, 927.7424, 797.3984
Charge, Multiplicity	0, 1
Predicted log column density	10.069±4.210
Electronic energy	-360.11215

geom73



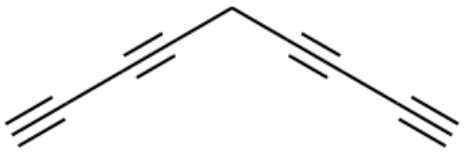
SMILES: CC#CC#CC(O)C#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.44)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	4.7, 1.6, 0.0
A, B, C	4561.3740, 547.1291, 500.0396
A_s, B_s, C_s	4548.1460, 545.5424, 498.5895
Charge, Multiplicity	0, 1
Predicted log column density	10.248±4.235
Electronic energy	-399.43315

geom74



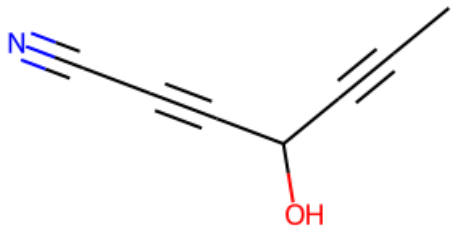
SMILES: C#CC#CCC#CC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#CC#C (3.01)

Is DFT optimized?: True

Property	Value
Formula	C9H4
Molecular weight	112.131
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.7, 0.0
A, B, C	4354.9438, 533.8614, 476.9631
A_s, B_s, C_s	4342.3144, 532.3132, 475.5800
Charge, Multiplicity	0, 1
Predicted log column density	9.835±2.656
Electronic energy	-344.96254

geom75



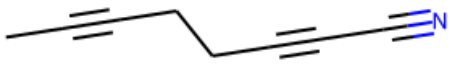
SMILES: CC#CC(O)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.75)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	5.2, 0.5, 0.2
A, B, C	2647.0510, 691.5017, 563.9588
A_s, B_s, C_s	2639.3746, 689.4963, 562.3233
Charge, Multiplicity	0, 1
Predicted log column density	9.867±4.404
Electronic energy	-399.42790

geom76



SMILES: CC#CCCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.81)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	5.8, 0.9, 0.0
A, B, C	17371.5478, 405.5445, 399.2517
A_s, B_s, C_s	17321.1703, 404.3684, 398.0938
Charge, Multiplicity	0, 1
Predicted log column density	9.685±3.254
Electronic energy	-363.55191

geom77

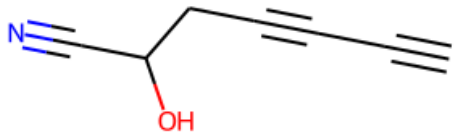
SMILES: C#CCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#C (4.30)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	hexa-2,5-diynal
$\mu_{a,b,c}$	3.5, 0.5, 0.4
A, B, C	13004.2326, 949.2548, 890.7341
A_s, B_s, C_s	12966.5203, 946.5020, 888.1510
Charge, Multiplicity	0, 1
Predicted log column density	9.928±2.385
Electronic energy	-306.00325

geom78



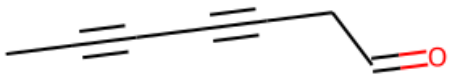
SMILES: C#CC#CCC(O)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	1.4, 2.9, 1.0
A, B, C	2870.0200, 815.7501, 740.3645
A_s, B_s, C_s	2861.6970, 813.3845, 738.2175
Charge, Multiplicity	0, 1
Predicted log column density	9.999±4.739
Electronic energy	-399.43275

geom79



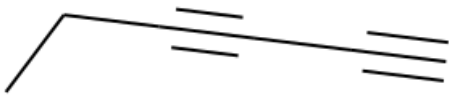
SMILES: CC#CC#CCC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (6.01)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	3.4, 0.4, 0.5
A, B, C	15360.6676, 543.7791, 529.2641
A_s, B_s, C_s	15316.1216, 542.2022, 527.7292
Charge, Multiplicity	0, 1
Predicted log column density	8.377±3.078
Electronic energy	-345.33124

geom80



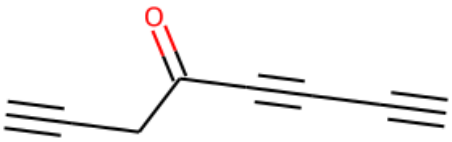
SMILES: C#CC#CCC

Nearest TMC-1 molecule (distance): CC#CC#C (2.63)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	hexa-1,3-diyne
$\mu_{a,b,c}$	1.3, 0.0, 0.0
A, B, C	21546.1432, 1331.6170, 1273.9559
A_s, B_s, C_s	21483.6594, 1327.7553, 1270.2615
Charge, Multiplicity	0, 1
Predicted log column density	11.012±2.880
Electronic energy	-232.03948

geom81



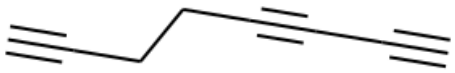
SMILES: C#CC#CC(=O)CC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (4.89)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	1.5, 2.7, 1.0
A, B, C	2372.7146, 952.6073, 696.5130
A_s, B_s, C_s	2365.8337, 949.8447, 694.4931
Charge, Multiplicity	0, 1
Predicted log column density	11.436±3.825
Electronic energy	-382.12910

geom82



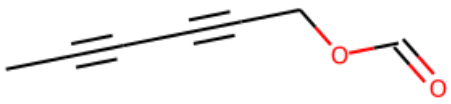
SMILES: C#CC#CCCC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (4.85)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	19824.0268, 610.2723, 596.4067
A_s, B_s, C_s	19766.5371, 608.5026, 594.6771
Charge, Multiplicity	0, 1
Predicted log column density	10.919±2.638
Electronic energy	-308.15017

geom83



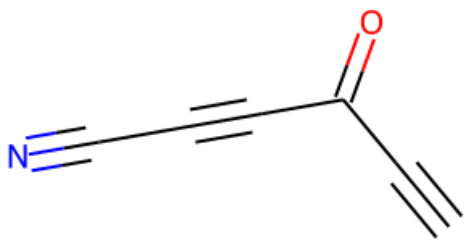
SMILES: CC#CC#CCOC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#C (6.21)

Is DFT optimized?: True

Property	Value
Formula	C7H6O2
Molecular weight	122.123
IUPAC name	hexa-2,4-diynyl formate
$\mu_{a,b,c}$	1.5, 1.3, 0.8
A, B, C	4999.4762, 526.2545, 497.0411
A_s, B_s, C_s	4984.9777, 524.7284, 495.5996
Charge, Multiplicity	0, 1
Predicted log column density	10.868±3.926
Electronic energy	-420.54344

geom84



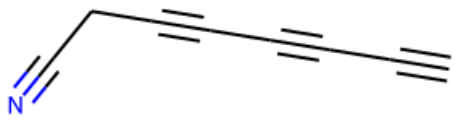
SMILES: C#CC(=O)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (3.90)

Is DFT optimized?: True

Property	Value
Formula	C6HNO
Molecular weight	103.080
IUPAC name	
$\mu_{a,b,c}$	2.9, 2.7, 0.0
A, B, C	5239.4371, 936.8852, 794.7693
A_s, B_s, C_s	5224.2427, 934.1683, 792.4645
Charge, Multiplicity	0, 1
Predicted log column density	10.268±3.740
Electronic energy	-358.90091

geom85



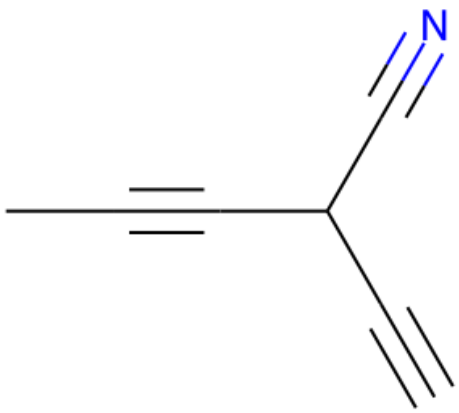
SMILES: C#CC#CC#CCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (2.91)

Is DFT optimized?: True

Property	Value
Formula	C8H3N
Molecular weight	113.119
IUPAC name	octa-3,5,7-triynenitrile
$\mu_{a,b,c}$	2.0, 3.2, 0.0
A, B, C	9941.8807, 449.0573, 430.7987
A_s, B_s, C_s	9913.0493, 447.7551, 429.5494
Charge, Multiplicity	0, 1
Predicted log column density	9.920±2.136
Electronic energy	-361.05673

geom86



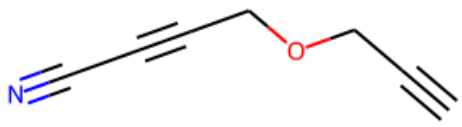
SMILES: C#CC(C#N)C#CC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.42)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	2.6, 3.1, 1.1
A, B, C	2736.2949, 1288.8159, 920.0407
A_s, B_s, C_s	2728.3596, 1285.0784, 917.3726
Charge, Multiplicity	0, 1
Predicted log column density	9.626±4.140
Electronic energy	-324.22302

geom87



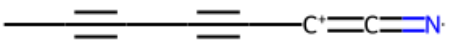
SMILES: C#CCOCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#C (6.23)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	4.8, 3.3, 0.0
A, B, C	6300.6924, 497.6447, 463.9160
A_s, B_s, C_s	6282.4204, 496.2016, 462.5707
Charge, Multiplicity	0, 1
Predicted log column density	12.463±4.913
Electronic energy	-399.40625

geom88



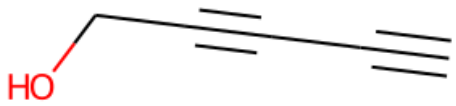
SMILES: CC#CC#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): CC#CC#CC#N (3.98)

Is DFT optimized?: False

Property	Value
Formula	C7H3N+
Molecular weight	101.108
IUPAC name	
$\mu_{a,b,c}$	-, -, -
A, B, C	45926.5312, 488.0174, 484.3647
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 2
Predicted log column density	12.285±1.832
Electronic energy	-

geom89



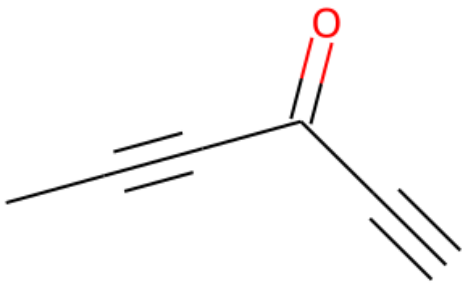
SMILES: C#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#C (3.55)

Is DFT optimized?: True

Property	Value
Formula	C5H4O
Molecular weight	80.086
IUPAC name	penta-2,4-diyn-1-ol
$\mu_{a,b,c}$	0.8, 0.4, 1.3
A, B, C	26412.6235, 1311.8645, 1262.7983
A_s, B_s, C_s	26336.0269, 1308.0601, 1259.1362
Charge, Multiplicity	0, 1
Predicted log column density	10.872±3.199
Electronic energy	-267.92037

geom90



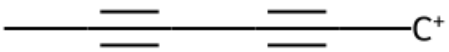
SMILES: C#CC(=O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (3.90)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	hexa-1,4-diyn-3-one
$\mu_{a,b,c}$	2.4, 3.6, 0.0
A, B, C	5314.4810, 1435.8007, 1138.4589
A_s, B_s, C_s	5299.0690, 1431.6369, 1135.1574
Charge, Multiplicity	0, 1
Predicted log column density	10.746±3.819
Electronic energy	-306.01280

geom91



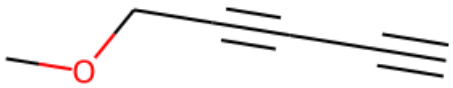
SMILES: CC#CC#C[CH4+]

Nearest TMC-1 molecule (distance): CC#CC#N (2.51)

Is DFT optimized?: True

Property	Value
Formula	C6H7+
Molecular weight	79.122
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.3, 0.1
A, B, C	26087.7752, 1215.6191, 1179.0225
A_s, B_s, C_s	26012.1206, 1212.0938, 1175.6034
Charge, Multiplicity	1, 1
Predicted log column density	12.100±1.557
Electronic energy	-232.37166

geom92



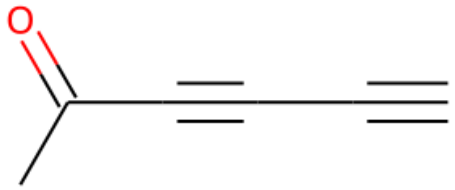
SMILES: C#CC#CCOC

Nearest TMC-1 molecule (distance): CC#CC#C (4.08)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	5-methoxypenta-1,3-diyne
$\mu_{a,b,c}$	1.4, 1.4, 0.0
A, B, C	22415.0490, 856.9841, 834.1615
A_s, B_s, C_s	22350.0453, 854.4989, 831.7424
Charge, Multiplicity	0, 1
Predicted log column density	12.882±3.732
Electronic energy	-307.21179

geom93



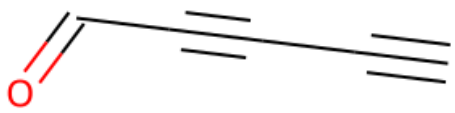
SMILES: C#CC#CC(C)=O

Nearest TMC-1 molecule (distance): CC#CC#C (4.24)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	hexa-3,5-diyn-2-one
$\mu_{a,b,c}$	1.8, 2.8, 0.0
A, B, C	10262.9880, 1094.6605, 995.2854
A_s, B_s, C_s	10233.2253, 1091.4860, 992.3991
Charge, Multiplicity	0, 1
Predicted log column density	9.977±3.727
Electronic energy	-306.02164

geom94



SMILES: C#CC#CC=O

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (4.11)

Is DFT optimized?: True

Property	Value
Formula	C5H2O
Molecular weight	78.070
IUPAC name	penta-2,4-diynal
$\mu_{a,b,c}$	3.0, 1.8, 0.0
A, B, C	53642.9626, 1338.5035, 1305.9182
A_s, B_s, C_s	53487.3980, 1334.6219, 1302.1310
Charge, Multiplicity	0, 1
Predicted log column density	10.764±1.960
Electronic energy	-266.70602

geom95

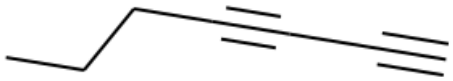
SMILES: C#CCC#CCC

Nearest TMC-1 molecule (distance): CC#CC#C (4.47)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	hepta-1,4-diyne
$\mu_{a,b,c}$	0.8, 0.3, 0.0
A, B, C	8685.4675, 944.9596, 908.5736
A_s, B_s, C_s	8660.2796, 942.2192, 905.9387
Charge, Multiplicity	0, 1
Predicted log column density	10.067±3.696
Electronic energy	-271.33311

geom96



SMILES: C#CC#CCCC

Nearest TMC-1 molecule (distance): CC#CC#C (4.49)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	hepta-1,3-diyne
$\mu_{a,b,c}$	1.4, 0.0, 0.0
A, B, C	18140.7312, 828.3142, 803.9888
A_s, B_s, C_s	18088.1230, 825.9121, 801.6572
Charge, Multiplicity	0, 1
Predicted log column density	10.454±3.511
Electronic energy	-271.34348

geom97

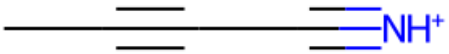
SMILES: [CH+]=[C]C#CC

Nearest TMC-1 molecule (distance): CC#CC#N (3.16)

Is DFT optimized?: True

Property	Value
Formula	C5H4+
Molecular weight	64.087
IUPAC name	
$\mu_{a,b,c}$	0.3, 0.0, 0.1
A, B, C	156850.9041, 2049.9413, 2049.3088
A_s, B_s, C_s	156396.0365, 2043.9964, 2043.3659
Charge, Multiplicity	1, 2
Predicted log column density	12.865±1.564
Electronic energy	-192.39975

geom98



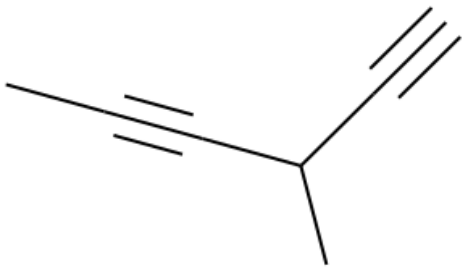
SMILES: CC#CC#[NH+]

Nearest TMC-1 molecule (distance): CC#CC#N (3.27)

Is DFT optimized?: True

Property	Value
Formula	C4H4N+
Molecular weight	66.083
IUPAC name	
$\mu_{a,b,c}$	2.0, 0.0, 0.0
A, B, C	157352.6488, 1996.4491, 1996.4423
A_s, B_s, C_s	156896.3261, 1990.6594, 1990.6526
Charge, Multiplicity	1, 1
Predicted log column density	11.820±1.599
Electronic energy	-209.13870

geom99



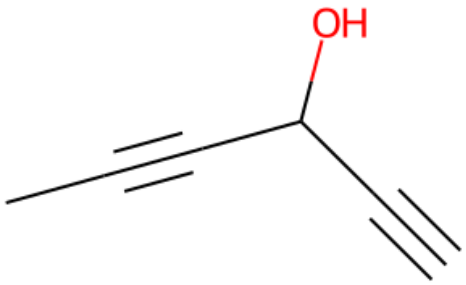
SMILES: C#CC(C)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.58)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	3-methylhexa-1,4-diyne
$\mu_{a,b,c}$	0.7, 0.5, 0.0
A, B, C	4601.8150, 1401.9383, 1130.0800
A_s, B_s, C_s	4588.4698, 1397.8727, 1126.8027
Charge, Multiplicity	0, 1
Predicted log column density	10.472±4.229
Electronic energy	-271.33475

geom100



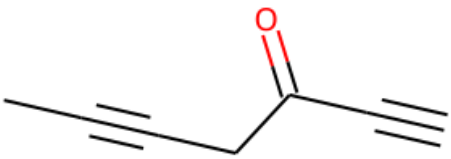
SMILES: C#CC(O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.58)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hexa-1,4-diyn-3-ol
$\mu_{a,b,c}$	1.6, 1.5, 0.8
A, B, C	4707.8257, 1422.2200, 1144.0467
A_s, B_s, C_s	4694.1730, 1418.0955, 1140.7290
Charge, Multiplicity	0, 1
Predicted log column density	10.574±4.314
Electronic energy	-307.21753

geom101



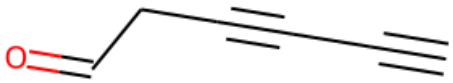
SMILES: C#CC(=O)CC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.75)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	2.7, 2.0, 1.4
A, B, C	3309.1340, 1163.9100, 924.0341
A_s, B_s, C_s	3299.5375, 1160.5346, 921.3544
Charge, Multiplicity	0, 1
Predicted log column density	11.446±4.038
Electronic energy	-345.31991

geom102



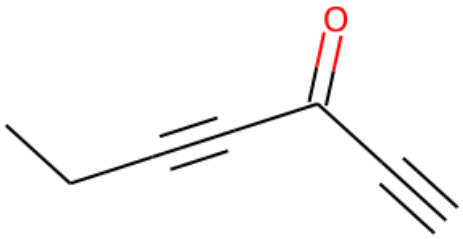
SMILES: C#CC#CCC=O

Nearest TMC-1 molecule (distance): CC#CC#C (4.77)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	
$\mu_{a,b,c}$	2.1, 0.4, 0.5
A, B, C	19100.2261, 883.8337, 850.6910
A_s, B_s, C_s	19044.8354, 881.2705, 848.2240
Charge, Multiplicity	0, 1
Predicted log column density	8.234±2.913
Electronic energy	-306.01591

geom103



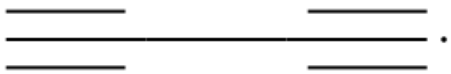
SMILES: C#CC(=O)C#CCC

Nearest TMC-1 molecule (distance): CC#CC#C (4.79)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	2.3, 3.6, 0.0
A, B, C	4893.9489, 874.5563, 756.8524
A_s, B_s, C_s	4879.7565, 872.0200, 754.6576
Charge, Multiplicity	0, 1
Predicted log column density	8.967±4.273
Electronic energy	-345.31609

geom104



SMILES: [C]#CC#C

Nearest TMC-1 molecule (distance): C#CC#[NH+] (1.67)

Is DFT optimized?: True

Property	Value
Formula	C4H
Molecular weight	49.052
IUPAC name	buta-1,3-diyne
$\mu_{a,b,c}$	0.9, 0.0, 0.0
A, B, C	∞, 4742.7988, 4742.7988
A_s, B_s, C_s	∞, 4729.0446, 4729.0446
Charge, Multiplicity	0, 2
Predicted log column density	12.801±1.467
Electronic energy	-152.69697

geom105

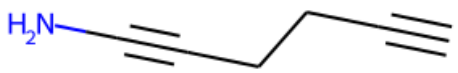
SMILES: C#CCC#CCO

Nearest TMC-1 molecule (distance): CC#CC#C (4.82)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hexa-2,5-diyn-1-ol
$\mu_{a,b,c}$	1.5, 0.3, 0.3
A, B, C	8445.3129, 950.7216, 907.7167
A_s, B_s, C_s	8420.8215, 947.9645, 905.0844
Charge, Multiplicity	0, 1
Predicted log column density	10.011±4.068
Electronic energy	-307.21564

geom106



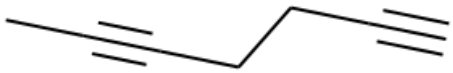
SMILES: C#CCCC#CN

Nearest TMC-1 molecule (distance): C#CCC#N (3.66)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	hexa-1,5-diyn-1-amine
$\mu_{a,b,c}$	1.9, 0.9, 0.0
A, B, C	20988.4673, 844.6393, 823.9358
A_s, B_s, C_s	20927.6007, 842.1898, 821.5464
Charge, Multiplicity	0, 1
Predicted log column density	10.598±2.846
Electronic energy	-287.36414

geom107



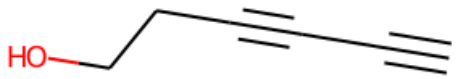
SMILES: C#CCCC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.85)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	hepta-1,5-diyne
$\mu_{a,b,c}$	0.9, 0.2, 0.0
A, B, C	19479.5488, 846.1634, 823.3564
A_s, B_s, C_s	19423.0581, 843.7095, 820.9687
Charge, Multiplicity	0, 1
Predicted log column density	11.355±2.741
Electronic energy	-271.33975

geom108



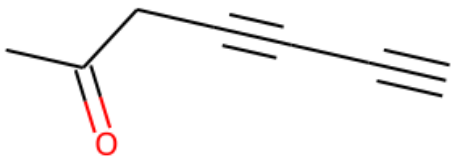
SMILES: C#CC#CCCO

Nearest TMC-1 molecule (distance): CC#CC#C (4.85)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hexa-3,5-diyn-1-ol
$\mu_{a,b,c}$	0.5, 1.0, 0.8
A, B, C	7842.0943, 1080.2192, 979.1246
A_s, B_s, C_s	7819.3522, 1077.0866, 976.2852
Charge, Multiplicity	0, 1
Predicted log column density	10.401±3.881
Electronic energy	-307.23073

geom109



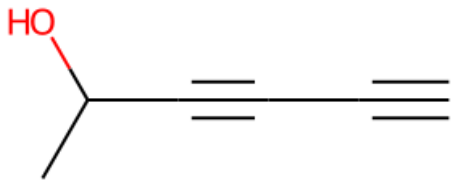
SMILES: C#CC#CCC(C)=O

Nearest TMC-1 molecule (distance): CC#CC#C (4.86)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	2.1, 0.8, 0.9
A, B, C	6971.5818, 810.9331, 741.1102
A_s, B_s, C_s	6951.3642, 808.5814, 738.9610
Charge, Multiplicity	0, 1
Predicted log column density	11.072±3.886
Electronic energy	-345.33252

geom110



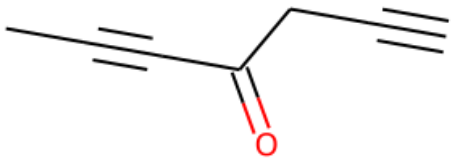
SMILES: C#CC#CC(C)O

Nearest TMC-1 molecule (distance): CC#CC#C (4.87)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hexa-3,5-diyn-2-ol
$\mu_{a,b,c}$	0.4, 1.4, 0.9
A, B, C	8373.6266, 1085.5579, 996.0242
A_s, B_s, C_s	8349.3431, 1082.4098, 993.1357
Charge, Multiplicity	0, 1
Predicted log column density	11.419±4.407
Electronic energy	-307.22930

geom111



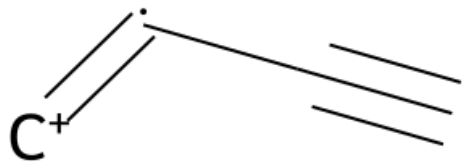
SMILES: C#CCC(=O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.89)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	hepta-1,5-diyn-4-one
$\mu_{a,b,c}$	1.8, 3.1, 1.1
A, B, C	2427.0631, 1459.2576, 950.8064
A_s, B_s, C_s	2420.0246, 1455.0257, 948.0491
Charge, Multiplicity	0, 1
Predicted log column density	11.883±3.869
Electronic energy	-345.32298

geom112



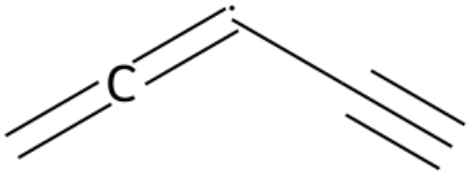
SMILES: C#C[C]=[CH+]

Nearest TMC-1 molecule (distance): C#CC#[NH+] (1.66)

Is DFT optimized?: True

Property	Value
Formula	C4H2+
Molecular weight	50.060
IUPAC name	but-1-en-3-yne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 4391.4175, 4391.4175
A_s, B_s, C_s	∞, 4378.6824, 4378.6824
Charge, Multiplicity	1, 2
Predicted log column density	12.822±1.488
Electronic energy	-153.05958

geom113



SMILES: C#C[C]=C=C

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (3.34)

Is DFT optimized?: True

Property	Value
Formula	C5H3
Molecular weight	63.079
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	288585.3159, 2158.5395, 2142.5157
A_s, B_s, C_s	287748.4184, 2152.2798, 2136.3024
Charge, Multiplicity	0, 2
Predicted log column density	11.673±1.562
Electronic energy	-192.08630

geom114

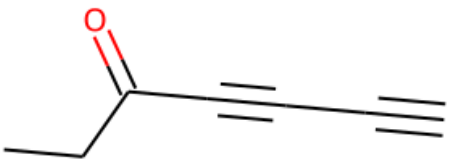
SMILES: C#CCC#CC(C)=O

Nearest TMC-1 molecule (distance): CC#CC#C (4.93)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	1.5, 3.3, 0.7
A, B, C	5557.4651, 795.9666, 736.1542
A_s, B_s, C_s	5541.3485, 793.6583, 734.0193
Charge, Multiplicity	0, 1
Predicted log column density	9.131±4.122
Electronic energy	-345.31886

geom115



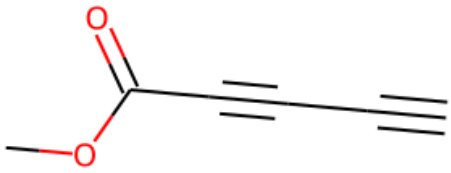
SMILES: C#CC#CC(=O)CC

Nearest TMC-1 molecule (distance): CC#CC#C (4.94)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	hepta-4,6-diyn-3-one
$\mu_{a,b,c}$	1.4, 3.0, 0.0
A, B, C	7825.6856, 775.2232, 711.5224
A_s, B_s, C_s	7802.9911, 772.9751, 709.4590
Charge, Multiplicity	0, 1
Predicted log column density	9.821±3.939
Electronic energy	-345.32722

geom116



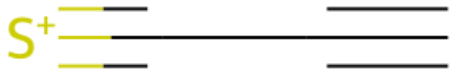
SMILES: C#CC#CC(=O)OC

Nearest TMC-1 molecule (distance): CC#CC#C (4.99)

Is DFT optimized?: True

Property	Value
Formula	C6H4O2
Molecular weight	108.096
IUPAC name	methyl penta-2,4-diynoate
$\mu_{a,b,c}$	0.4, 2.0, 0.0
A, B, C	8793.0202, 805.8887, 741.7053
A_s, B_s, C_s	8767.5205, 803.5516, 739.5544
Charge, Multiplicity	0, 1
Predicted log column density	11.061±4.377
Electronic energy	-381.23041

geom117



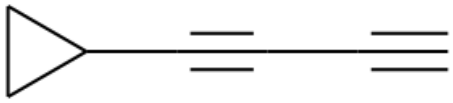
SMILES: C#CC#[S+]

Nearest TMC-1 molecule (distance): C#CC#[NH+] (1.78)

Is DFT optimized?: True

Property	Value
Formula	C3HS+
Molecular weight	69.108
IUPAC name	prop-2-yne-1-thione
$\mu_{a,b,c}$	2.3, 0.0, 0.0
A, B, C	22490823713.9077, 2731.0628, 2731.0625
A_s, B_s, C_s	22425600325.1373, 2723.1427, 2723.1424
Charge, Multiplicity	1, 1
Predicted log column density	12.575±1.458
Electronic energy	-512.63081

geom118



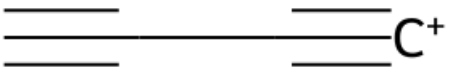
SMILES: C#CC#CC1CC1

Nearest TMC-1 molecule (distance): CC#CC#C (5.04)

Is DFT optimized?: True

Property	Value
Formula	C7H6
Molecular weight	90.125
IUPAC name	buta-1,3-diynylcyclopropane
$\mu_{a,b,c}$	1.6, 0.0, 0.1
A, B, C	14194.7806, 1036.8589, 1028.0712
A_s, B_s, C_s	14153.6158, 1033.8520, 1025.0898
Charge, Multiplicity	0, 1
Predicted log column density	10.426±4.021
Electronic energy	-270.09988

geom119



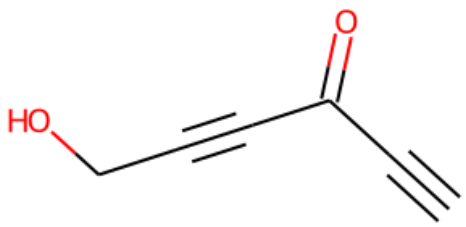
SMILES: [C+]#CC#C

Nearest TMC-1 molecule (distance): C#CC#[NH+] (2.02)

Is DFT optimized?: True

Property	Value
Formula	C4H+
Molecular weight	49.052
IUPAC name	buta-1,3-diyne
$\mu_{a,b,c}$	2.9, 0.0, 0.0
A, B, C	6704332413.1092, 4805.4004, 4805.3969
A_s, B_s, C_s	6684889849.1112, 4791.4647, 4791.4613
Charge, Multiplicity	1, 1
Predicted log column density	12.458±1.567
Electronic energy	-152.17425

geom120



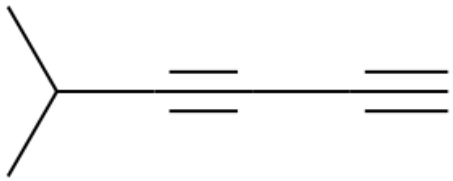
SMILES: C#CC(=O)C#CCO

Nearest TMC-1 molecule (distance): CC#CC#C (5.07)

Is DFT optimized?: True

Property	Value
Formula	C6H4O2
Molecular weight	108.096
IUPAC name	
$\mu_{a,b,c}$	1.4, 2.3, 1.2
A, B, C	4026.3461, 942.0274, 768.6066
A_s, B_s, C_s	4014.6697, 939.2955, 766.3776
Charge, Multiplicity	0, 1
Predicted log column density	8.927±4.955
Electronic energy	-381.19643

geom121



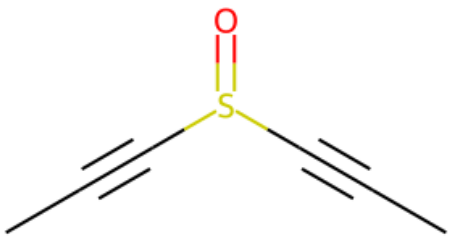
SMILES: C#CC#CC(C)C

Nearest TMC-1 molecule (distance): CC#CC#C (5.11)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	5-methylhexa-1,3-diyne
$\mu_{a,b,c}$	1.3, 0.0, 0.1
A, B, C	7760.3930, 1091.8363, 995.3733
A_s, B_s, C_s	7737.8879, 1088.6700, 992.4867
Charge, Multiplicity	0, 1
Predicted log column density	11.567±4.437
Electronic energy	-271.34424

geom122



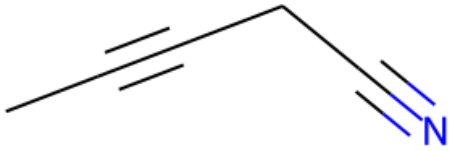
SMILES: CC#CS(=O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.20)

Is DFT optimized?: True

Property	Value
Formula	C6H6OS
Molecular weight	126.180
IUPAC name	1-prop-1-ynylsulfinylprop-1-yne
$\mu_{a,b,c}$	0.0, 4.6, 1.3
A, B, C	2558.0516, 853.9592, 669.0505
A_s, B_s, C_s	2550.6333, 851.4827, 667.1103
Charge, Multiplicity	0, 1
Predicted log column density	11.544±4.933
Electronic energy	-705.33903

geom123



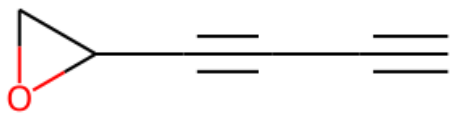
SMILES: CC#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#N (2.91)

Is DFT optimized?: True

Property	Value
Formula	C5H5N
Molecular weight	79.102
IUPAC name	pent-3-ynenitrile
$\mu_{a,b,c}$	3.5, 2.5, 0.0
A, B, C	12666.2105, 1511.1698, 1373.1930
A_s, B_s, C_s	12629.4785, 1506.7874, 1369.2108
Charge, Multiplicity	0, 1
Predicted log column density	10.564±2.280
Electronic energy	-248.12524

geom124



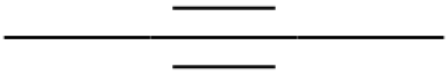
SMILES: C#CC#CC1CO1

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (5.14)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	
$\mu_{a,b,c}$	0.2, 1.8, 0.9
A, B, C	16588.0729, 1030.9233, 1024.4517
A_s, B_s, C_s	16539.9675, 1027.9337, 1021.4808
Charge, Multiplicity	0, 1
Predicted log column density	10.377±4.549
Electronic energy	-305.97922

geom125



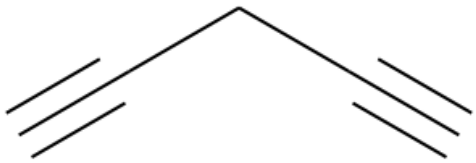
SMILES: CC#CC

Nearest TMC-1 molecule (distance): CC#C (4.29)

Is DFT optimized?: True

Property	Value
Formula	C4H6
Molecular weight	54.092
IUPAC name	but-2-yne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	79915.2750, 3345.2270, 3345.2194
A_s, B_s, C_s	79683.5207, 3335.5259, 3335.5183
Charge, Multiplicity	0, 1
Predicted log column density	13.046±1.758
Electronic energy	-155.92510

geom126



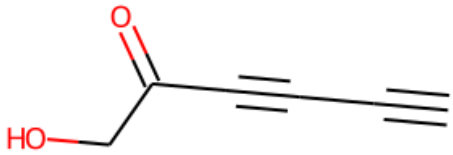
SMILES: C#CCC#C

Nearest TMC-1 molecule (distance): [C]#CC#C (3.16)

Is DFT optimized?: True

Property	Value
Formula	C5H4
Molecular weight	64.087
IUPAC name	penta-1,4-diyne
$\mu_{a,b,c}$	0.0, 0.5, 0.0
A, B, C	19054.6948, 2842.8638, 2512.0657
A_s, B_s, C_s	18999.4362, 2834.6195, 2504.7807
Charge, Multiplicity	0, 1
Predicted log column density	12.883±2.243
Electronic energy	-192.71662

geom127



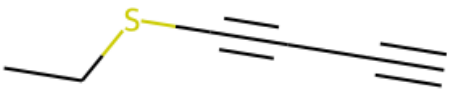
SMILES: C#CC#CC(=O)CO

Nearest TMC-1 molecule (distance): CC#CC#C (5.36)

Is DFT optimized?: True

Property	Value
Formula	C6H4O2
Molecular weight	108.096
IUPAC name	
$\mu_{a,b,c}$	3.8, 1.5, 0.0
A, B, C	8418.1115, 775.1645, 712.9671
A_s, B_s, C_s	8393.6990, 772.9166, 710.8995
Charge, Multiplicity	0, 1
Predicted log column density	9.181±4.601
Electronic energy	-381.21358

geom128



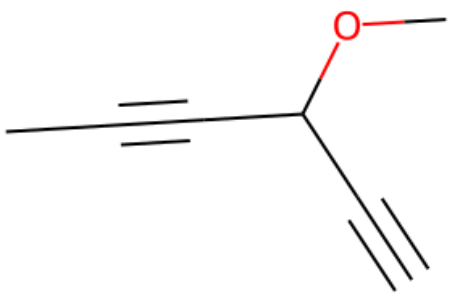
SMILES: C#CC#CSCC

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (5.08)

Is DFT optimized?: True

Property	Value
Formula	C6H6S
Molecular weight	110.181
IUPAC name	1-ethylsulfanylbuta-1,3-diyne
$\mu_{a,b,c}$	1.4, 1.7, 0.0
A, B, C	10359.7653, 754.6944, 709.7361
A_s, B_s, C_s	10329.7220, 752.5058, 707.6778
Charge, Multiplicity	0, 1
Predicted log column density	9.999±5.072
Electronic energy	-630.20402

geom129



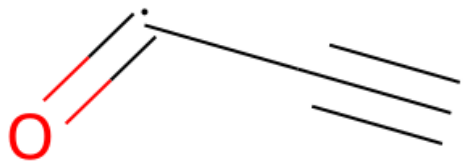
SMILES: C#CC(C#CC)OC

Nearest TMC-1 molecule (distance): CC#CC#C (5.41)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	1.9, 0.4, 0.9
A, B, C	2404.4243, 1386.8322, 914.6639
A_s, B_s, C_s	2397.4515, 1382.8104, 912.0114
Charge, Multiplicity	0, 1
Predicted log column density	11.222±4.665
Electronic energy	-346.50849

geom130



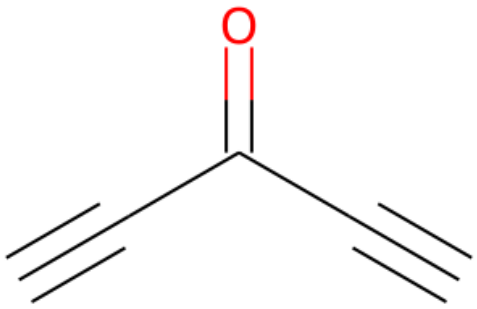
SMILES: C#C[C]=O

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (2.67)

Is DFT optimized?: True

Property	Value
Formula	C3HO
Molecular weight	53.040
IUPAC name	prop-2-ynal
$\mu_{a,b,c}$	2.5, 0.0, 0.0
A, B, C	∞, 4360.6707, 4360.6707
A_s, B_s, C_s	∞, 4348.0248, 4348.0248
Charge, Multiplicity	0, 2
Predicted log column density	11.171±1.041
Electronic energy	-189.92960

geom131



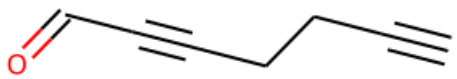
SMILES: C#CC(=O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (3.99)

Is DFT optimized?: True

Property	Value
Formula	C5H2O
Molecular weight	78.070
IUPAC name	penta-1,4-diyn-3-one
$\mu_{a,b,c}$	0.0, 3.5, 0.0
A, B, C	6461.1948, 2885.0264, 1994.4657
A_s, B_s, C_s	6442.4573, 2876.6598, 1988.6817
Charge, Multiplicity	0, 1
Predicted log column density	11.368±4.003
Electronic energy	-266.69559

geom132



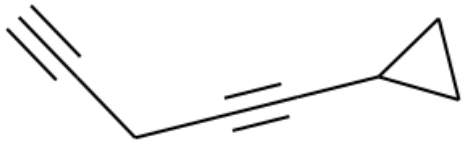
SMILES: C#CCCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#C (5.44)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	3.3, 1.3, 0.2
A, B, C	18957.4940, 583.4768, 570.1999
A_s, B_s, C_s	18902.5172, 581.7847, 568.5464
Charge, Multiplicity	0, 1
Predicted log column density	9.449±2.978
Electronic energy	-345.31361

geom133



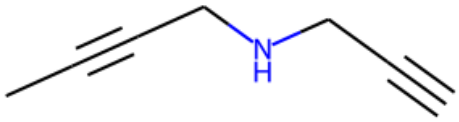
SMILES: C#CCC#CC1CC1

Nearest TMC-1 molecule (distance): CC#CC#C (5.45)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	
$\mu_{a,b,c}$	0.7, 0.2, 0.1
A, B, C	5343.0829, 831.7065, 763.0752
A_s, B_s, C_s	5327.5880, 829.2946, 760.8623
Charge, Multiplicity	0, 1
Predicted log column density	9.586±4.311
Electronic energy	-309.39312

geom134



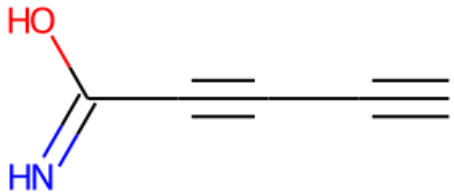
SMILES: C#CCNCC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.46)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	N-prop-2-ynylbut-2-yn-1-amine
$\mu_{a,b,c}$	0.8, 0.4, 1.1
A, B, C	7519.2056, 644.4175, 601.0306
A_s, B_s, C_s	7497.3999, 642.5487, 599.2876
Charge, Multiplicity	0, 1
Predicted log column density	12.855±4.934
Electronic energy	-326.65700

geom135



SMILES: C#CC#CC(=N)O

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (5.01)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	penta-2,4-diynamide
$\mu_{a,b,c}$	4.6, 1.0, 0.0
A, B, C	11130.1256, 1109.2941, 1008.7555
A_s, B_s, C_s	11097.8482, 1106.0771, 1005.8301
Charge, Multiplicity	0, 1
Predicted log column density	11.284±3.833
Electronic energy	-322.04672

geom136

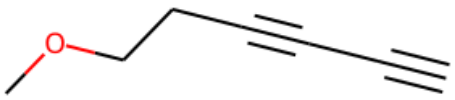
SMILES: CC#CCC

Nearest TMC-1 molecule (distance): CC#C (4.84)

Is DFT optimized?: True

Property	Value
Formula	C5H8
Molecular weight	68.119
IUPAC name	pent-2-yne
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	20320.8280, 2072.5780, 1949.1826
A_s, B_s, C_s	20261.8976, 2066.5675, 1943.5300
Charge, Multiplicity	0, 1
Predicted log column density	11.282±3.026
Electronic energy	-195.22811

geom137



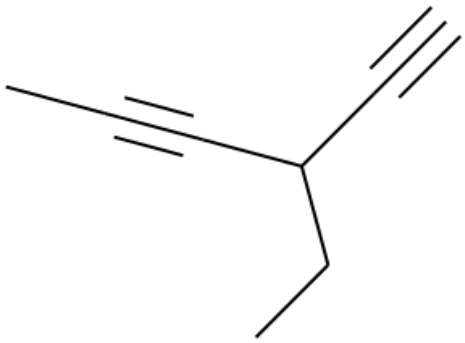
SMILES: C#CC#CCCOC

Nearest TMC-1 molecule (distance): CC#CC#C (5.56)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	0.9, 1.1, 0.0
A, B, C	11558.9642, 593.9290, 571.0034
A_s, B_s, C_s	11525.4432, 592.2066, 569.3475
Charge, Multiplicity	0, 1
Predicted log column density	11.900±4.561
Electronic energy	-346.52331

geom138



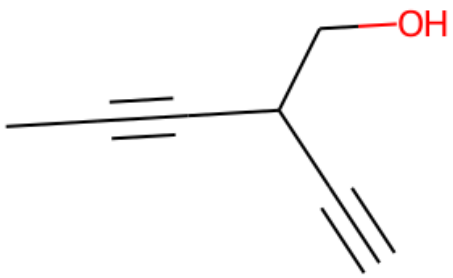
SMILES: C#CC(C#CC)CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.58)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	3-ethylhexa-1,4-diyne
$\mu_{a,b,c}$	0.7, 0.6, 0.1
A, B, C	2212.6516, 1380.1483, 889.3788
A_s, B_s, C_s	2206.2350, 1376.1459, 886.7996
Charge, Multiplicity	0, 1
Predicted log column density	8.990±5.171
Electronic energy	-310.63912

geom139



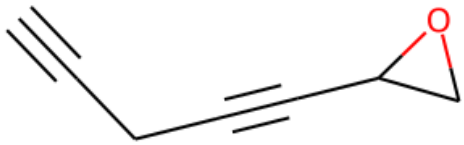
SMILES: C#CC(C#CC)CO

Nearest TMC-1 molecule (distance): CC#CC#C (5.59)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	2.1, 0.4, 1.0
A, B, C	2713.3921, 1266.9119, 987.4459
A_s, B_s, C_s	2705.5233, 1263.2379, 984.5823
Charge, Multiplicity	0, 1
Predicted log column density	8.560±4.769
Electronic energy	-346.52532

geom140



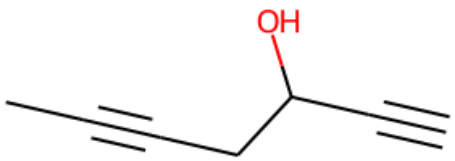
SMILES: C#CCC#CC1CO1

Nearest TMC-1 molecule (distance): CC#CC#C (5.61)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	0.1, 2.4, 0.4
A, B, C	6855.2919, 780.7625, 729.4784
A_s, B_s, C_s	6835.4115, 778.4983, 727.3630
Charge, Multiplicity	0, 1
Predicted log column density	9.553±4.824
Electronic energy	-345.27420

geom141



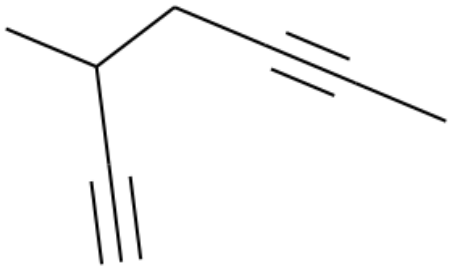
SMILES: C#CC(O)CC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.61)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	1.6, 1.1, 0.8
A, B, C	2968.9511, 1186.9859, 1029.9074
A_s, B_s, C_s	2960.3412, 1183.5436, 1026.9207
Charge, Multiplicity	0, 1
Predicted log column density	10.455±4.917
Electronic energy	-346.53082

geom142



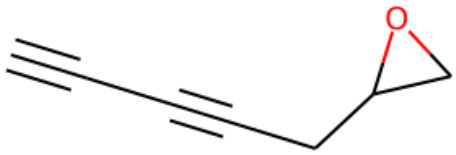
SMILES: C#CC(C)CC#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.62)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	3-methylhepta-1,5-diyne
$\mu_{a,b,c}$	0.9, 0.3, 0.1
A, B, C	6290.1992, 819.0073, 752.5398
A_s, B_s, C_s	6271.9577, 816.6322, 750.3574
Charge, Multiplicity	0, 1
Predicted log column density	11.407±4.665
Electronic energy	-310.64474

geom143



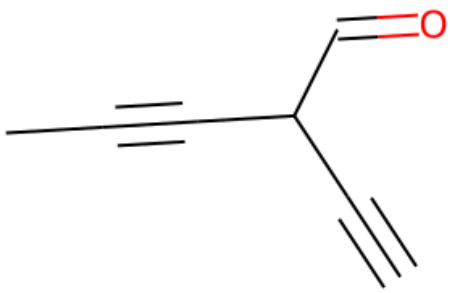
SMILES: C#CC#CCC1CO1

Nearest TMC-1 molecule (distance): CC#CC#C (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.8, 0.2
A, B, C	9066.0401, 733.7412, 699.1492
A_s, B_s, C_s	9039.7486, 731.6134, 697.1216
Charge, Multiplicity	0, 1
Predicted log column density	10.055±5.205
Electronic energy	-345.28826

geom144



SMILES: C#CC(C#CC)C=O

Nearest TMC-1 molecule (distance): CC#CC#C (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	2.2, 2.0, 0.8
A, B, C	2638.6232, 1263.5926, 894.2977
A_s, B_s, C_s	2630.9712, 1259.9282, 891.7042
Charge, Multiplicity	0, 1
Predicted log column density	8.213±4.286
Electronic energy	-345.31043

geom145

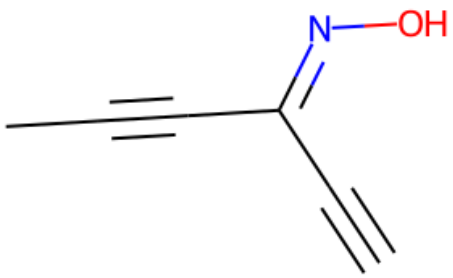
SMILES: C#CCC#CC(C)O

Nearest TMC-1 molecule (distance): CC#CC#C (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	hepta-3,6-diyn-2-ol
$\mu_{a,b,c}$	0.8, 0.4, 1.6
A, B, C	5334.7758, 767.3945, 714.4693
A_s, B_s, C_s	5319.3050, 765.1691, 712.3974
Charge, Multiplicity	0, 1
Predicted log column density	10.577±4.938
Electronic energy	-346.52401

geom146



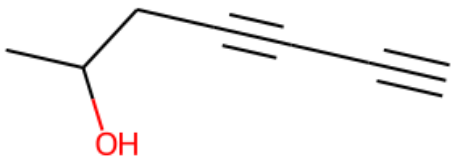
SMILES: C#CC(C#CC)=NO

Nearest TMC-1 molecule (distance): CC#CC#C (5.63)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	1.6, 0.2, 0.0
A, B, C	2576.6385, 1415.9746, 919.0616
A_s, B_s, C_s	2569.1663, 1411.8683, 916.3964
Charge, Multiplicity	0, 1
Predicted log column density	7.776±5.379
Electronic energy	-361.30112

geom147



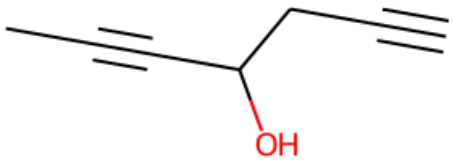
SMILES: C#CC#CCC(C)O

Nearest TMC-1 molecule (distance): CC#CC#C (5.64)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	hepta-4,6-diyn-2-ol
$\mu_{a,b,c}$	0.2, 0.1, 1.4
A, B, C	4508.0136, 879.6215, 867.0188
A_s, B_s, C_s	4494.9403, 877.0706, 864.5045
Charge, Multiplicity	0, 1
Predicted log column density	12.080±4.953
Electronic energy	-346.53995

geom148



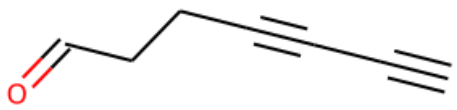
SMILES: C#CCC(O)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.64)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	hepta-1,5-diyn-4-ol
$\mu_{a,b,c}$	1.1, 1.6, 0.6
A, B, C	2805.2495, 1237.5090, 1003.4081
A_s, B_s, C_s	2797.1143, 1233.9202, 1000.4982
Charge, Multiplicity	0, 1
Predicted log column density	11.455±4.610
Electronic energy	-346.53145

geom149



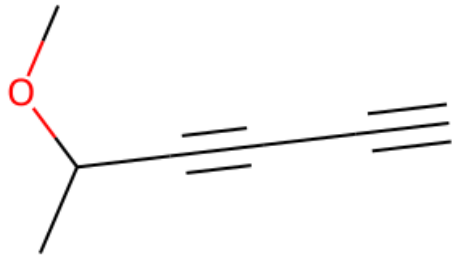
SMILES: C#CC#CCCC=O

Nearest TMC-1 molecule (distance): CC#CC#C (5.65)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	0.6, 2.2, 0.0
A, B, C	15297.9759, 621.0183, 601.1713
A_s, B_s, C_s	15253.6118, 619.2174, 599.4279
Charge, Multiplicity	0, 1
Predicted log column density	7.053±3.539
Electronic energy	-345.32388

geom150



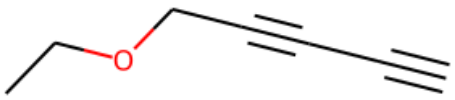
SMILES: C#CC#CC(C)OC

Nearest TMC-1 molecule (distance): CC#CC#C (5.66)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	1.5, 1.0, 0.9
A, B, C	6004.0041, 811.3601, 735.2408
A_s, B_s, C_s	5986.5925, 809.0072, 733.1086
Charge, Multiplicity	0, 1
Predicted log column density	11.654±4.763
Electronic energy	-346.51903

geom151



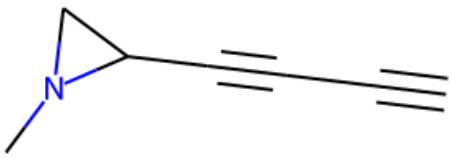
SMILES: C#CC#CCOCC

Nearest TMC-1 molecule (distance): CC#CC#C (5.66)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	
$\mu_{a,b,c}$	1.3, 1.4, 0.0
A, B, C	9829.4066, 622.4746, 591.9482
A_s, B_s, C_s	9800.9013, 620.6695, 590.2315
Charge, Multiplicity	0, 1
Predicted log column density	12.118±5.067
Electronic energy	-346.52024

geom152



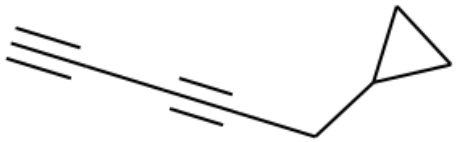
SMILES: C#CC#CC1CN1C

Nearest TMC-1 molecule (distance): CC#CC#C (5.67)

Is DFT optimized?: True

Property	Value
Formula	C7H7N
Molecular weight	105.140
IUPAC name	
$\mu_{a,b,c}$	1.7, 0.6, 1.1
A, B, C	9060.7669, 771.3397, 742.4662
A_s, B_s, C_s	9034.4907, 769.1028, 740.3131
Charge, Multiplicity	0, 1
Predicted log column density	13.169±4.685
Electronic energy	-325.41838

geom153



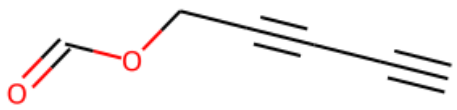
SMILES: C#CC#CCC1CC1

Nearest TMC-1 molecule (distance): CC#CC#C (5.69)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	penta-2,4-diynylcyclopropane
$\mu_{a,b,c}$	1.3, 0.2, 0.1
A, B, C	8177.3312, 752.5419, 711.4406
A_s, B_s, C_s	8153.6169, 750.3596, 709.3775
Charge, Multiplicity	0, 1
Predicted log column density	9.441±4.601
Electronic energy	-309.40176

geom154



SMILES: C#CC#CCOC=O

Nearest TMC-1 molecule (distance): CC#CC#C (5.71)

Is DFT optimized?: True

Property	Value
Formula	C6H4O2
Molecular weight	108.096
IUPAC name	
$\mu_{a,b,c}$	0.2, 1.6, 0.6
A, B, C	5592.1378, 879.0291, 807.3251
A_s, B_s, C_s	5575.9206, 876.4800, 804.9838
Charge, Multiplicity	0, 1
Predicted log column density	10.708±3.838
Electronic energy	-381.22788

geom155

SMILES: CC#CCO

Nearest TMC-1 molecule (distance): CC#C (5.14)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	but-2-yn-1-ol
$\mu_{a,b,c}$	2.0, 0.2, 1.1
A, B, C	24121.4404, 2063.6449, 1953.9262
A_s, B_s, C_s	24051.4882, 2057.6604, 1948.2598
Charge, Multiplicity	0, 1
Predicted log column density	11.247±3.314
Electronic energy	-231.11102

geom156

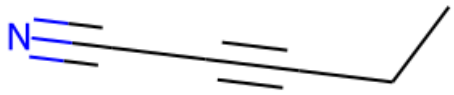
SMILES: C#CC#CC(=O)C=O

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (5.52)

Is DFT optimized?: True

Property	Value
Formula	C6H2O2
Molecular weight	106.080
IUPAC name	
$\mu_{a,b,c}$	2.0, 0.4, 0.0
A, B, C	4643.8275, 1005.8350, 826.7617
A_s, B_s, C_s	4630.3604, 1002.9181, 824.3641
Charge, Multiplicity	0, 1
Predicted log column density	9.133±2.930
Electronic energy	-379.98934

geom157



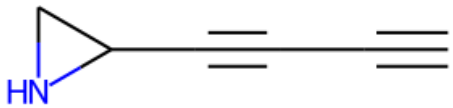
SMILES: CCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (2.63)

Is DFT optimized?: True

Property	Value
Formula	C5H5N
Molecular weight	79.102
IUPAC name	pent-2-ynenitrile
$\mu_{a,b,c}$	5.5, 0.7, 0.0
A, B, C	21510.6154, 1342.0914, 1283.4399
A_s, B_s, C_s	21448.2346, 1338.1993, 1279.7179
Charge, Multiplicity	0, 1
Predicted log column density	10.787±2.886
Electronic energy	-248.12862

geom158



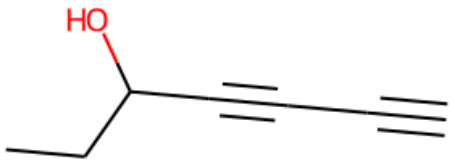
SMILES: C#CC#CC1CN1

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (5.54)

Is DFT optimized?: True

Property	Value
Formula	C6H5N
Molecular weight	91.113
IUPAC name	
$\mu_{a,b,c}$	0.5, 1.1, 0.7
A, B, C	15096.3299, 1040.8499, 1035.3590
A_s, B_s, C_s	15052.5505, 1037.8314, 1032.3564
Charge, Multiplicity	0, 1
Predicted log column density	9.180±5.130
Electronic energy	-286.12039

geom159



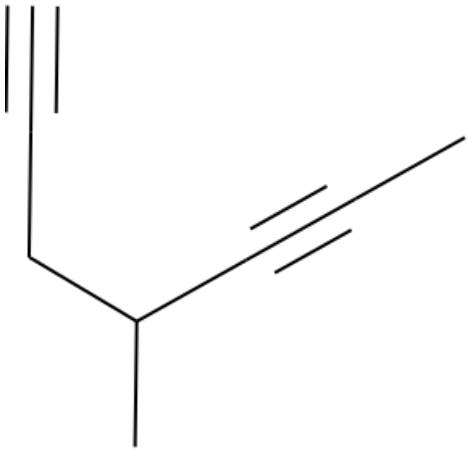
SMILES: C#CC#CC(O)CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.73)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	hepta-4,6-diyn-3-ol
$\mu_{a,b,c}$	0.1, 1.4, 0.9
A, B, C	6342.8641, 777.9307, 713.9664
A_s, B_s, C_s	6324.4697, 775.6747, 711.8958
Charge, Multiplicity	0, 1
Predicted log column density	9.657±4.856
Electronic energy	-346.53318

geom160



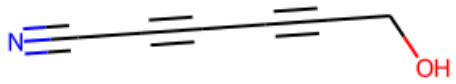
SMILES: C#CCC(C)C#CC

Nearest TMC-1 molecule (distance): CC#CC#C (5.75)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	4-methylhepta-1,5-diyne
$\mu_{a,b,c}$	0.9, 0.0, 0.1
A, B, C	5816.3387, 834.6223, 755.1183
A_s, B_s, C_s	5799.4713, 832.2019, 752.9285
Charge, Multiplicity	0, 1
Predicted log column density	12.401±4.511
Electronic energy	-310.64475

geom161



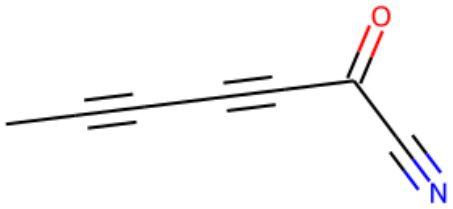
SMILES: N#CC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#N (3.55)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO
Molecular weight	105.096
IUPAC name	
$\mu_{a,b,c}$	4.5, 0.9, 1.4
A, B, C	23641.1348, 542.8947, 533.1055
A_s, B_s, C_s	23572.5755, 541.3203, 531.5595
Charge, Multiplicity	0, 1
Predicted log column density	10.464±3.184
Electronic energy	-360.13007

geom162



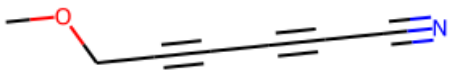
SMILES: CC#CC#CC(=O)C#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.02)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	6.8, 0.1, 0.0
A, B, C	5119.0007, 550.6962, 498.7640
A_s, B_s, C_s	5104.1556, 549.0992, 497.3176
Charge, Multiplicity	0, 1
Predicted log column density	9.958±3.399
Electronic energy	-398.22112

geom163



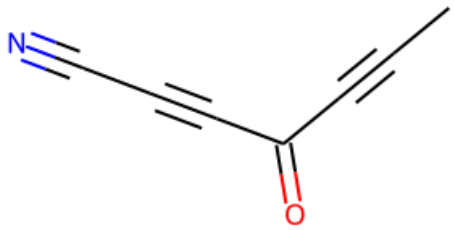
SMILES: COCC#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.08)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	6.6, 1.9, 0.0
A, B, C	18445.5949, 393.5772, 387.2495
A_s, B_s, C_s	18392.1027, 392.4358, 386.1265
Charge, Multiplicity	0, 1
Predicted log column density	12.471±3.773
Electronic energy	-399.42208

geom164



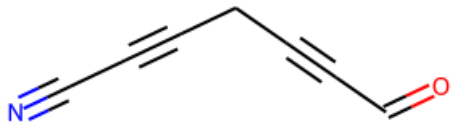
SMILES: CC#CC(=O)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.14)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	4.8, 2.8, 0.0
A, B, C	2891.2286, 687.2133, 557.1766
A_s, B_s, C_s	2882.8441, 685.2203, 555.5608
Charge, Multiplicity	0, 1
Predicted log column density	9.458±3.877
Electronic energy	-398.21945

geom165



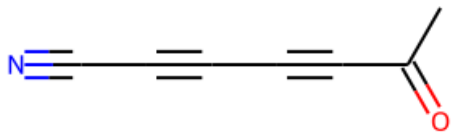
SMILES: N#CC#CCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.24)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	0.7, 2.2, 0.3
A, B, C	5808.0963, 476.7190, 441.9550
A_s, B_s, C_s	5791.2528, 475.3365, 440.6734
Charge, Multiplicity	0, 1
Predicted log column density	8.180±3.203
Electronic energy	-398.21228

geom166



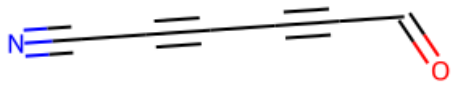
SMILES: CC(=O)C#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.24)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	3.1, 2.8, 0.0
A, B, C	10126.4988, 458.1381, 439.5055
A_s, B_s, C_s	10097.1319, 456.8095, 438.2310
Charge, Multiplicity	0, 1
Predicted log column density	9.535±3.749
Electronic energy	-398.23014

geom167



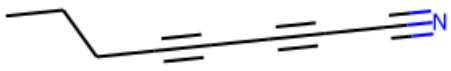
SMILES: N#CC#CC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.36)

Is DFT optimized?: True

Property	Value
Formula	C6HNO
Molecular weight	103.080
IUPAC name	
$\mu_{a,b,c}$	2.0, 2.2, 0.0
A, B, C	46436.9355, 554.1407, 547.6060
A_s, B_s, C_s	46302.2684, 552.5337, 546.0179
Charge, Multiplicity	0, 1
Predicted log column density	10.294±2.025
Electronic energy	-358.91237

geom168



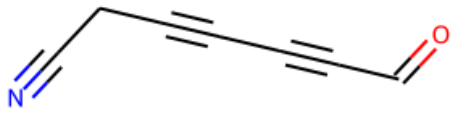
SMILES: CCCC#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.49)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	6.7, 0.5, 0.0
A, B, C	15521.4035, 387.4595, 380.7015
A_s, B_s, C_s	15476.3914, 386.3358, 379.5974
Charge, Multiplicity	0, 1
Predicted log column density	10.028±3.536
Electronic energy	-363.55509

geom169



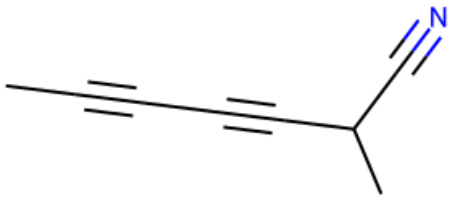
SMILES: N#CCC#CC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.53)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	0.9, 4.1, 1.4
A, B, C	7979.2981, 438.1975, 423.5097
A_s, B_s, C_s	7956.1581, 436.9268, 422.2816
Charge, Multiplicity	0, 1
Predicted log column density	8.348±2.876
Electronic energy	-398.21722

geom170



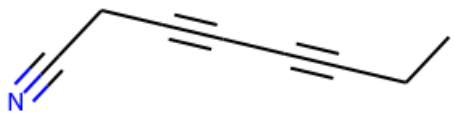
SMILES: CC#CC#CC(C)C#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.54)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	3.0, 3.4, 0.7
A, B, C	4444.1953, 547.2223, 499.9325
A_s, B_s, C_s	4431.3071, 545.6354, 498.4827
Charge, Multiplicity	0, 1
Predicted log column density	10.135±4.049
Electronic energy	-363.55384

geom171



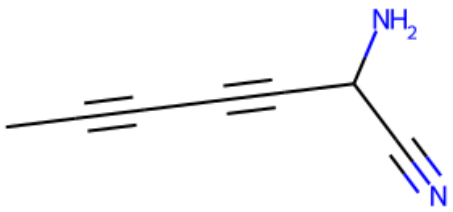
SMILES: CCC#CC#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.64)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	3.7, 2.8, 0.2
A, B, C	8255.4771, 428.0227, 410.4905
A_s, B_s, C_s	8231.5362, 426.7814, 409.3001
Charge, Multiplicity	0, 1
Predicted log column density	8.536±3.563
Electronic energy	-363.55171

geom172



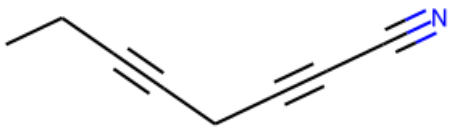
SMILES: CC#CC#CC(N)C#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.65)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	4.7, 3.2, 0.4
A, B, C	4497.2887, 547.1326, 499.7621
A_s, B_s, C_s	4484.2466, 545.5459, 498.3128
Charge, Multiplicity	0, 1
Predicted log column density	9.190±4.109
Electronic energy	-379.57628

geom173



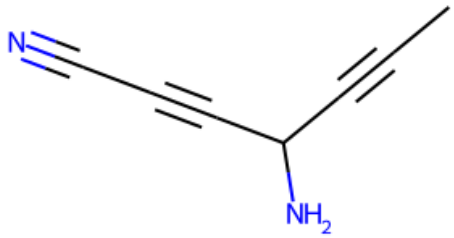
SMILES: CCC#CCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.75)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	4.8, 2.5, 0.3
A, B, C	3265.7675, 543.0359, 477.3746
A_s, B_s, C_s	3256.2968, 541.4611, 475.9902
Charge, Multiplicity	0, 1
Predicted log column density	8.361±4.199
Electronic energy	-363.54486

geom174



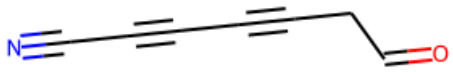
SMILES: CC#CC(N)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.75)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	6.3, 0.7, 0.0
A, B, C	2603.9043, 694.6101, 564.6198
A_s, B_s, C_s	2596.3530, 692.5958, 562.9824
Charge, Multiplicity	0, 1
Predicted log column density	8.809±4.196
Electronic energy	-379.57006

geom175



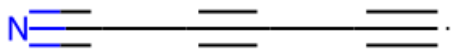
SMILES: N#CC#CC#CCC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.77)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	3.1, 1.2, 0.5
A, B, C	15822.5788, 403.1088, 394.4142
A_s, B_s, C_s	15776.6933, 401.9398, 393.2704
Charge, Multiplicity	0, 1
Predicted log column density	7.824±2.988
Electronic energy	-398.22517

geom176



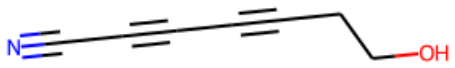
SMILES: [C]#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.52)

Is DFT optimized?: True

Property	Value
Formula	C5N
Molecular weight	74.062
IUPAC name	penta-2,4-diynenitrile
$\mu_{a,b,c}$	3.7, 0.0, 0.0
A, B, C	∞, 1394.5930, 1394.5930
A_s, B_s, C_s	∞, 1390.5487, 1390.5487
Charge, Multiplicity	0, 2
Predicted log column density	12.272±1.509
Electronic energy	-244.90483

geom177



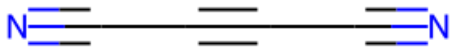
SMILES: N#CC#CC#CCCO

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.85)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	4.8, 1.8, 0.8
A, B, C	6832.3187, 459.3817, 436.7699
A_s, B_s, C_s	6812.5050, 458.0495, 435.5033
Charge, Multiplicity	0, 1
Predicted log column density	10.012±3.901
Electronic energy	-399.44100

geom178



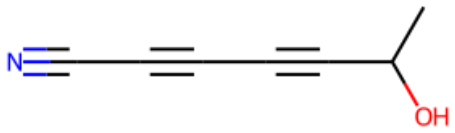
SMILES: N#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.87)

Is DFT optimized?: True

Property	Value
Formula	C4N2
Molecular weight	76.058
IUPAC name	but-2-ynedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 1333.0641, 1333.0641
A_s, B_s, C_s	∞, 1329.1983, 1329.1983
Charge, Multiplicity	0, 1
Predicted log column density	11.972±1.612
Electronic energy	-261.70936

geom179



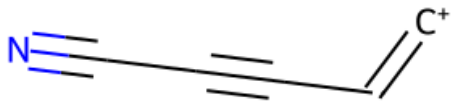
SMILES: CC(O)C#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.87)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	5.0, 1.5, 0.6
A, B, C	8219.6464, 453.5388, 437.5271
A_s, B_s, C_s	8195.8094, 452.2235, 436.2583
Charge, Multiplicity	0, 1
Predicted log column density	11.018±4.405
Electronic energy	-399.43936

geom180



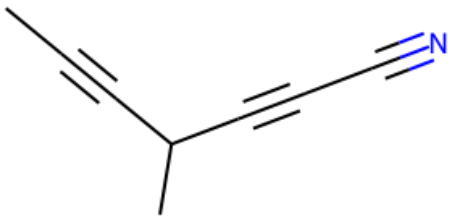
SMILES: [CH+]=[C]C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.57)

Is DFT optimized?: True

Property	Value
Formula	C5HN+
Molecular weight	75.070
IUPAC name	
$\mu_{a,b,c}$	6.9, 0.0, 0.0
A, B, C	523019796.5224, 1333.7462, 1333.7428
A_s, B_s, C_s	521503039.1125, 1329.8783, 1329.8749
Charge, Multiplicity	1, 2
Predicted log column density	12.289±1.522
Electronic energy	-245.25261

geom181



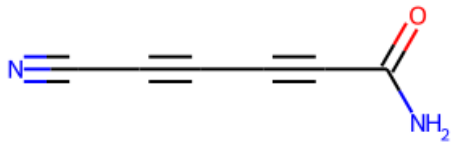
SMILES: CC#CC(C)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.89)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	5.3, 1.9, 0.3
A, B, C	2670.7460, 681.2441, 560.0924
A_s, B_s, C_s	2663.0008, 679.2685, 558.4681
Charge, Multiplicity	0, 1
Predicted log column density	9.749±4.398
Electronic energy	-363.54697

geom182



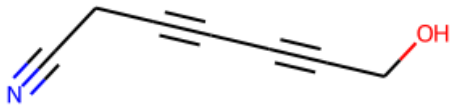
SMILES: N#CC#CC#CC(N)=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (4.90)

Is DFT optimized?: True

Property	Value
Formula	C6H2N2O
Molecular weight	118.095
IUPAC name	
$\mu_{a,b,c}$	3.6, 3.9, 0.0
A, B, C	11361.7728, 457.0975, 439.4191
A_s, B_s, C_s	11328.8237, 455.7719, 438.1448
Charge, Multiplicity	0, 1
Predicted log column density	9.976±3.333
Electronic energy	-414.28581

geom183



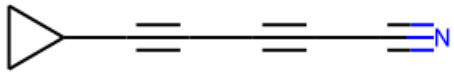
SMILES: N#CCC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.02)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	1.6, 3.2, 1.7
A, B, C	8577.7622, 419.4362, 404.0763
A_s, B_s, C_s	8552.8867, 418.2198, 402.9045
Charge, Multiplicity	0, 1
Predicted log column density	8.502±4.008
Electronic energy	-399.43220

geom184



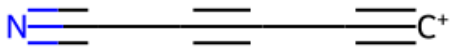
SMILES: N#CC#CC#CC1CC1

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.04)

Is DFT optimized?: True

Property	Value
Formula	C8H5N
Molecular weight	115.135
IUPAC name	
$\mu_{a,b,c}$	7.1, 0.0, 0.3
A, B, C	13123.1025, 450.1710, 449.7047
A_s, B_s, C_s	13085.0455, 448.8656, 448.4006
Charge, Multiplicity	0, 1
Predicted log column density	9.996±4.072
Electronic energy	-362.31175

geom185



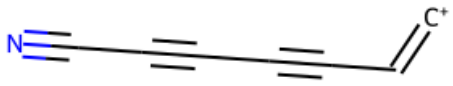
SMILES: [C+]#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.83)

Is DFT optimized?: True

Property	Value
Formula	C5N+
Molecular weight	74.062
IUPAC name	penta-2,4-diynenitrile
$\mu_{a,b,c}$	11.1, 0.0, 0.0
A, B, C	1615729454.2394, 1404.3719, 1404.3707
A_s, B_s, C_s	1611043838.8221, 1400.2992, 1400.2980
Charge, Multiplicity	1, 1
Predicted log column density	12.004±1.609
Electronic energy	-244.36149

geom186



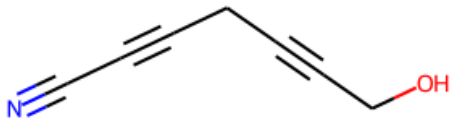
SMILES: [CH+]=[C]C#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (4.57)

Is DFT optimized?: True

Property	Value
Formula	C7HN+
Molecular weight	99.092
IUPAC name	
$\mu_{a,b,c}$	8.1, 0.0, 0.0
A, B, C	251454403.6219, 565.8685, 565.8673
A_s, B_s, C_s	250725185.8513, 564.2275, 564.2263
Charge, Multiplicity	1, 2
Predicted log column density	11.977±1.574
Electronic energy	-321.40145

geom187



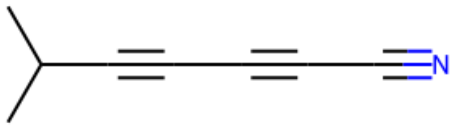
SMILES: N#CC#CCC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.07)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	2.8, 3.1, 0.8
A, B, C	3355.4837, 533.4831, 469.7883
A_s, B_s, C_s	3345.7528, 531.9360, 468.4259
Charge, Multiplicity	0, 1
Predicted log column density	8.335±4.630
Electronic energy	-399.42622

geom188



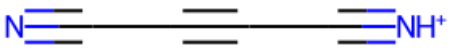
SMILES: CC(C)C#CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.11)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	6.7, 0.0, 0.3
A, B, C	7598.1575, 459.7726, 442.1637
A_s, B_s, C_s	7576.1228, 458.4392, 440.8815
Charge, Multiplicity	0, 1
Predicted log column density	11.164±4.432
Electronic energy	-363.55593

geom189



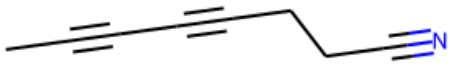
SMILES: N#CC#CC#[NH+]

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.58)

Is DFT optimized?: True

Property	Value
Formula	C4HN2+
Molecular weight	77.066
IUPAC name	4-iminobut-2-ynenitrile
$\mu_{a,b,c}$	9.0, 0.0, 0.0
A, B, C	∞, 1289.6699, 1289.6699
A_s, B_s, C_s	∞, 1285.9298, 1285.9298
Charge, Multiplicity	1, 1
Predicted log column density	11.238±1.552
Electronic energy	-261.98941

geom190



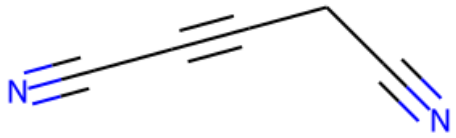
SMILES: CC#CC#CCCC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.14)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	4.8, 0.6, 0.0
A, B, C	15256.4498, 400.0836, 392.7172
A_s, B_s, C_s	15212.2061, 398.9234, 391.5783
Charge, Multiplicity	0, 1
Predicted log column density	9.851±3.200
Electronic energy	-363.56025

geom191



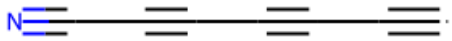
SMILES: N#CC#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.18)

Is DFT optimized?: True

Property	Value
Formula	C5H2N2
Molecular weight	90.085
IUPAC name	
$\mu_{a,b,c}$	1.9, 4.1, 0.0
A, B, C	12080.0258, 1013.9915, 940.9386
A_s, B_s, C_s	12044.9937, 1011.0509, 938.2098
Charge, Multiplicity	0, 1
Predicted log column density	10.014±2.205
Electronic energy	-301.01780

geom192



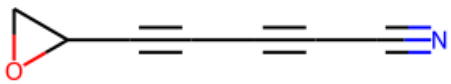
SMILES: [C]#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (4.52)

Is DFT optimized?: True

Property	Value
Formula	C7N
Molecular weight	98.084
IUPAC name	hepta-2,4,6-triynenitrile
$\mu_{a,b,c}$	4.2, 0.0, 0.0
A, B, C	∞, 582.2047, 582.2047
A_s, B_s, C_s	∞, 580.5163, 580.5163
Charge, Multiplicity	0, 2
Predicted log column density	11.963±1.566
Electronic energy	-321.02906

geom193



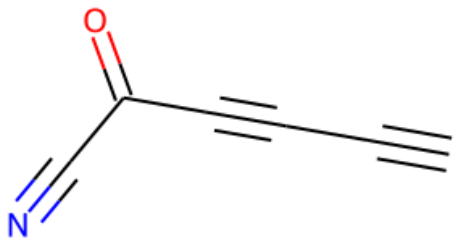
SMILES: N#CC#CC#CC1CO1

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.25)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	5.1, 0.9, 2.0
A, B, C	15301.6393, 444.3359, 443.9350
A_s, B_s, C_s	15257.2645, 443.0473, 442.6476
Charge, Multiplicity	0, 1
Predicted log column density	9.967±4.569
Electronic energy	-398.18869

geom194



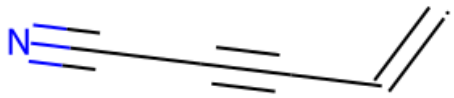
SMILES: C#CC#CC(=O)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.02)

Is DFT optimized?: True

Property	Value
Formula	C6HNO
Molecular weight	103.080
IUPAC name	
$\mu_{a,b,c}$	5.0, 0.2, 0.0
A, B, C	5430.4402, 931.8420, 795.3612
A_s, B_s, C_s	5414.6919, 929.1396, 793.0546
Charge, Multiplicity	0, 1
Predicted log column density	9.933±3.312
Electronic energy	-358.90272

geom195



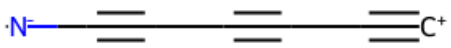
SMILES: [CH]=CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (3.37)

Is DFT optimized?: True

Property	Value
Formula	C5H2N
Molecular weight	76.078
IUPAC name	pent-4-en-2-ynenitrile
$\mu_{a,b,c}$	4.4, 0.0, 0.0
A, B, C	39479.0028, 1436.4098, 1385.9825
A_s, B_s, C_s	39364.5137, 1432.2442, 1381.9632
Charge, Multiplicity	0, 2
Predicted log column density	11.760±1.636
Electronic energy	-246.19853

geom196



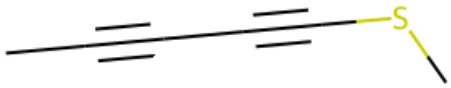
SMILES: [C+]#CC#CC#C[N−]

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (4.76)

Is DFT optimized?: True

Property	Value
Formula	C6N
Molecular weight	86.073
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.0, 0.0
A, B, C	∞, 869.7294, 869.7294
A_s, B_s, C_s	∞, 867.2072, 867.2072
Charge, Multiplicity	0, 2
Predicted log column density	12.308±2.305
Electronic energy	-282.97260

geom197



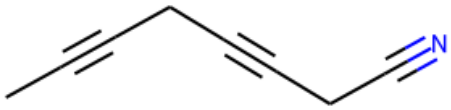
SMILES: CC#CC#CSC

Nearest TMC-1 molecule (distance): CC#CC#N (4.58)

Is DFT optimized?: True

Property	Value
Formula	C6H6S
Molecular weight	110.181
IUPAC name	1-methylsulfanylpenta-1,3-diyne
$\mu_{a,b,c}$	0.5, 1.7, 0.0
A, B, C	12760.7066, 627.1494, 602.3401
A_s, B_s, C_s	12723.7005, 625.3306, 600.5933
Charge, Multiplicity	0, 1
Predicted log column density	11.679±4.234
Electronic energy	-630.21432

geom198



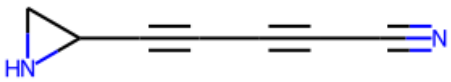
SMILES: CC#CCC#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.72)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	1.6, 3.4, 0.8
A, B, C	2619.0019, 629.0205, 516.0319
A_s, B_s, C_s	2611.4068, 627.1964, 514.5354
Charge, Multiplicity	0, 1
Predicted log column density	8.161±4.135
Electronic energy	-363.54250

geom199



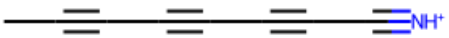
SMILES: N#CC#CC#CC1CN1

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.73)

Is DFT optimized?: True

Property	Value
Formula	C7H4N2
Molecular weight	116.123
IUPAC name	
$\mu_{a,b,c}$	4.7, 0.4, 1.1
A, B, C	13875.9820, 449.4246, 449.2477
A_s, B_s, C_s	13835.7416, 448.1212, 447.9449
Charge, Multiplicity	0, 1
Predicted log column density	8.768±5.136
Electronic energy	-378.33064

geom200



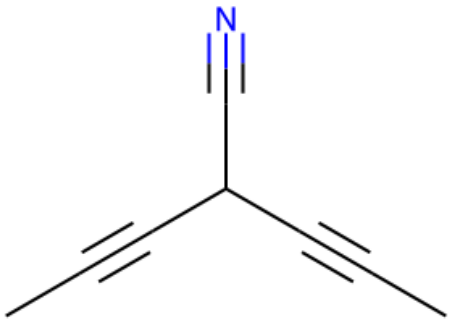
SMILES: CC#CC#CC#CC#[NH+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (4.68)

Is DFT optimized?: True

Property	Value
Formula	C8H4N+
Molecular weight	114.127
IUPAC name	
$\mu_{a,b,c}$	5.3, 0.0, 0.0
A, B, C	158143.3545, 367.8853, 367.8852
A_s, B_s, C_s	157684.7387, 366.8184, 366.8184
Charge, Multiplicity	1, 1
Predicted log column density	11.260±1.732
Electronic energy	-361.39367

geom201



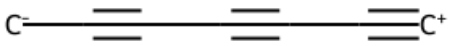
SMILES: CC#CC(C#N)C#CC

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.77)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	0.0, 4.4, 1.1
A, B, C	1810.4438, 920.8826, 641.1812
A_s, B_s, C_s	1805.1935, 918.2120, 639.3218
Charge, Multiplicity	0, 1
Predicted log column density	9.413±4.432
Electronic energy	-363.53821

geom202



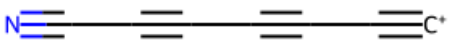
SMILES: [C+]#CC#CC#C[CH2−]

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (4.94)

Is DFT optimized?: True

Property	Value
Formula	C7H2
Molecular weight	86.093
IUPAC name	hepta-1,3,5-triyne
$\mu_{a,b,c}$	8.1, 0.0, 0.0
A, B, C	289638.4411, 850.1755, 847.6872
A_s, B_s, C_s	288798.4897, 847.7100, 845.2289
Charge, Multiplicity	0, 1
Predicted log column density	11.923±2.209
Electronic energy	-267.53031

geom203



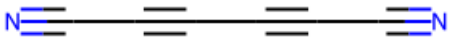
SMILES: [C+]#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (4.83)

Is DFT optimized?: True

Property	Value
Formula	C7N+
Molecular weight	98.084
IUPAC name	hepta-2,4,6-triynenitrile
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	4034555097132.0391, 583.2294, 583.2294
A_s, B_s, C_s	4022854887350.3560, 581.5380, 581.5380
Charge, Multiplicity	1, 1
Predicted log column density	11.705±1.663
Electronic energy	-320.66595

geom204



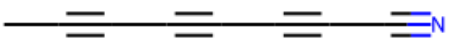
SMILES: N#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C6N2
Molecular weight	100.080
IUPAC name	hexa-2,4-diynedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 559.6794, 559.6794
A_s, B_s, C_s	∞, 558.0563, 558.0563
Charge, Multiplicity	0, 1
Predicted log column density	11.697±1.642
Electronic energy	-337.83450

geom205



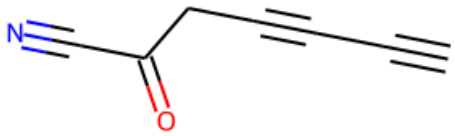
SMILES: CC#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (4.19)

Is DFT optimized?: True

Property	Value
Formula	C8H3N
Molecular weight	113.119
IUPAC name	octa-2,4,6-triynenitrile
$\mu_{a,b,c}$	7.3, 0.0, 0.0
A, B, C	159010.2611, 373.2508, 373.2505
A_s, B_s, C_s	158549.1313, 372.1684, 372.1681
Charge, Multiplicity	0, 1
Predicted log column density	12.020±1.577
Electronic energy	-361.07148

geom206



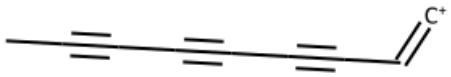
SMILES: C#CC#CCC(=O)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.89)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	2.5, 2.0, 0.0
A, B, C	8536.0735, 589.6954, 553.4578
A_s, B_s, C_s	8511.3189, 587.9853, 551.8528
Charge, Multiplicity	0, 1
Predicted log column density	10.592±3.690
Electronic energy	-398.21361

geom207



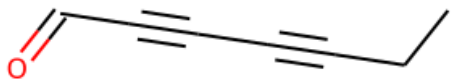
SMILES: [CH+]=[C]C#CC#CC#CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (4.75)

Is DFT optimized?: True

Property	Value
Formula	C9H4+
Molecular weight	112.131
IUPAC name	
$\mu_{a,b,c}$	0.6, 0.0, 0.1
A, B, C	157614.0280, 379.1336, 379.1218
A_s, B_s, C_s	157156.9474, 378.0341, 378.0224
Charge, Multiplicity	1, 2
Predicted log column density	12.294±1.680
Electronic energy	-344.68017

geom208



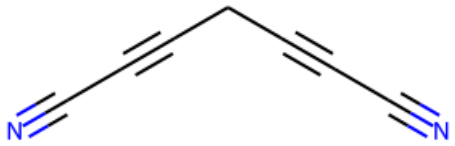
SMILES: CCC#CC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (5.97)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	hepta-2,4-diynal
$\mu_{a,b,c}$	4.6, 1.4, 1.3
A, B, C	13287.9421, 545.3508, 535.0897
A_s, B_s, C_s	13249.4071, 543.7693, 533.5380
Charge, Multiplicity	0, 1
Predicted log column density	9.083±3.297
Electronic energy	-345.32620

geom209



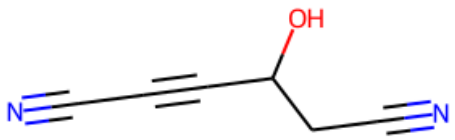
SMILES: N#CC#CCC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (5.13)

Is DFT optimized?: True

Property	Value
Formula	C7H2N2
Molecular weight	114.107
IUPAC name	
$\mu_{a,b,c}$	0.0, 5.0, 0.0
A, B, C	4492.9119, 527.0847, 473.1253
A_s, B_s, C_s	4479.8824, 525.5562, 471.7532
Charge, Multiplicity	0, 1
Predicted log column density	9.583±2.711
Electronic energy	-377.13497

geom210



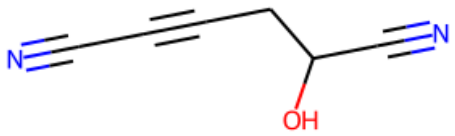
SMILES: N#CC#CC(O)CC#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (6.08)

Is DFT optimized?: True

Property	Value
Formula	C6H4N2O
Molecular weight	120.111
IUPAC name	
$\mu_{a,b,c}$	3.1, 3.8, 1.7
A, B, C	2216.9138, 916.8364, 669.5995
A_s, B_s, C_s	2210.4848, 914.1776, 667.6576
Charge, Multiplicity	0, 1
Predicted log column density	9.643±4.615
Electronic energy	-415.51746

geom211



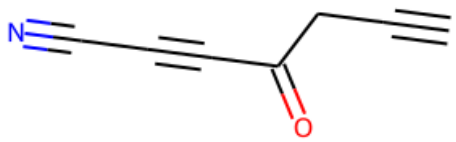
SMILES: N#CC#CCC(O)C#N

Nearest TMC-1 molecule (distance): CC#CC#CC#N (6.16)

Is DFT optimized?: True

Property	Value
Formula	C6H4N2O
Molecular weight	120.111
IUPAC name	
$\mu_{a,b,c}$	1.8, 1.2, 1.2
A, B, C	6961.2945, 583.3675, 550.5128
A_s, B_s, C_s	6941.1067, 581.6757, 548.9163
Charge, Multiplicity	0, 1
Predicted log column density	9.848±4.766
Electronic energy	-415.51640

geom212



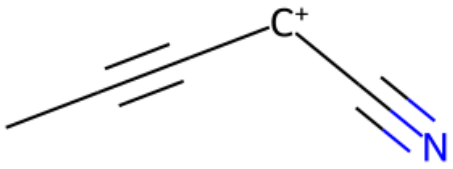
SMILES: C#CCC(=O)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.89)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	3.1, 1.5, 0.9
A, B, C	2380.3208, 955.1796, 697.9180
A_s, B_s, C_s	2373.4178, 952.4096, 695.8940
Charge, Multiplicity	0, 1
Predicted log column density	11.415±3.773
Electronic energy	-398.21224

geom213



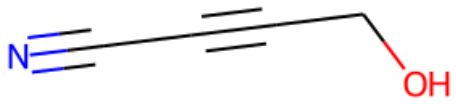
SMILES: CC#C[CH+]C#N

Nearest TMC-1 molecule (distance): CC#CC#N (2.72)

Is DFT optimized?: True

Property	Value
Formula	C5H4N+
Molecular weight	78.094
IUPAC name	
$\mu_{a,b,c}$	5.4, 2.3, 0.1
A, B, C	17780.2358, 1476.4374, 1374.7522
A_s, B_s, C_s	17728.6731, 1472.1558, 1370.7654
Charge, Multiplicity	1, 1
Predicted log column density	11.195±1.826
Electronic energy	-247.16833

geom214



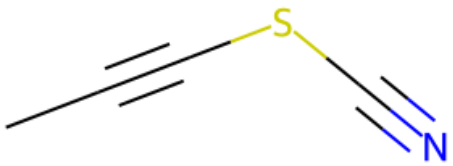
SMILES: N#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#N (3.55)

Is DFT optimized?: True

Property	Value
Formula	C4H3NO
Molecular weight	81.074
IUPAC name	4-hydroxybut-2-ynenitrile
$\mu_{a,b,c}$	3.6, 1.1, 1.4
A, B, C	26270.5810, 1320.7583, 1271.1203
A_s, B_s, C_s	26194.3963, 1316.9281, 1267.4340
Charge, Multiplicity	0, 1
Predicted log column density	10.725±3.167
Electronic energy	-284.00731

geom215



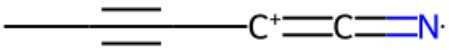
SMILES: CC#CSC#N

Nearest TMC-1 molecule (distance): CC#CC#N (3.87)

Is DFT optimized?: True

Property	Value
Formula	C4H3NS
Molecular weight	97.142
IUPAC name	prop-1-ynyl thiocyanate
$\mu_{a,b,c}$	4.2, 1.6, 0.0
A, B, C	7530.5086, 1379.6634, 1174.6725
A_s, B_s, C_s	7508.6701, 1375.6624, 1171.2660
Charge, Multiplicity	0, 1
Predicted log column density	10.601±4.171
Electronic energy	-606.97579

geom216



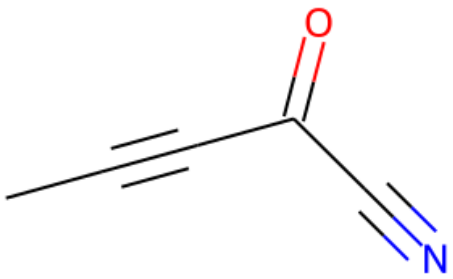
SMILES: CC#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): CC#CC#N (3.98)

Is DFT optimized?: True

Property	Value
Formula	C5H3N+
Molecular weight	77.086
IUPAC name	
$\mu_{a,b,c}$	6.7, 0.0, 0.2
A, B, C	156188.8857, 1223.5070, 1223.2565
A_s, B_s, C_s	155735.9379, 1219.9589, 1219.7091
Charge, Multiplicity	1, 2
Predicted log column density	12.608±1.840
Electronic energy	-246.50773

geom217



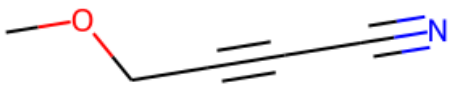
SMILES: CC#CC(=O)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.02)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	5.5, 0.6, 0.0
A, B, C	5414.9896, 1439.4793, 1145.3367
A_s, B_s, C_s	5399.2861, 1435.3048, 1142.0153
Charge, Multiplicity	0, 1
Predicted log column density	10.225±3.398
Electronic energy	-322.09920

geom218



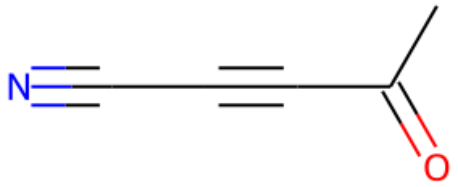
SMILES: COCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.08)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	
$\mu_{a,b,c}$	5.6, 2.1, 0.0
A, B, C	22017.1486, 860.4805, 836.9181
A_s, B_s, C_s	21953.2989, 857.9851, 834.4911
Charge, Multiplicity	0, 1
Predicted log column density	12.732±3.749
Electronic energy	-323.29936

geom219



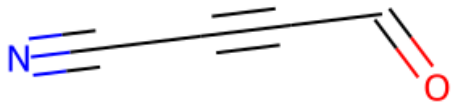
SMILES: CC(=O)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.24)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	4-oxopent-2-ynenitrile
$\mu_{a,b,c}$	2.7, 2.8, 0.0
A, B, C	10146.4208, 1099.8545, 998.4449
A_s, B_s, C_s	10116.9962, 1096.6649, 995.5494
Charge, Multiplicity	0, 1
Predicted log column density	9.809±3.732
Electronic energy	-322.10644

geom220



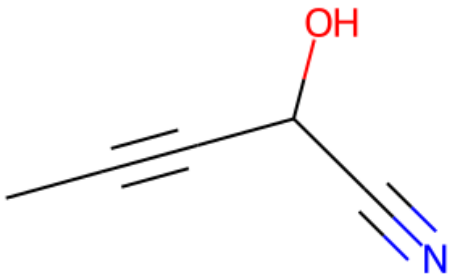
SMILES: N#CC#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (4.30)

Is DFT optimized?: True

Property	Value
Formula	C4HNO
Molecular weight	79.058
IUPAC name	4-oxobut-2-ynenitrile
$\mu_{a,b,c}$	1.6, 2.2, 0.0
A, B, C	52952.6969, 1346.0397, 1312.6721
A_s, B_s, C_s	52799.1340, 1342.1362, 1308.8653
Charge, Multiplicity	0, 1
Predicted log column density	10.565±1.988
Electronic energy	-282.78826

geom221



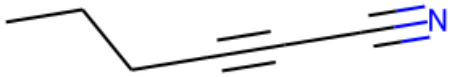
SMILES: CC#CC(O)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.44)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	
$\mu_{a,b,c}$	4.2, 1.2, 0.1
A, B, C	4801.0354, 1429.9884, 1153.8700
A_s, B_s, C_s	4787.1124, 1425.8414, 1150.5238
Charge, Multiplicity	0, 1
Predicted log column density	10.498±4.242
Electronic energy	-323.31035

geom222



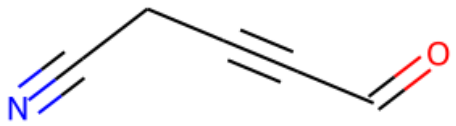
SMILES: CCCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.49)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	hex-2-ynenitrile
$\mu_{a,b,c}$	5.6, 0.8, 0.0
A, B, C	18133.1175, 829.8744, 805.4557
A_s, B_s, C_s	18080.5314, 827.4678, 803.1199
Charge, Multiplicity	0, 1
Predicted log column density	10.304±3.515
Electronic energy	-287.43272

geom223



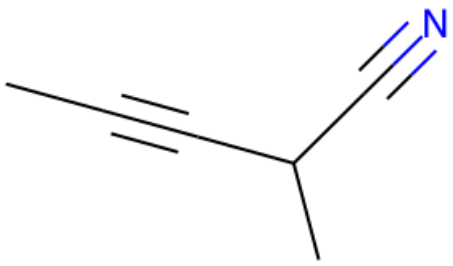
SMILES: N#CCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#N (4.53)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	0.5, 1.7, 0.3
A, B, C	13525.7334, 950.8611, 893.7411
A_s, B_s, C_s	13486.5088, 948.1036, 891.1492
Charge, Multiplicity	0, 1
Predicted log column density	8.601±2.844
Electronic energy	-322.09543

geom224



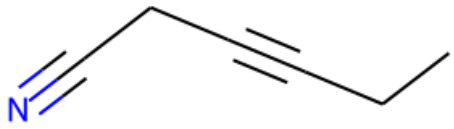
SMILES: CC#CC(C)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.54)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	2-methylpent-3-ynenitrile
$\mu_{a,b,c}$	3.1, 3.1, 0.7
A, B, C	4706.4722, 1406.5509, 1138.9937
A_s, B_s, C_s	4692.8235, 1402.4719, 1135.6906
Charge, Multiplicity	0, 1
Predicted log column density	10.393±4.071
Electronic energy	-287.43028

geom225



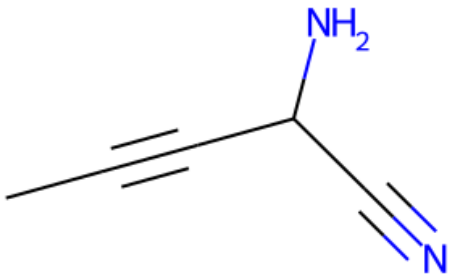
SMILES: CCC#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.64)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	hex-3-ynenitrile
$\mu_{a,b,c}$	3.4, 2.7, 0.4
A, B, C	8190.8382, 964.0521, 926.3308
A_s, B_s, C_s	8167.0847, 961.2563, 923.6444
Charge, Multiplicity	0, 1
Predicted log column density	8.784±3.557
Electronic energy	-287.42838

geom226



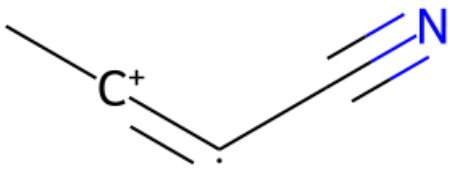
SMILES: CC#CC(N)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.65)

Is DFT optimized?: True

Property	Value
Formula	C5H6N2
Molecular weight	94.117
IUPAC name	
$\mu_{a,b,c}$	4.6, 2.7, 0.4
A, B, C	4750.3513, 1418.9506, 1145.5517
A_s, B_s, C_s	4736.5753, 1414.8356, 1142.2296
Charge, Multiplicity	0, 1
Predicted log column density	9.439±4.114
Electronic energy	-303.45282

geom227



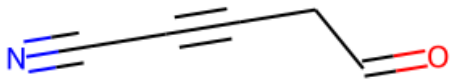
SMILES: C[C+]=[C]C#N

Nearest TMC-1 molecule (distance): N#CC#[NH+] (1.97)

Is DFT optimized?: True

Property	Value
Formula	C4H3N+
Molecular weight	65.075
IUPAC name	
$\mu_{a,b,c}$	5.6, 0.2, 0.0
A, B, C	155852.6787, 2074.9794, 2073.8725
A_s, B_s, C_s	155400.7059, 2068.9619, 2067.8583
Charge, Multiplicity	1, 2
Predicted log column density	13.092±1.561
Electronic energy	-208.43948

geom228



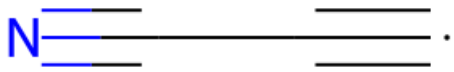
SMILES: N#CC#CCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (4.46)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	2.3, 1.5, 0.9
A, B, C	17724.5425, 893.8719, 860.2617
A_s, B_s, C_s	17673.1413, 891.2797, 857.7670
Charge, Multiplicity	0, 1
Predicted log column density	8.084±2.949
Electronic energy	-322.10242

geom229



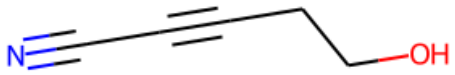
SMILES: [C]#CC#N

Nearest TMC-1 molecule (distance): N#CC#[NH+] (1.67)

Is DFT optimized?: True

Property	Value
Formula	C3N
Molecular weight	50.040
IUPAC name	prop-2-ynenitrile
$\mu_{a,b,c}$	3.0, 0.0, 0.0
A, B, C	∞, 4930.8968, 4930.8968
A_s, B_s, C_s	∞, 4916.5972, 4916.5972
Charge, Multiplicity	0, 2
Predicted log column density	13.296±1.071
Electronic energy	-168.78158

geom230



SMILES: N#CC#CCCO

Nearest TMC-1 molecule (distance): CC#CC#N (4.85)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	5-hydroxypent-2-ynenitrile
$\mu_{a,b,c}$	3.7, 2.1, 0.8
A, B, C	7933.4081, 1072.3966, 974.6611
A_s, B_s, C_s	7910.4012, 1069.2866, 971.8346
Charge, Multiplicity	0, 1
Predicted log column density	10.262±3.869
Electronic energy	-323.31850

geom231

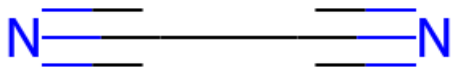
SMILES: CC(=O)CC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.86)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	5-oxohex-2-ynenitrile
$\mu_{a,b,c}$	6.2, 3.9, 0.0
A, B, C	8573.4906, 777.5397, 719.2139
A_s, B_s, C_s	8548.6275, 775.2848, 717.1282
Charge, Multiplicity	0, 1
Predicted log column density	10.938±3.889
Electronic energy	-361.41773

geom232



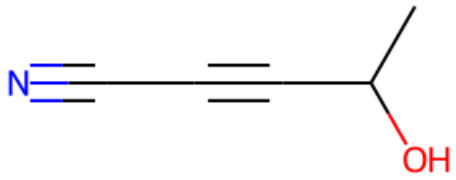
SMILES: N#CC#N

Nearest TMC-1 molecule (distance): N#CC#[NH+] (3.27)

Is DFT optimized?: True

Property	Value
Formula	C2N2
Molecular weight	52.036
IUPAC name	oxalonitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 4699.1625, 4699.1625
A_s, B_s, C_s	∞, 4685.5349, 4685.5349
Charge, Multiplicity	0, 1
Predicted log column density	12.234±1.612
Electronic energy	-185.58406

geom233



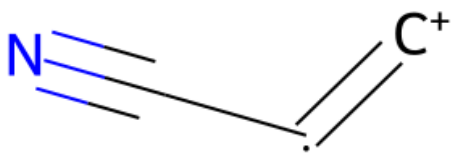
SMILES: CC(O)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.87)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	4-hydroxypent-2-ynenitrile
$\mu_{a,b,c}$	4.1, 1.5, 0.5
A, B, C	8368.3559, 1087.8549, 997.7420
A_s, B_s, C_s	8344.0877, 1084.7001, 994.8485
Charge, Multiplicity	0, 1
Predicted log column density	11.282±4.406
Electronic energy	-323.31666

geom234



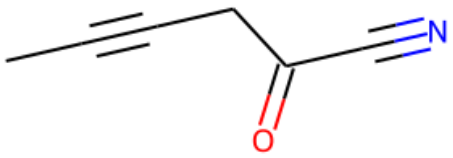
SMILES: [CH+]=[C]C#N

Nearest TMC-1 molecule (distance): N#CC#[NH+] (1.66)

Is DFT optimized?: True

Property	Value
Formula	C3HN+
Molecular weight	51.048
IUPAC name	prop-2-enenitrile
$\mu_{a,b,c}$	5.4, 0.0, 0.0
A, B, C	∞, 4525.2088, 4525.2088
A_s, B_s, C_s	∞, 4512.0857, 4512.0857
Charge, Multiplicity	1, 2
Predicted log column density	13.143±1.248
Electronic energy	-169.08958

geom235



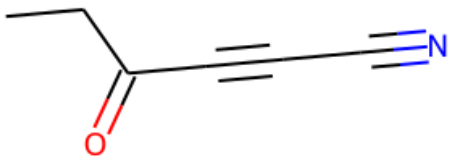
SMILES: CC#CCC(=O)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.89)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	3.1, 2.1, 1.0
A, B, C	3397.1756, 1192.3881, 940.5120
A_s, B_s, C_s	3387.3238, 1188.9302, 937.7845
Charge, Multiplicity	0, 1
Predicted log column density	10.929±3.813
Electronic energy	-361.40675

geom236



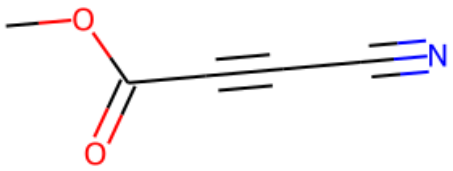
SMILES: CCC(=O)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.94)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	4-oxohex-2-ynenitrile
$\mu_{a,b,c}$	3.3, 2.4, 0.0
A, B, C	7878.3089, 771.1599, 708.5312
A_s, B_s, C_s	7855.4618, 768.9236, 706.4765
Charge, Multiplicity	0, 1
Predicted log column density	9.669±3.916
Electronic energy	-361.41109

geom237



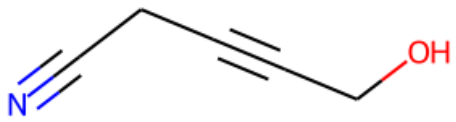
SMILES: COC(=O)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (4.99)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	methyl 3-cyanoprop-2-ynoate
$\mu_{a,b,c}$	4.3, 1.6, 0.0
A, B, C	8750.4467, 803.7506, 739.5978
A_s, B_s, C_s	8725.0704, 801.4197, 737.4530
Charge, Multiplicity	0, 1
Predicted log column density	10.899±4.399
Electronic energy	-397.31387

geom238



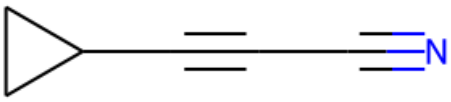
SMILES: N#CCC#CCO

Nearest TMC-1 molecule (distance): CC#CC#N (5.02)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	
$\mu_{a,b,c}$	2.0, 3.9, 1.2
A, B, C	9734.0670, 930.4786, 893.5712
A_s, B_s, C_s	9705.8382, 927.7802, 890.9799
Charge, Multiplicity	0, 1
Predicted log column density	8.730±3.989
Electronic energy	-323.30924

geom239



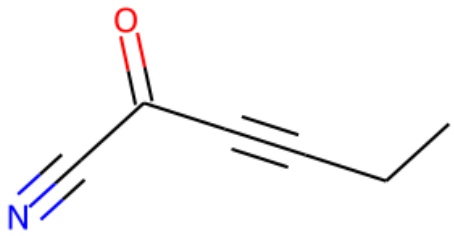
SMILES: N#CC#CC1CC1

Nearest TMC-1 molecule (distance): CC#CC#N (5.04)

Is DFT optimized?: True

Property	Value
Formula	C6H5N
Molecular weight	91.113
IUPAC name	3-cyclopropylprop-2-ynenitrile
$\mu_{a,b,c}$	5.9, 0.0, 0.5
A, B, C	14063.1602, 1042.9344, 1034.9443
A_s, B_s, C_s	14022.3770, 1039.9099, 1031.9430
Charge, Multiplicity	0, 1
Predicted log column density	10.263±4.044
Electronic energy	-286.18925

geom240



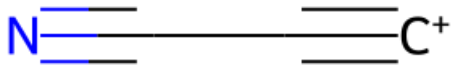
SMILES: CCC#CC(=O)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.05)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	5.6, 0.5, 0.1
A, B, C	3942.8884, 967.4196, 785.6347
A_s, B_s, C_s	3931.4540, 964.6141, 783.3564
Charge, Multiplicity	0, 1
Predicted log column density	8.451±4.269
Electronic energy	-361.40263

geom241



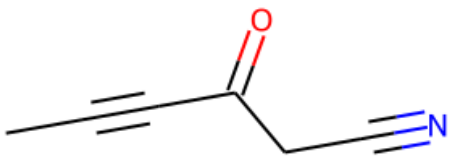
SMILES: [C+]#CC#N

Nearest TMC-1 molecule (distance): N#CC#[NH+] (2.02)

Is DFT optimized?: True

Property	Value
Formula	C3N+
Molecular weight	50.040
IUPAC name	prop-2-ynenitrile
$\mu_{a,b,c}$	0.0, 7.2, 0.0
A, B, C	7260167609.1681, 4939.0048, 4939.0014
A_s, B_s, C_s	7239113123.1015, 4924.6817, 4924.6783
Charge, Multiplicity	1, 1
Predicted log column density	12.624±1.481
Electronic energy	-168.21934

geom242



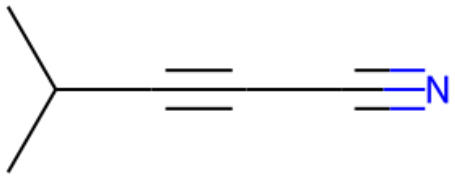
SMILES: CC#CC(=O)CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.08)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	3-oxohex-4-ynenitrile
$\mu_{a,b,c}$	1.6, 0.1, 0.5
A, B, C	2346.3586, 1607.4491, 967.0555
A_s, B_s, C_s	2339.5542, 1602.7875, 964.2510
Charge, Multiplicity	0, 1
Predicted log column density	10.598±3.949
Electronic energy	-361.41732

geom243



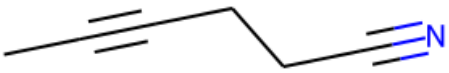
SMILES: CC(C)C#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.11)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	4-methylpent-2-ynenitrile
$\mu_{a,b,c}$	5.6, 0.0, 0.4
A, B, C	7736.7466, 1096.7267, 999.0563
A_s, B_s, C_s	7714.3100, 1093.5462, 996.1591
Charge, Multiplicity	0, 1
Predicted log column density	11.427±4.440
Electronic energy	-287.43351

geom244



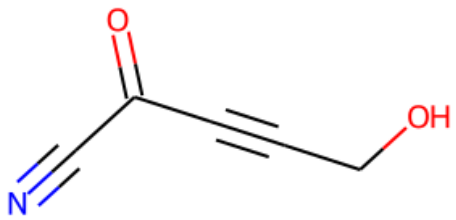
SMILES: CC#CCCC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.14)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	hex-4-ynenitrile
$\mu_{a,b,c}$	4.5, 0.9, 0.0
A, B, C	19288.5465, 850.6803, 827.3136
A_s, B_s, C_s	19232.6097, 848.2133, 824.9144
Charge, Multiplicity	0, 1
Predicted log column density	10.076±3.168
Electronic energy	-287.43570

geom245



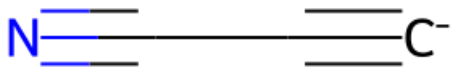
SMILES: N#CC(=O)C#CCO

Nearest TMC-1 molecule (distance): CC#CC#N (5.20)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	
$\mu_{a,b,c}$	3.7, 0.7, 1.5
A, B, C	5183.1689, 857.3690, 741.7829
A_s, B_s, C_s	5168.1377, 854.8826, 739.6317
Charge, Multiplicity	0, 1
Predicted log column density	8.417±4.620
Electronic energy	-397.28154

geom246



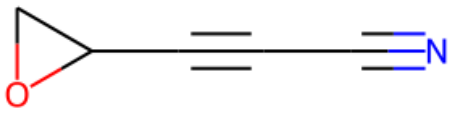
SMILES: [C−]#CC#N

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.55)

Is DFT optimized?: True

Property	Value
Formula	C3N-
Molecular weight	50.040
IUPAC name	prop-2-ynenitrile
$\mu_{a,b,c}$	2.8, 0.0, 0.0
A, B, C	∞, 4838.5969, 4838.5969
A_s, B_s, C_s	∞, 4824.5649, 4824.5649
Charge, Multiplicity	-1, 1
Predicted log column density	11.890±1.521
Electronic energy	-168.94531

geom247



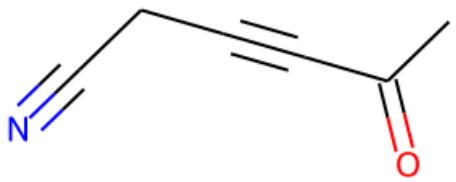
SMILES: N#CC#CC1CO1

Nearest TMC-1 molecule (distance): CC#CC#N (5.25)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	4.2, 1.7, 1.5
A, B, C	16540.1102, 1035.0472, 1028.7788
A_s, B_s, C_s	16492.1439, 1032.0456, 1025.7953
Charge, Multiplicity	0, 1
Predicted log column density	10.216±4.535
Electronic energy	-322.06570

geom248



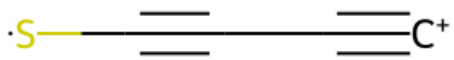
SMILES: CC(=O)C#CCC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.26)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.7, 1.2
A, B, C	5502.9907, 820.1247, 726.4291
A_s, B_s, C_s	5487.0320, 817.7463, 724.3225
Charge, Multiplicity	0, 1
Predicted log column density	7.831±4.385
Electronic energy	-361.41248

geom249



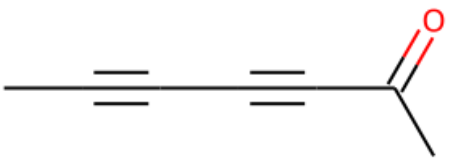
SMILES: [C+]#CC#C[S]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.86)

Is DFT optimized?: True

Property	Value
Formula	C4S+
Molecular weight	80.111
IUPAC name	buta-1,3-diyne-1-thiol
$\mu_{a,b,c}$	1.8, 0.0, 0.0
A, B, C	∞, 1518.7341, 1518.7341
A_s, B_s, C_s	∞, 1514.3297, 1514.3297
Charge, Multiplicity	1, 2
Predicted log column density	13.269±1.834
Electronic energy	-549.95609

geom250



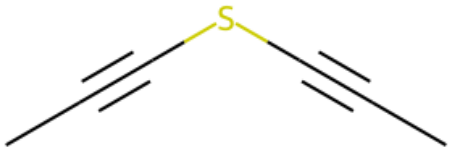
SMILES: CC#CC#CC(C)=O

Nearest TMC-1 molecule (distance): CC#CC#N (5.32)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	hepta-3,5-diyn-2-one
$\mu_{a,b,c}$	3.4, 2.8, 0.0
A, B, C	9651.9057, 634.6095, 599.9207
A_s, B_s, C_s	9623.9152, 632.7691, 598.1809
Charge, Multiplicity	0, 1
Predicted log column density	10.081±3.790
Electronic energy	-345.33824

geom251



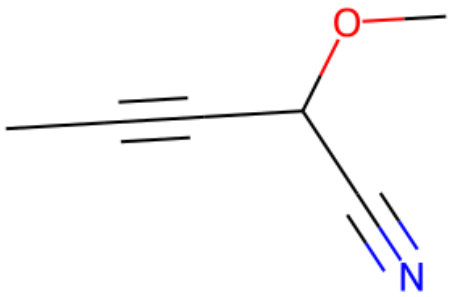
SMILES: CC#CSC#CC

Nearest TMC-1 molecule (distance): CC#CC#N (5.34)

Is DFT optimized?: True

Property	Value
Formula	C6H6S
Molecular weight	110.181
IUPAC name	1-prop-1-ynylsulfanylprop-1-yne
$\mu_{a,b,c}$	0.0, 1.9, 0.0
A, B, C	4340.6025, 889.9356, 745.4501
A_s, B_s, C_s	4328.0147, 887.3548, 743.2883
Charge, Multiplicity	0, 1
Predicted log column density	10.711±4.454
Electronic energy	-630.19981

geom252



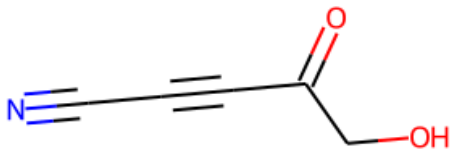
SMILES: CC#CC(C#N)OC

Nearest TMC-1 molecule (distance): CC#CC#N (5.34)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	1.6, 2.7, 1.5
A, B, C	3368.4299, 1131.5002, 878.9267
A_s, B_s, C_s	3358.6615, 1128.2188, 876.3778
Charge, Multiplicity	0, 1
Predicted log column density	11.166±4.676
Electronic energy	-362.60189

geom253



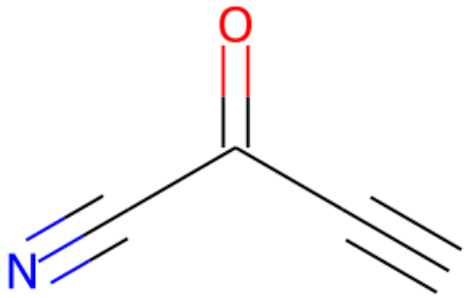
SMILES: N#CC#CC(=O)CO

Nearest TMC-1 molecule (distance): CC#CC#N (5.36)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	
$\mu_{a,b,c}$	1.0, 0.9, 0.0
A, B, C	8405.5958, 771.5974, 709.8585
A_s, B_s, C_s	8381.2196, 769.3598, 707.7999
Charge, Multiplicity	0, 1
Predicted log column density	9.039±4.576
Electronic energy	-397.29520

geom254



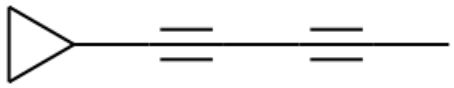
SMILES: C#CC(=O)C#N

Nearest TMC-1 molecule (distance): [C]#CC#N (3.98)

Is DFT optimized?: True

Property	Value
Formula	C4HNO
Molecular weight	79.058
IUPAC name	
$\mu_{a,b,c}$	3.7, 1.5, 0.0
A, B, C	6569.2335, 2912.5403, 2017.8881
A_s, B_s, C_s	6550.1828, 2904.0940, 2012.0362
Charge, Multiplicity	0, 1
Predicted log column density	11.064±3.370
Electronic energy	-282.77994

geom255



SMILES: CC#CC#CC1CC1

Nearest TMC-1 molecule (distance): CC#CC#N (5.39)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	penta-1,3-diynylcyclopropane
$\mu_{a,b,c}$	0.2, 0.0, 0.3
A, B, C	12483.5828, 616.5320, 614.6663
A_s, B_s, C_s	12447.3804, 614.7441, 612.8838
Charge, Multiplicity	0, 1
Predicted log column density	10.548±4.076
Electronic energy	-309.41420

geom256

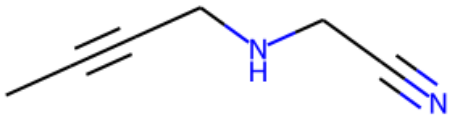
SMILES: CC#CC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.33)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	but-2-ynal
$\mu_{a,b,c}$	3.8, 1.6, 0.0
A, B, C	42400.2804, 2111.1416, 2036.6349
A_s, B_s, C_s	42277.3196, 2105.0193, 2030.7287
Charge, Multiplicity	0, 1
Predicted log column density	11.137±2.044
Electronic energy	-229.90015

geom257



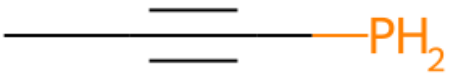
SMILES: CC#CCNCC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.47)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	2-(but-2-ynylamino)acetonitrile
$\mu_{a,b,c}$	3.7, 2.7, 1.2
A, B, C	7649.5683, 643.8788, 601.4595
A_s, B_s, C_s	7627.3846, 642.0115, 599.7152
Charge, Multiplicity	0, 1
Predicted log column density	11.590±4.759
Electronic energy	-342.75169

geom258



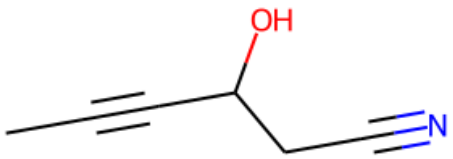
SMILES: CC#CP

Nearest TMC-1 molecule (distance): CC#N (3.17)

Is DFT optimized?: True

Property	Value
Formula	C3H5P
Molecular weight	72.047
IUPAC name	prop-1-ynylphosphane
$\mu_{a,b,c}$	1.3, 0.0, 0.7
A, B, C	71773.3069, 2106.3127, 2102.1568
A_s, B_s, C_s	71565.1643, 2100.2044, 2096.0605
Charge, Multiplicity	0, 1
Predicted log column density	12.679±1.776
Electronic energy	-458.54619

geom259



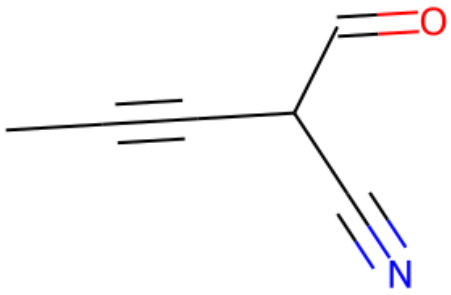
SMILES: CC#CC(O)CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.51)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	3-hydroxyhex-4-ynenitrile
$\mu_{a,b,c}$	2.8, 1.9, 1.8
A, B, C	2285.5020, 1412.4720, 912.9389
A_s, B_s, C_s	2278.8740, 1408.3758, 910.2913
Charge, Multiplicity	0, 1
Predicted log column density	10.189±4.700
Electronic energy	-362.62561

geom260



SMILES: CC#CC(C#N)C=O

Nearest TMC-1 molecule (distance): CC#CC#N (5.51)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	4.0, 1.2, 0.1
A, B, C	2638.2593, 1275.4179, 899.0499
A_s, B_s, C_s	2630.6084, 1271.7191, 896.4427
Charge, Multiplicity	0, 1
Predicted log column density	8.138±4.145
Electronic energy	-361.40196

geom261

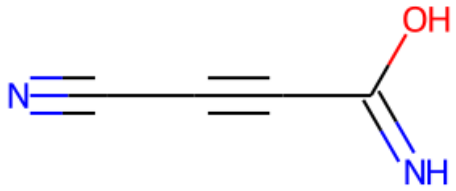
SMILES: CC#CCN

Nearest TMC-1 molecule (distance): CC#C (4.93)

Is DFT optimized?: True

Property	Value
Formula	C4H7N
Molecular weight	69.107
IUPAC name	but-2-yn-1-amine
$\mu_{a,b,c}$	0.0, 0.6, 1.3
A, B, C	23173.1081, 2064.9133, 1950.4376
A_s, B_s, C_s	23105.9061, 2058.9250, 1944.7813
Charge, Multiplicity	0, 1
Predicted log column density	10.494±3.051
Electronic energy	-211.25071

geom262



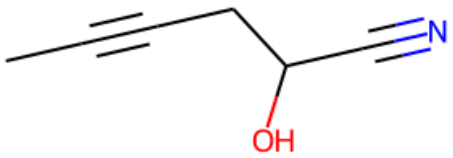
SMILES: N#CC#CC(=N)O

Nearest TMC-1 molecule (distance): CC#CC#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C4H2N2O
Molecular weight	94.073
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.9, 0.0
A, B, C	11109.7808, 1110.7851, 1009.8206
A_s, B_s, C_s	11077.5624, 1107.5638, 1006.8921
Charge, Multiplicity	0, 1
Predicted log column density	11.162±3.742
Electronic energy	-338.12951

geom263



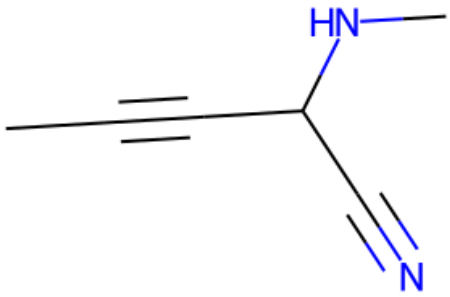
SMILES: CC#CCC(O)C#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	2.8, 2.4, 1.0
A, B, C	3014.0992, 1199.9708, 1047.1780
A_s, B_s, C_s	3005.3583, 1196.4909, 1044.1411
Charge, Multiplicity	0, 1
Predicted log column density	10.394±4.850
Electronic energy	-362.62480

geom264



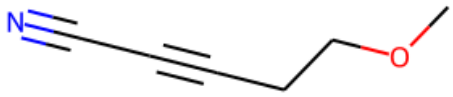
SMILES: CC#CC(C#N)NC

Nearest TMC-1 molecule (distance): CC#CC#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	
$\mu_{a,b,c}$	2.4, 4.1, 1.6
A, B, C	3252.6695, 1117.4146, 862.8943
A_s, B_s, C_s	3243.2368, 1114.1741, 860.3919
Charge, Multiplicity	0, 1
Predicted log column density	10.086±5.412
Electronic energy	-342.74743

geom265



SMILES: COCCC#CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	5.8, 2.2, 1.0
A, B, C	4547.7142, 813.7486, 711.5082
A_s, B_s, C_s	4534.5259, 811.3887, 709.4448
Charge, Multiplicity	0, 1
Predicted log column density	11.762±4.574
Electronic energy	-362.61107

geom266

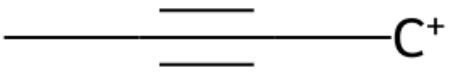
SMILES: CC#COC

Nearest TMC-1 molecule (distance): CC#N (3.83)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	1-methoxyprop-1-yne
$\mu_{a,b,c}$	0.5, 1.7, 0.0
A, B, C	27294.4481, 2210.0159, 2098.9033
A_s, B_s, C_s	27215.2942, 2203.6069, 2092.8165
Charge, Multiplicity	0, 1
Predicted log column density	12.639±2.616
Electronic energy	-231.09066

geom267



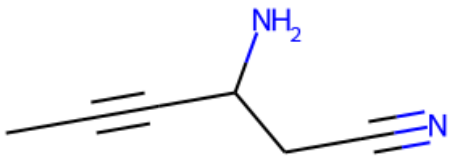
SMILES: CC#C[CH4+]

Nearest TMC-1 molecule (distance): CC#N (2.84)

Is DFT optimized?: True

Property	Value
Formula	C4H7+
Molecular weight	55.100
IUPAC name	
$\mu_{a,b,c}$	1.4, 0.1, 0.0
A, B, C	32660.9372, 3834.8456, 3592.2679
A_s, B_s, C_s	32566.2205, 3823.7245, 3581.8503
Charge, Multiplicity	1, 1
Predicted log column density	12.456±1.561
Electronic energy	-156.22749

geom268



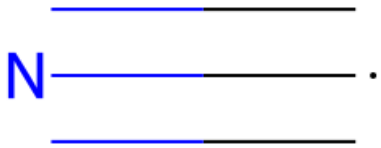
SMILES: CC#CC(N)CC#N

Nearest TMC-1 molecule (distance): CC#CC#N (5.59)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	
$\mu_{a,b,c}$	2.9, 3.1, 1.0
A, B, C	2256.1933, 1419.4965, 912.3516
A_s, B_s, C_s	2249.6503, 1415.3800, 909.7058
Charge, Multiplicity	0, 1
Predicted log column density	8.612±4.447
Electronic energy	-342.76731

geom269



SMILES: [C]#N

Nearest TMC-1 molecule (distance): N#[NH+] (0.74)

Is DFT optimized?: False

Property	Value
Formula	CN
Molecular weight	26.018
IUPAC name	formonitrile
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	∞, 63096.4669, 63096.4669
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	12.959±1.054
Electronic energy	-92.66819

geom270

SMILES: N#[S+]

Nearest TMC-1 molecule (distance): N#[NH+] (0.78)

Is DFT optimized?: True

Property	Value
Formula	NS+
Molecular weight	46.074
IUPAC name	azanylidynesulfanium
$\mu_{a,b,c}$	2.0, 0.0, 0.0
A, B, C	∞, 25430.4501, 25430.4501
A_s, B_s, C_s	∞, 25356.7018, 25356.7018
Charge, Multiplicity	1, 1
Predicted log column density	12.905±1.162
Electronic energy	-452.48379

geom271

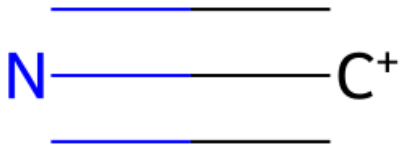
SMILES: [CH+]=[N]

Nearest TMC-1 molecule (distance): N#[NH+] (0.82)

Is DFT optimized?: True

Property	Value
Formula	CHN+
Molecular weight	27.026
IUPAC name	methanimine
$\mu_{a,b,c}$	0.0, 2.0, 0.0
A, B, C	11760533841088.5977, 44804.0771, 44804.0770
A_s, B_s, C_s	11726428292949.4414, 44674.1453, 44674.1451
Charge, Multiplicity	1, 2
Predicted log column density	13.057±1.115
Electronic energy	-92.87449

geom272



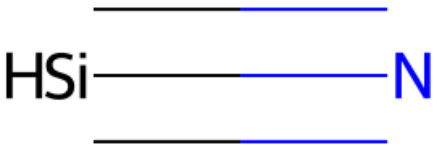
SMILES: [C+]#N

Nearest TMC-1 molecule (distance): N#[NH+] (0.82)

Is DFT optimized?: False

Property	Value
Formula	CN+
Molecular weight	26.018
IUPAC name	azanylidynemethane
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	∞, 63096.4669, 63096.4669
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 1
Predicted log column density	12.899±1.175
Electronic energy	-92.10563

geom273



SMILES: N#[SiH]

Nearest TMC-1 molecule (distance): N#[NH+] (1.15)

Is DFT optimized?: True

Property	Value
Formula	HNSi
Molecular weight	43.101
IUPAC name	azanylidynesilane
$\mu_{a,b,c}$	5.0, 0.0, 0.0
A, B, C	29806889662131.6602, 19032.8948, 19032.8948
A_s, B_s, C_s	29720449682111.4766, 18977.6994, 18977.6994
Charge, Multiplicity	0, 1
Predicted log column density	12.536±1.318
Electronic energy	-344.66088

geom274

SMILES: [C]#[S+]

Nearest TMC-1 molecule (distance): N#[NH+] (1.53)

Is DFT optimized?: False

Property	Value
Formula	CS+
Molecular weight	44.078
IUPAC name	methanethione
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	∞, 27535.7218, 27535.7218
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	13.142±1.376
Electronic energy	-435.74982

geom275

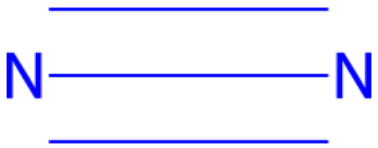
SMILES: [N]=O

Nearest TMC-1 molecule (distance): N#[NH+] (1.62)

Is DFT optimized?: True

Property	Value
Formula	NO
Molecular weight	30.006
IUPAC name	nitroxyl
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	∞, 51000.7365, 51000.7365
A_s, B_s, C_s	∞, 50852.8344, 50852.8344
Charge, Multiplicity	0, 2
Predicted log column density	12.153±1.418
Electronic energy	-129.84983

geom276



SMILES: N#N

Nearest TMC-1 molecule (distance): N#[NH+] (1.62)

Is DFT optimized?: True

Property	Value
Formula	N2
Molecular weight	28.014
IUPAC name	molecular nitrogen
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 59520.8768, 59520.8768
A_s, B_s, C_s	∞, 59348.2663, 59348.2663
Charge, Multiplicity	0, 1
Predicted log column density	12.323±1.397
Electronic energy	-109.48932

geom277

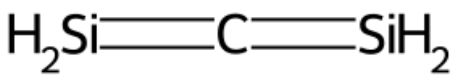
SMILES: [SiH]#[S+]

Nearest TMC-1 molecule (distance): [CH] (1.14)

Is DFT optimized?: False

Property	Value
Formula	HSSi+
Molecular weight	61.161
IUPAC name	sulfanylidenesilanylium
$\mu_{a,b,c}$	0.0, 3.8, 0.4
A, B, C	269138.2799, 10231.4975, 9856.7843
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 1
Predicted log column density	12.959±1.343
Electronic energy	-687.84341

geom278



SMILES: [SiH2]=C=[SiH2]

Nearest TMC-1 molecule (distance): N#[NH+] (1.74)

Is DFT optimized?: True

Property	Value
Formula	CH4Si2
Molecular weight	72.215
IUPAC name	silylidenemethylidenesilane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	82830.4511, 2721.7962, 2721.6929
A_s, B_s, C_s	82590.2428, 2713.9030, 2713.8000
Charge, Multiplicity	0, 1
Predicted log column density	11.709±1.630
Electronic energy	-619.31413

geom279

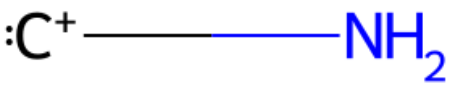
SMILES: [N]=S

Nearest TMC-1 molecule (distance): S=O (1.60)

Is DFT optimized?: False

Property	Value
Formula	NS
Molecular weight	46.074
IUPAC name	
$\mu_{a,b,c}$	1.9, 0.0, 0.0
A, B, C	∞, 22837.2095, 22837.2095
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	13.731±1.425
Electronic energy	-452.81805

geom280



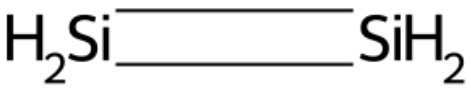
SMILES: [C+]N

Nearest TMC-1 molecule (distance): N#[NH+] (1.75)

Is DFT optimized?: True

Property	Value
Formula	CH2N+
Molecular weight	28.034
IUPAC name	methylideneazanium
$\mu_{a,b,c}$	1.0, 0.0, 0.0
A, B, C	324438.0918, 40100.6054, 35689.3911
A_s, B_s, C_s	323497.2213, 39984.3137, 35585.8918
Charge, Multiplicity	1, 3
Predicted log column density	12.863±1.658
Electronic energy	-93.50530

geom281



SMILES: [SiH2]=[SiH2]

Nearest TMC-1 molecule (distance): [CH] (1.43)

Is DFT optimized?: True

Property	Value
Formula	H4Si2
Molecular weight	60.204
IUPAC name	silylidenesilane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	77474.2197, 6478.5627, 6029.2233
A_s, B_s, C_s	77249.5445, 6459.7749, 6011.7386
Charge, Multiplicity	0, 1
Predicted log column density	12.444±1.462
Electronic energy	-581.27021

geom282

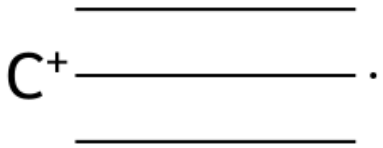
SMILES: [N]=N

Nearest TMC-1 molecule (distance): N#[NH+] (1.77)

Is DFT optimized?: True

Property	Value
Formula	HN2
Molecular weight	29.022
IUPAC name	diazene
$\mu_{a,b,c}$	0.0, 1.5, 1.5
A, B, C	667297.8773, 46354.2939, 43343.4146
A_s, B_s, C_s	665362.7135, 46219.8665, 43217.7187
Charge, Multiplicity	0, 2
Predicted log column density	13.449±1.793
Electronic energy	-109.99295

geom283



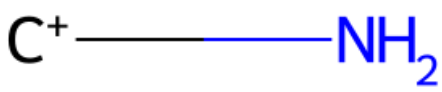
SMILES: [C]#[C+]

Nearest TMC-1 molecule (distance): N#[NH+] (1.83)

Is DFT optimized?: True

Property	Value
Formula	C2+
Molecular weight	24.022
IUPAC name	ethyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 58343.4859, 58343.4859
A_s, B_s, C_s	∞, 58174.2898, 58174.2898
Charge, Multiplicity	1, 2
Predicted log column density	13.046±1.444
Electronic energy	-75.32023

geom284



SMILES: [CH2+]N

Nearest TMC-1 molecule (distance): N (1.57)

Is DFT optimized?: True

Property	Value
Formula	CH4N+
Molecular weight	30.050
IUPAC name	methylideneazanium
$\mu_{a,b,c}$	-, -, -
A, B, C	152551.8688, 31369.5375, 26019.1660
A_s, B_s, C_s	152109.4684, 31278.5659, 25943.7105
Charge, Multiplicity	1, 1
Predicted log column density	12.719±1.633
Electronic energy	-

geom285

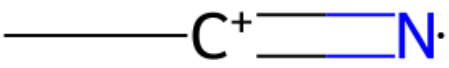
SMILES: [C+]S

Nearest TMC-1 molecule (distance): N#[NH+] (1.85)

Is DFT optimized?: True

Property	Value
Formula	CHS+
Molecular weight	45.086
IUPAC name	methylidenesulfanium
$\mu_{a,b,c}$	0.0, 1.3, 0.5
A, B, C	286417.9800, 22150.9830, 20560.8489
A_s, B_s, C_s	285587.3679, 22086.7452, 20501.2224
Charge, Multiplicity	1, 3
Predicted log column density	13.816±2.128
Electronic energy	-436.31113

geom286



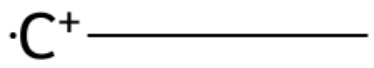
SMILES: C[C+]=[N]

Nearest TMC-1 molecule (distance): N#[NH+] (1.86)

Is DFT optimized?: True

Property	Value
Formula	C2H3N+
Molecular weight	41.053
IUPAC name	acetonitrilium
$\mu_{a,b,c}$	3.6, 0.2, 0.3
A, B, C	153762.5611, 9245.9692, 9211.6173
A_s, B_s, C_s	153316.6497, 9219.1558, 9184.9036
Charge, Multiplicity	1, 2
Predicted log column density	13.412±1.567
Electronic energy	-132.26760

geom287



SMILES: [CH+]C

Nearest TMC-1 molecule (distance): [CH] (1.47)

Is DFT optimized?: True

Property	Value
Formula	C2H4+
Molecular weight	28.054
IUPAC name	ethane
$\mu_{a,b,c}$	0.2, 0.7, 1.0
A, B, C	145399.4081, 28804.0046, 27280.1957
A_s, B_s, C_s	144977.7498, 28720.4730, 27201.0831
Charge, Multiplicity	1, 2
Predicted log column density	13.199±1.474
Electronic energy	-78.13449

geom288

SMILES: [S+]S

Nearest TMC-1 molecule (distance): [CH] (1.74)

Is DFT optimized?: True

Property	Value
Formula	HS2+
Molecular weight	65.142
IUPAC name	sulfanylsulfanium
$\mu_{a,b,c}$	0.0, 0.3, 1.5
A, B, C	286257.5552, 7935.8336, 7721.7654
A_s, B_s, C_s	285427.4083, 7912.8197, 7699.3723
Charge, Multiplicity	1, 3
Predicted log column density	13.811±2.081
Electronic energy	-796.55631

geom289

SMILES: [C]=N

Nearest TMC-1 molecule (distance): C=[N] (1.86)

Is DFT optimized?: True

Property	Value
Formula	CHN
Molecular weight	27.026
IUPAC name	methanimine
$\mu_{a,b,c}$	0.0, 0.2, 1.3
A, B, C	626839.1768, 44594.3170, 41632.5150
A_s, B_s, C_s	625021.3432, 44464.9935, 41511.7807
Charge, Multiplicity	0, 3
Predicted log column density	13.689±1.803
Electronic energy	-93.20087

geom290

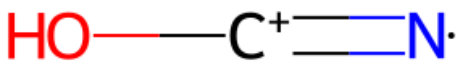
SMILES: [CH+]=N

Nearest TMC-1 molecule (distance): C=[N] (1.92)

Is DFT optimized?: True

Property	Value
Formula	CH2N+
Molecular weight	28.034
IUPAC name	methanimine
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	13976355293.4079, 37058.3053, 37058.2079
A_s, B_s, C_s	13935823863.0570, 36950.8362, 36950.7391
Charge, Multiplicity	1, 1
Predicted log column density	13.844±1.802
Electronic energy	-93.66878

geom291



SMILES: [N]=[C+]O

Nearest TMC-1 molecule (distance): N#[NH+] (1.92)

Is DFT optimized?: True

Property	Value
Formula	CHNO+
Molecular weight	43.025
IUPAC name	
$\mu_{a,b,c}$	2.9, 1.9, 0.0
A, B, C	744501.2813, 10692.2472, 10540.8633
A_s, B_s, C_s	742342.2276, 10661.2397, 10510.2948
Charge, Multiplicity	1, 2
Predicted log column density	12.692±1.544
Electronic energy	-168.15019

geom292

SMILES: N=[S+]

Nearest TMC-1 molecule (distance): C=[N] (1.76)

Is DFT optimized?: False

Property	Value
Formula	HNS+
Molecular weight	47.082
IUPAC name	sulfanylideneazanium
$\mu_{a,b,c}$	0.0, 0.1, 1.9
A, B, C	587080.4158, 21007.2879, 20281.5601
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	13.721±1.793
Electronic energy	-453.08389

geom293

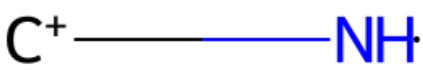
SMILES: [C+]=N

Nearest TMC-1 molecule (distance): N#[NH+] (1.97)

Is DFT optimized?: True

Property	Value
Formula	CHN+
Molecular weight	27.026
IUPAC name	methanimine
$\mu_{a,b,c}$	0.0, 0.6, 0.0
A, B, C	82120647300.6753, 47208.9543, 47208.9272
A_s, B_s, C_s	81882497423.5033, 47072.0483, 47072.0213
Charge, Multiplicity	1, 2
Predicted log column density	13.719±1.825
Electronic energy	-92.92206

geom294



SMILES: [CH2+][NH]

Nearest TMC-1 molecule (distance): C=[N] (1.77)

Is DFT optimized?: True

Property	Value
Formula	CH3N+
Molecular weight	29.042
IUPAC name	methylideneazanium
$\mu_{a,b,c}$	0.0, 0.1, 0.8
A, B, C	249661.5554, 33726.1337, 29712.3669
A_s, B_s, C_s	248937.5369, 33628.3279, 29626.2011
Charge, Multiplicity	1, 2
Predicted log column density	13.541±1.770
Electronic energy	-94.23309

geom295

SMILES: [SH3+]

Nearest TMC-1 molecule (distance): [CH] (1.40)

Is DFT optimized?: True

Property	Value
Formula	H3S+
Molecular weight	35.091
IUPAC name	sulfanium
$\mu_{a,b,c}$	0.0, 0.0, 2.1
A, B, C	150134.5685, 150095.3495, 125089.5834
A_s, B_s, C_s	149699.1783, 149660.0729, 124726.8236
Charge, Multiplicity	1, 1
Predicted log column density	12.869±1.521
Electronic energy	-399.64217

geom296

SMILES: C=[N]

Nearest TMC-1 molecule (distance): C=S (1.91)

Is DFT optimized?: True

Property	Value
Formula	CH2N
Molecular weight	28.034
IUPAC name	methanimine
$\mu_{a,b,c}$	2.6, 0.0, 0.0
A, B, C	284689.8066, 39083.1500, 34365.3607
A_s, B_s, C_s	283864.2061, 38969.8089, 34265.7011
Charge, Multiplicity	0, 2
Predicted log column density	11.427±1.033
Electronic energy	-93.94921

geom297

SMILES: C[S+]

Nearest TMC-1 molecule (distance): [CH] (1.21)

Is DFT optimized?: True

Property	Value
Formula	CH3S+
Molecular weight	47.102
IUPAC name	methylsulfanium
$\mu_{a,b,c}$	1.3, 0.0, 0.0
A, B, C	155053.3962, 14128.6454, 14128.2796
A_s, B_s, C_s	154603.7414, 14087.6724, 14087.3076
Charge, Multiplicity	1, 3
Predicted log column density	13.109±1.466
Electronic energy	-437.68535

geom298

SMILES: [S−2]

Nearest TMC-1 molecule (distance): [CH] (1.60)

Is DFT optimized?: False

Property	Value
Formula	S-2
Molecular weight	32.067
IUPAC name	sulfide
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-2, 1
Predicted log column density	12.125±1.672
Electronic energy	-398.01281

geom299

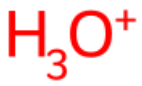
SMILES: O=[SiH2]

Nearest TMC-1 molecule (distance): [CH] (1.00)

Is DFT optimized?: True

Property	Value
Formula	H2OSi
Molecular weight	46.101
IUPAC name	oxosilane
$\mu_{a,b,c}$	4.0, 0.0, 0.0
A, B, C	166630.8291, 18402.1627, 16572.0058
A_s, B_s, C_s	166147.5997, 18348.7964, 16523.9470
Charge, Multiplicity	0, 1
Predicted log column density	12.177±1.439
Electronic energy	-365.85060

geom300



SMILES: [OH3+]

Nearest TMC-1 molecule (distance): [CH] (0.89)

Is DFT optimized?: True

Property	Value
Formula	H3O+
Molecular weight	19.023
IUPAC name	oxidanium
$\mu_{a,b,c}$	0.0, 0.0, 1.8
A, B, C	327125.9370, 327124.0579, 188561.0212
A_s, B_s, C_s	326177.2718, 326175.3981, 188014.1942
Charge, Multiplicity	1, 1
Predicted log column density	12.593±1.454
Electronic energy	-76.67115

geom301

SMILES: S=[S+]

Nearest TMC-1 molecule (distance): S=O (1.25)

Is DFT optimized?: True

Property	Value
Formula	S2+
Molecular weight	64.134
IUPAC name	sulfanylidenesulfanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 9541.3444, 9541.3444
A_s, B_s, C_s	∞, 9513.6745, 9513.6745
Charge, Multiplicity	1, 2
Predicted log column density	14.052±1.446
Electronic energy	-795.95982

geom302

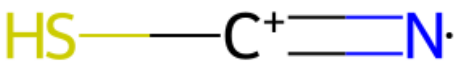
SMILES: [CH2+]O

Nearest TMC-1 molecule (distance): [CH] (1.57)

Is DFT optimized?: True

Property	Value
Formula	CH3O+
Molecular weight	31.034
IUPAC name	methylideneoxidanium
$\mu_{a,b,c}$	1.5, 1.9, 0.0
A, B, C	198940.8209, 34410.3988, 29336.1783
A_s, B_s, C_s	198363.8926, 34310.6086, 29251.1033
Charge, Multiplicity	1, 1
Predicted log column density	12.267±1.463
Electronic energy	-114.74728

geom303



SMILES: [N]=[C+]S

Nearest TMC-1 molecule (distance): N#[NH+] (2.10)

Is DFT optimized?: True

Property	Value
Formula	CHNS+
Molecular weight	59.093
IUPAC name	
$\mu_{a,b,c}$	3.5, 1.4, 0.0
A, B, C	284380.1817, 5923.7225, 5802.8475
A_s, B_s, C_s	283555.4792, 5906.5437, 5786.0192
Charge, Multiplicity	1, 2
Predicted log column density	14.031±2.157
Electronic energy	-491.16257

geom304

SMILES: S[SH2+]

Nearest TMC-1 molecule (distance): N (2.00)

Is DFT optimized?: True

Property	Value
Formula	H3S2+
Molecular weight	67.158
IUPAC name	sulfanylsulfanium
$\mu_{a,b,c}$	2.7, 0.4, 0.0
A, B, C	98179.7840, 6595.8865, 6500.9834
A_s, B_s, C_s	97895.0626, 6576.7584, 6482.1305
Charge, Multiplicity	1, 1
Predicted log column density	13.569±2.297
Electronic energy	-797.81153

geom305

SMILES: [NH4+]

Nearest TMC-1 molecule (distance): N (1.11)

Is DFT optimized?: True

Property	Value
Formula	H4N+
Molecular weight	18.039
IUPAC name	azanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	178336.7872, 178318.9937, 178312.1305
A_s, B_s, C_s	177819.6105, 177801.8686, 177795.0254
Charge, Multiplicity	1, 1
Predicted log column density	13.003±1.733
Electronic energy	-56.87875

geom306

SMILES: O

Nearest TMC-1 molecule (distance): N (1.22)

Is DFT optimized?: True

Property	Value
Formula	H2O
Molecular weight	18.015
IUPAC name	oxidane
$\mu_{a,b,c}$	2.3, 0.0, 0.0
A, B, C	833483.5240, 424897.3141, 281429.0396
A_s, B_s, C_s	831066.4218, 423665.1119, 280612.8954
Charge, Multiplicity	0, 1
Predicted log column density	14.019±2.013
Electronic energy	-76.39813

geom307

SMILES: S

Nearest TMC-1 molecule (distance): [CH] (1.01)

Is DFT optimized?: True

Property	Value
Formula	H2S
Molecular weight	34.083
IUPAC name	sulfane
$\mu_{a,b,c}$	0.0, 0.0, 1.5
A, B, C	313753.6386, 262955.0913, 143058.5535
A_s, B_s, C_s	312843.7531, 262192.5215, 142643.6837
Charge, Multiplicity	0, 1
Predicted log column density	13.068±1.514
Electronic energy	-399.36506

geom308

SMILES: [SiH4]

Nearest TMC-1 molecule (distance): [CH] (0.55)

Is DFT optimized?: True

Property	Value
Formula	H4Si
Molecular weight	32.118
IUPAC name	silane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	85458.0009, 85452.4876, 85448.1551
A_s, B_s, C_s	85210.1727, 85204.6754, 85200.3555
Charge, Multiplicity	0, 1
Predicted log column density	12.690±1.415
Electronic energy	-291.85766

geom309

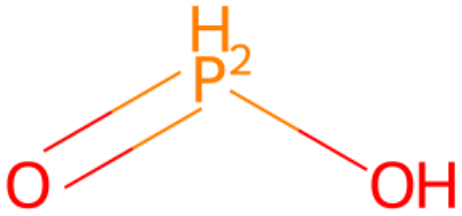
SMILES: C

Nearest TMC-1 molecule (distance): [CH] (1.36)

Is DFT optimized?: True

Property	Value
Formula	CH4
Molecular weight	16.043
IUPAC name	methane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	157380.9040, 157363.9626, 157338.4155
A_s, B_s, C_s	156924.4993, 156907.6071, 156882.1341
Charge, Multiplicity	0, 1
Predicted log column density	12.371±1.729
Electronic energy	-40.50320

geom310



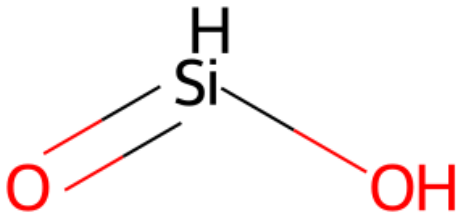
SMILES: O=[PH2]O

Nearest TMC-1 molecule (distance): CO (1.46)

Is DFT optimized?: True

Property	Value
Formula	H3O2P
Molecular weight	65.996
IUPAC name	hydroxy(oxo)phosphanium
$\mu_{a,b,c}$	2.3, 1.2, 1.0
A, B, C	29073.8857, 8268.5372, 6917.6662
A_s, B_s, C_s	28989.5714, 8244.5585, 6897.6050
Charge, Multiplicity	0, 1
Predicted log column density	11.901±1.549
Electronic energy	-493.56042

geom311



SMILES: O=[SiH]O

Nearest TMC-1 molecule (distance): CO (1.46)

Is DFT optimized?: False

Property	Value
Formula	H2O2Si
Molecular weight	62.100
IUPAC name	hydroxy(oxo)silane
$\mu_{a,b,c}$	1.0, 0.6, 2.5
A, B, C	27646.0486, 9639.9163, 7440.4955
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.809±1.529
Electronic energy	-441.05550

geom312

SMILES: [O]O

Nearest TMC-1 molecule (distance): [CH] (1.48)

Is DFT optimized?: True

Property	Value
Formula	HO2
Molecular weight	33.006
IUPAC name	hydrogen peroxide
$\mu_{a,b,c}$	0.0, 1.6, 1.8
A, B, C	620486.1359, 34261.2732, 32468.4675
A_s, B_s, C_s	618686.7261, 34161.9155, 32374.3090
Charge, Multiplicity	0, 2
Predicted log column density	11.900±1.519
Electronic energy	-150.85922

geom313

SMILES: OP

Nearest TMC-1 molecule (distance): [CH] (1.67)

Is DFT optimized?: True

Property	Value
Formula	H3OP
Molecular weight	49.997
IUPAC name	phosphinous acid
$\mu_{a,b,c}$	0.3, 0.8, 0.0
A, B, C	111413.5844, 14300.5935, 14199.7353
A_s, B_s, C_s	111090.4850, 14259.1218, 14158.5560
Charge, Multiplicity	0, 1
Predicted log column density	12.532±1.628
Electronic energy	-418.32440

geom314

SMILES: OO

Nearest TMC-1 molecule (distance): CO (1.73)

Is DFT optimized?: True

Property	Value
Formula	H2O2
Molecular weight	34.014
IUPAC name	hydrogen peroxide
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	303459.7894, 27560.6025, 25265.9197
A_s, B_s, C_s	302579.7560, 27480.6768, 25192.6485
Charge, Multiplicity	0, 1
Predicted log column density	11.894±1.916
Electronic energy	-151.49617

geom315

SMILES: CC

Nearest TMC-1 molecule (distance): CO (1.75)

Is DFT optimized?: True

Property	Value
Formula	C2H6
Molecular weight	30.070
IUPAC name	ethane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	80140.8221, 19965.1443, 19963.5717
A_s, B_s, C_s	79908.4137, 19907.2453, 19905.6773
Charge, Multiplicity	0, 1
Predicted log column density	13.112±1.727
Electronic energy	-79.80393

geom316

SMILES: OS

Nearest TMC-1 molecule (distance): CO (1.78)

Is DFT optimized?: True

Property	Value
Formula	H2OS
Molecular weight	50.082
IUPAC name	sulfanol
$\mu_{a,b,c}$	0.3, 0.6, 0.0
A, B, C	200829.8727, 15062.7583, 14011.9588
A_s, B_s, C_s	200247.4660, 15019.0763, 13971.3241
Charge, Multiplicity	0, 1
Predicted log column density	13.365±2.182
Electronic energy	-474.52614

geom317

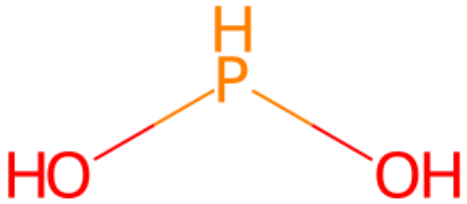
SMILES: [O−]O

Nearest TMC-1 molecule (distance): N (1.78)

Is DFT optimized?: True

Property	Value
Formula	HO2-
Molecular weight	33.006
IUPAC name	
$\mu_{a,b,c}$	0.0, 2.5, 1.6
A, B, C	600578.8143, 27167.3857, 25991.6448
A_s, B_s, C_s	598837.1357, 27088.6002, 25916.2690
Charge, Multiplicity	-1, 1
Predicted log column density	11.990±1.912
Electronic energy	-150.89006

geom318



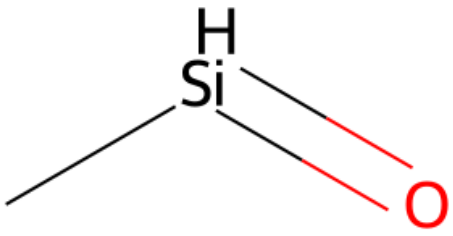
SMILES: OPO

Nearest TMC-1 molecule (distance): CO (1.79)

Is DFT optimized?: True

Property	Value
Formula	H3O2P
Molecular weight	65.996
IUPAC name	phosphonous acid
$\mu_{a,b,c}$	0.7, 0.6, 0.4
A, B, C	22942.7449, 8121.4016, 6476.0150
A_s, B_s, C_s	22876.2109, 8097.8495, 6457.2346
Charge, Multiplicity	0, 1
Predicted log column density	12.129±1.942
Electronic energy	-493.55481

geom319



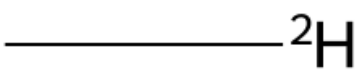
SMILES: C[SiH]=O

Nearest TMC-1 molecule (distance): S=O (1.63)

Is DFT optimized?: True

Property	Value
Formula	CH4OSi
Molecular weight	60.128
IUPAC name	methyl(oxo)silane
$\mu_{a,b,c}$	4.3, 1.7, 0.0
A, B, C	33126.7896, 6560.4229, 5668.4071
A_s, B_s, C_s	33030.7219, 6541.3977, 5651.9687
Charge, Multiplicity	0, 1
Predicted log column density	12.465±1.572
Electronic energy	-405.17523

geom320



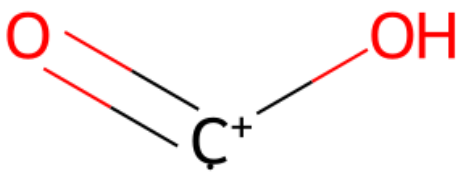
SMILES: [2H]C

Nearest TMC-1 molecule (distance): [CH] (1.53)

Is DFT optimized?: True

Property	Value
Formula	CH4
Molecular weight	17.049
IUPAC name	deuteriomethane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	157418.1069, 157384.8840, 157337.1460
A_s, B_s, C_s	156961.5944, 156928.4679, 156880.8682
Charge, Multiplicity	0, 1
Predicted log column density	12.833±1.741
Electronic energy	-40.50320

geom321



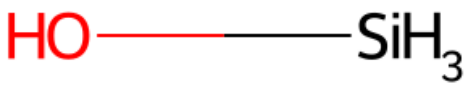
SMILES: O=[CH+]O

Nearest TMC-1 molecule (distance): CO (1.86)

Is DFT optimized?: True

Property	Value
Formula	CH2O2+
Molecular weight	46.025
IUPAC name	
$\mu_{a,b,c}$	2.1, 3.4, 0.0
A, B, C	87703.9655, 11922.6946, 10495.8614
A_s, B_s, C_s	87449.6240, 11888.1188, 10465.4234
Charge, Multiplicity	1, 2
Predicted log column density	11.409±1.702
Electronic energy	-189.29129

geom322



SMILES: O[SiH3]

Nearest TMC-1 molecule (distance): [CH] (1.80)

Is DFT optimized?: True

Property	Value
Formula	H4OSi
Molecular weight	48.117
IUPAC name	hydroxysilane
$\mu_{a,b,c}$	0.0, 0.2, 1.5
A, B, C	77090.8815, 13564.7721, 13304.3915
A_s, B_s, C_s	76867.3180, 13525.4343, 13265.8088
Charge, Multiplicity	0, 1
Predicted log column density	11.534±1.711
Electronic energy	-367.10101

geom323

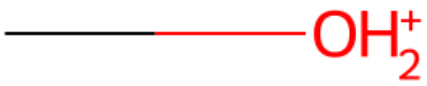
SMILES: NO

Nearest TMC-1 molecule (distance): N (1.86)

Is DFT optimized?: True

Property	Value
Formula	H3NO
Molecular weight	33.030
IUPAC name	hydroxylamine
$\mu_{a,b,c}$	0.7, 0.0, 0.1
A, B, C	192513.9860, 25860.8809, 25789.4347
A_s, B_s, C_s	191955.6955, 25785.8844, 25714.6454
Charge, Multiplicity	0, 1
Predicted log column density	12.190±1.887
Electronic energy	-131.67567

geom324



SMILES: C[OH2+]

Nearest TMC-1 molecule (distance): CO (1.88)

Is DFT optimized?: True

Property	Value
Formula	CH5O+
Molecular weight	33.050
IUPAC name	methyloxidanium
$\mu_{a,b,c}$	1.3, 0.0, 1.5
A, B, C	104111.6434, 21218.1540, 20374.5458
A_s, B_s, C_s	103809.7196, 21156.6214, 20315.4596
Charge, Multiplicity	1, 1
Predicted log column density	12.606±1.958
Electronic energy	-115.98281

geom325

SMILES: C[PH]

Nearest TMC-1 molecule (distance): [CH] (0.97)

Is DFT optimized?: True

Property	Value
Formula	CH4P
Molecular weight	47.017
IUPAC name	methylphosphane
$\mu_{a,b,c}$	1.3, 0.7, 0.0
A, B, C	98600.2721, 12504.8692, 11924.5600
A_s, B_s, C_s	98314.3313, 12468.6051, 11889.9788
Charge, Multiplicity	0, 2
Predicted log column density	12.842±1.520
Electronic energy	-381.78821

geom326

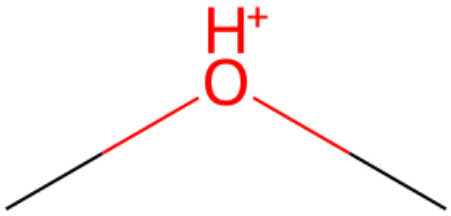
SMILES: C[SH2+]

Nearest TMC-1 molecule (distance): [CH] (1.49)

Is DFT optimized?: True

Property	Value
Formula	CH5S+
Molecular weight	49.118
IUPAC name	methylsulfanium
$\mu_{a,b,c}$	0.0, 0.0, 1.6
A, B, C	75643.5239, 12157.1848, 12003.6022
A_s, B_s, C_s	75424.1577, 12121.9290, 11968.7917
Charge, Multiplicity	1, 1
Predicted log column density	12.847±1.668
Electronic energy	-438.96770

geom327



SMILES: C[OH+]C

Nearest TMC-1 molecule (distance): CO (1.95)

Is DFT optimized?: True

Property	Value
Formula	C2H7O+
Molecular weight	47.077
IUPAC name	dimethyloxidanium
$\mu_{a,b,c}$	0.0, 0.5, 1.1
A, B, C	34724.1068, 8825.5308, 7840.5001
A_s, B_s, C_s	34623.4069, 8799.9368, 7817.7626
Charge, Multiplicity	1, 1
Predicted log column density	13.153±1.836
Electronic energy	-155.29085

geom328

SMILES: CS

Nearest TMC-1 molecule (distance): [CH] (1.64)

Is DFT optimized?: True

Property	Value
Formula	CH4S
Molecular weight	48.110
IUPAC name	methanethiol
$\mu_{a,b,c}$	1.5, 1.0, 0.0
A, B, C	102864.8512, 12845.3482, 12317.1429
A_s, B_s, C_s	102566.5431, 12808.0967, 12281.4232
Charge, Multiplicity	0, 1
Predicted log column density	13.839±2.138
Electronic energy	-438.66588

geom329

SMILES: CP

Nearest TMC-1 molecule (distance): [CH] (1.51)

Is DFT optimized?: True

Property	Value
Formula	CH5P
Molecular weight	48.025
IUPAC name	methylphosphane
$\mu_{a,b,c}$	1.1, 0.0, 0.8
A, B, C	71969.1144, 11720.4611, 11599.2438
A_s, B_s, C_s	71760.4040, 11686.4718, 11565.6060
Charge, Multiplicity	0, 1
Predicted log column density	13.113±1.686
Electronic energy	-382.42331

geom330

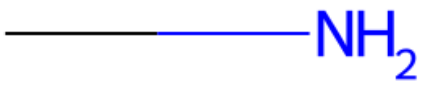
SMILES: C[O]

Nearest TMC-1 molecule (distance): [CH] (1.49)

Is DFT optimized?: True

Property	Value
Formula	CH3O
Molecular weight	31.034
IUPAC name	methanol
$\mu_{a,b,c}$	2.2, 0.0, 0.2
A, B, C	156665.1612, 28046.6600, 27864.7824
A_s, B_s, C_s	156210.8322, 27965.3246, 27783.9745
Charge, Multiplicity	0, 2
Predicted log column density	12.467±1.567
Electronic energy	-115.01650

geom331



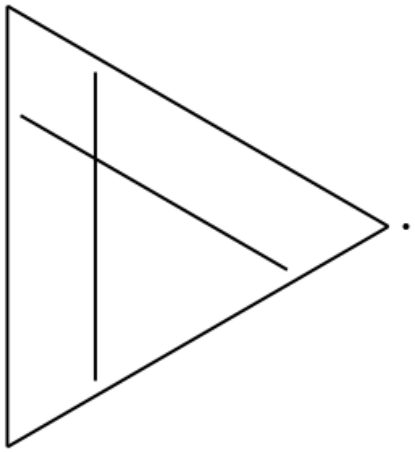
SMILES: CN

Nearest TMC-1 molecule (distance): N (1.95)

Is DFT optimized?: True

Property	Value
Formula	CH5N
Molecular weight	31.058
IUPAC name	methanamine
$\mu_{a,b,c}$	0.4, 0.0, 1.5
A, B, C	103337.5783, 22844.6612, 21922.2737
A_s, B_s, C_s	103037.8993, 22778.4117, 21858.6991
Charge, Multiplicity	0, 1
Predicted log column density	13.178±1.836
Electronic energy	-95.82775

geom332



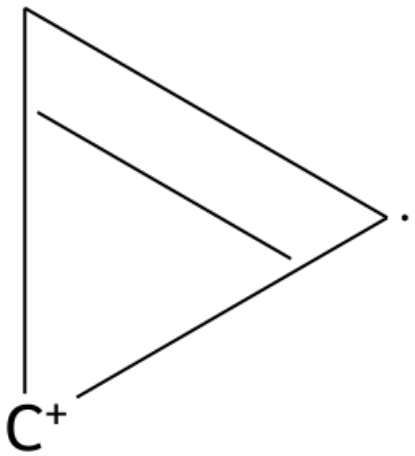
SMILES: [C]1=C=C1

Nearest TMC-1 molecule (distance): C1=C=C1 (3.00)

Is DFT optimized?: True

Property	Value
Formula	C3H
Molecular weight	37.041
IUPAC name	
$\mu_{a,b,c}$	2.4, 0.0, 0.0
A, B, C	44984.6244, 34180.8719, 19422.7758
A_s, B_s, C_s	44854.1690, 34081.7473, 19366.4497
Charge, Multiplicity	0, 2
Predicted log column density	13.470±1.032
Electronic energy	-114.63898

geom333



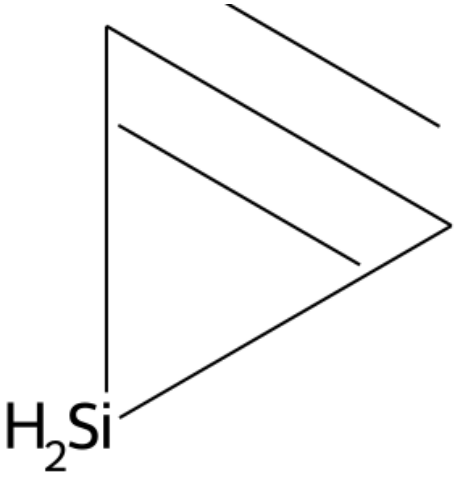
SMILES: `[c]1c[cH+]1`

Nearest TMC-1 molecule (distance): `C1=C=C1` (3.47)

Is DFT optimized?: True

Property	Value
Formula	C3H2+
Molecular weight	38.049
IUPAC name	cyclopropane
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	28094.9501, 23685.8388, 14017.8463
A_s, B_s, C_s	28013.4748, 23617.1498, 13977.1945
Charge, Multiplicity	1, 2
Predicted log column density	12.780±1.505
Electronic energy	-116.23261

geom334



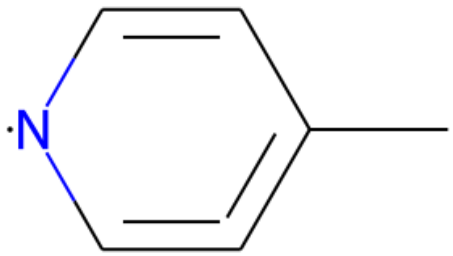
SMILES: C1#C[SiH2]1

Nearest TMC-1 molecule (distance): C1=C=[C]1 (3.49)

Is DFT optimized?: True

Property	Value
Formula	C2H2Si
Molecular weight	54.124
IUPAC name	1-silacycloprop-2-yne
$\mu_{a,b,c}$	3.6, 0.0, 0.0
A, B, C	40670.8495, 10921.4127, 9559.6329
A_s, B_s, C_s	40552.9041, 10889.7406, 9531.9100
Charge, Multiplicity	0, 1
Predicted log column density	12.675±1.644
Electronic energy	-366.67340

geom335



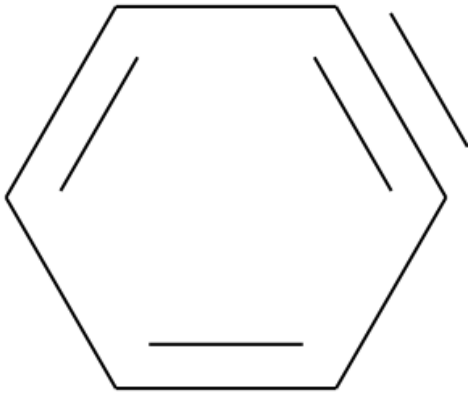
SMILES: CC1=C=C[N]C=C1

Nearest TMC-1 molecule (distance): C1=C=C1 (4.34)

Is DFT optimized?: True

Property	Value
Formula	C6H6N
Molecular weight	92.121
IUPAC name	4-methylpyridine
$\mu_{a,b,c}$	2.5, 0.8, 0.0
A, B, C	6289.1164, 2514.4003, 1816.6139
A_s, B_s, C_s	6270.8780, 2507.1085, 1811.3457
Charge, Multiplicity	0, 2
Predicted log column density	11.637±3.109
Electronic energy	-286.82180

geom336



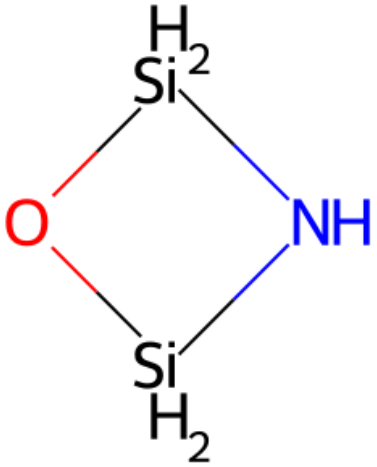
SMILES: `c1ccccc#1`

Nearest TMC-1 molecule (distance): `C1=C=C1` (4.49)

Is DFT optimized?: True

Property	Value
Formula	C6H4
Molecular weight	76.098
IUPAC name	cyclohexa-1,3-dien-5-yne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	5706.6815, 5703.9568, 2852.6594
A_s, B_s, C_s	5690.1321, 5687.4153, 2844.3867
Charge, Multiplicity	0, 1
Predicted log column density	12.842±2.574
Electronic energy	-232.17198

geom337



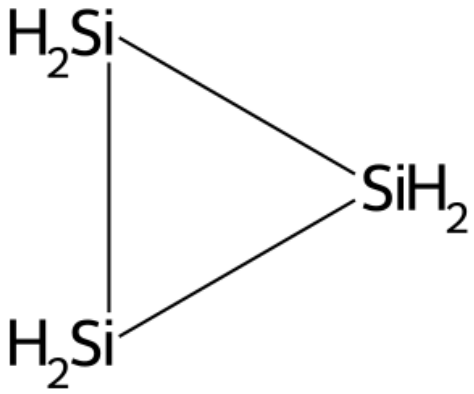
SMILES: N1[SiH2]O[SiH2]1

Nearest TMC-1 molecule (distance): [C-]#[S+] (3.99)

Is DFT optimized?: True

Property	Value
Formula	H5NOSi2
Molecular weight	91.218
IUPAC name	1,3,2,4-oxazadisiletidine
$\mu_{a,b,c}$	0.0, 2.3, 0.0
A, B, C	9459.8647, 4643.9011, 3358.0121
A_s, B_s, C_s	9432.4311, 4630.4338, 3348.2739
Charge, Multiplicity	0, 1
Predicted log column density	12.264±3.566
Electronic energy	-711.98609

geom338



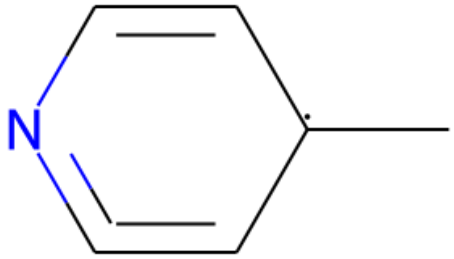
SMILES: `[SiH2]1[SiH2][SiH2]1`

Nearest TMC-1 molecule (distance): `C1=C=[C]1` (4.67)

Is DFT optimized?: True

Property	Value
Formula	H6Si3
Molecular weight	90.306
IUPAC name	trisilirane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	5086.7748, 5085.1804, 2803.8788
A_s, B_s, C_s	5072.0232, 5070.4333, 2795.7475
Charge, Multiplicity	0, 1
Predicted log column density	11.485±3.959
Electronic energy	-871.97638

geom339



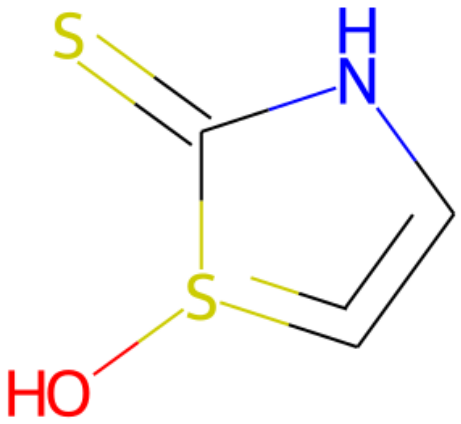
SMILES: C[C]1C=C=NC=C1

Nearest TMC-1 molecule (distance): C1=C=C1 (4.78)

Is DFT optimized?: True

Property	Value
Formula	C6H6N
Molecular weight	92.121
IUPAC name	
$\mu_{a,b,c}$	3.3, 1.3, 0.0
A, B, C	6193.1056, 2596.1064, 1850.4194
A_s, B_s, C_s	6175.1455, 2588.5777, 1845.0532
Charge, Multiplicity	0, 2
Predicted log column density	12.007±3.275
Electronic energy	-286.83176

geom340



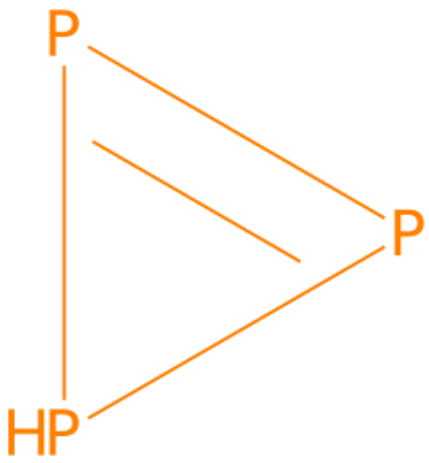
SMILES: OS1=C=CNC1=S

Nearest TMC-1 molecule (distance): C1=C=[C]1 (4.89)

Is DFT optimized?: True

Property	Value
Formula	C3H3NOS2
Molecular weight	133.197
IUPAC name	1-hydroxy-1,3-thiazole-2-thione
$\mu_{a,b,c}$	1.2, 2.4, 0.8
A, B, C	2888.5699, 1264.7080, 977.2532
A_s, B_s, C_s	2880.1930, 1261.0403, 974.4192
Charge, Multiplicity	0, 1
Predicted log column density	13.719±4.271
Electronic energy	-1042.25161

geom341



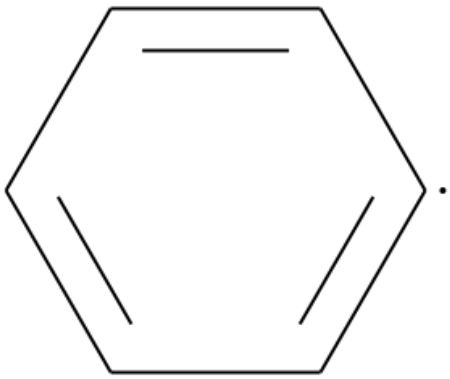
SMILES: P1=PP1

Nearest TMC-1 molecule (distance): [C−]#[S+] (3.30)

Is DFT optimized?: True

Property	Value
Formula	HP3
Molecular weight	93.930
IUPAC name	1H-triphosphirene
$\mu_{a,b,c}$	0.0, 0.1, 0.8
A, B, C	5965.9203, 5839.0379, 3164.0367
A_s, B_s, C_s	5948.6191, 5822.1047, 3154.8610
Charge, Multiplicity	0, 1
Predicted log column density	12.734±3.114
Electronic energy	-1025.78966

geom342



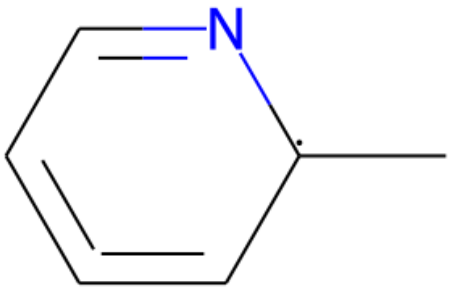
SMILES: `[c]1ccccc1`

Nearest TMC-1 molecule (distance): `C1=C=C1` (5.25)

Is DFT optimized?: True

Property	Value
Formula	C6H5
Molecular weight	77.106
IUPAC name	benzene
$\mu_{a,b,c}$	0.0, 0.0, 0.9
A, B, C	6290.8527, 5614.5981, 2966.7595
A_s, B_s, C_s	6272.6093, 5598.3158, 2958.1559
Charge, Multiplicity	0, 2
Predicted log column density	12.537±2.599
Electronic energy	-231.48278

geom343



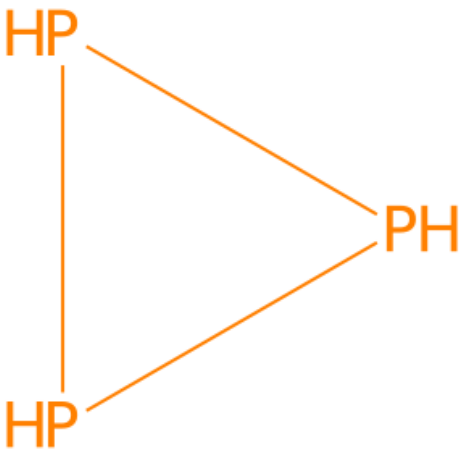
SMILES: C[C]1C=C=CC=N1

Nearest TMC-1 molecule (distance): C1=C=C1 (5.25)

Is DFT optimized?: True

Property	Value
Formula	C6H6N
Molecular weight	92.121
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.9, 0.0
A, B, C	6118.4271, 2672.5889, 1881.8206
A_s, B_s, C_s	6100.6837, 2664.8384, 1876.3633
Charge, Multiplicity	0, 2
Predicted log column density	11.766±4.183
Electronic energy	-286.82604

geom344



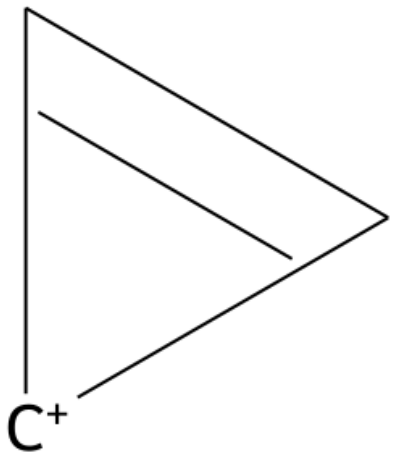
SMILES: [pH]1[pH][pH]1

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (3.98)

Is DFT optimized?: True

Property	Value
Formula	H3P3
Molecular weight	95.946
IUPAC name	triphosphirane
$\mu_{a,b,c}$	0.0, 0.1, 0.8
A, B, C	5964.3304, 5838.8125, 3163.5560
A_s, B_s, C_s	5947.0339, 5821.8800, 3154.3817
Charge, Multiplicity	0, 1
Predicted log column density	12.543±3.507
Electronic energy	-1025.78966

geom345



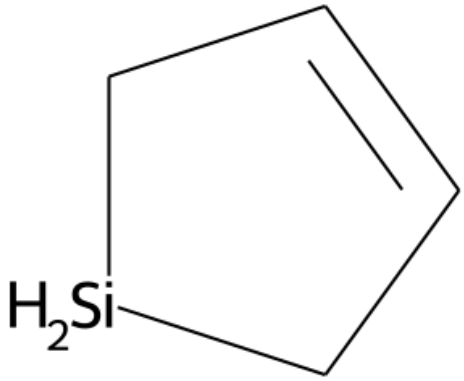
SMILES: `c1c[cH+]1`

Nearest TMC-1 molecule (distance): S=O (2.51)

Is DFT optimized?: True

Property	Value
Formula	C3H3+
Molecular weight	39.057
IUPAC name	cyclopropane
$\mu_{a,b,c}$	0.0, 0.7, 0.0
A, B, C	49848.6514, 11007.2581, 9016.3304
A_s, B_s, C_s	49704.0903, 10975.3370, 8990.1830
Charge, Multiplicity	1, 1
Predicted log column density	12.739±1.589
Electronic energy	-116.92551

geom346



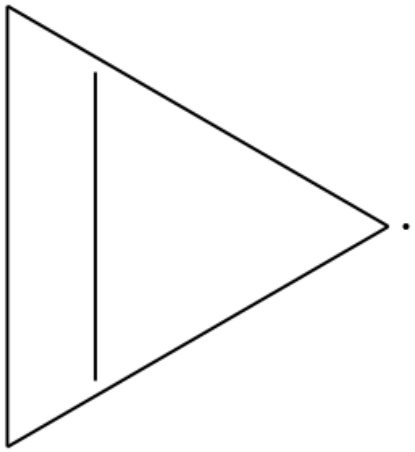
SMILES: C1=CC[SiH2]C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.67)

Is DFT optimized?: True

Property	Value
Formula	C4H8Si
Molecular weight	84.194
IUPAC name	2,5-dihydro-1H-silole
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	5929.7254, 4511.3128, 2729.5886
A_s, B_s, C_s	5912.5292, 4498.2300, 2721.6728
Charge, Multiplicity	0, 1
Predicted log column density	11.262±3.091
Electronic energy	-446.64982

geom347



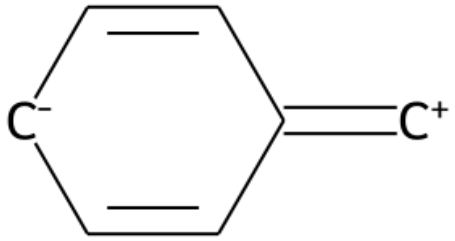
SMILES: [CH]1C=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (2.98)

Is DFT optimized?: True

Property	Value
Formula	C3H3
Molecular weight	39.057
IUPAC name	cyclopropene
$\mu_{a,b,c}$	1.3, 0.0, 0.9
A, B, C	31875.6282, 26680.9520, 14948.1012
A_s, B_s, C_s	31783.1889, 26603.5773, 14904.7517
Charge, Multiplicity	0, 2
Predicted log column density	12.961±2.327
Electronic energy	-115.91091

geom348



SMILES: [CH+]=C1C=C[CH−]C=C1

Nearest TMC-1 molecule (distance): C1=C=[C]1 (5.50)

Is DFT optimized?: False

Property	Value
Formula	C7H6
Molecular weight	90.125
IUPAC name	3-methylidenecyclohexa-1,4-diene
$\mu_{a,b,c}$	0.2, 0.1, 2.7
A, B, C	5218.0863, 2990.3463, 1901.2085
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.465±3.383
Electronic energy	-270.05619

geom349

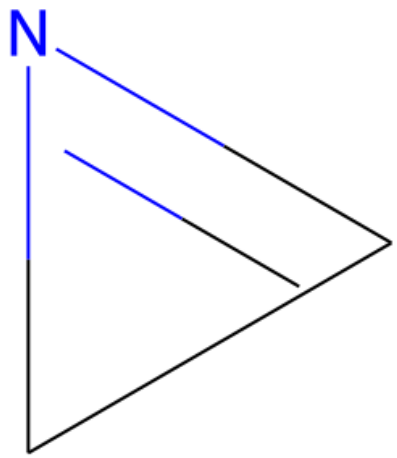
SMILES: [CH+]=C=[CH−]

Nearest TMC-1 molecule (distance): [C+]#C[O−] (1.70)

Is DFT optimized?: True

Property	Value
Formula	C3H2
Molecular weight	38.049
IUPAC name	propa-1,2-diene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 10180.7113, 10180.7113
A_s, B_s, C_s	∞, 10151.1872, 10151.1872
Charge, Multiplicity	0, 1
Predicted log column density	12.275±1.747
Electronic energy	-115.24693

geom350



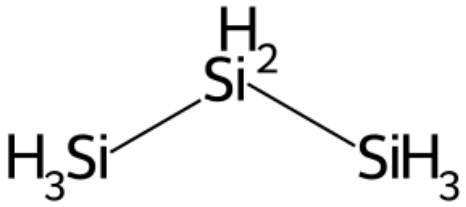
SMILES: C1=NC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.47)

Is DFT optimized?: True

Property	Value
Formula	C2H3N
Molecular weight	41.053
IUPAC name	2H-azirine
$\mu_{a,b,c}$	0.5, 2.3, 0.0
A, B, C	35923.1658, 22486.5058, 15260.9554
A_s, B_s, C_s	35818.9886, 22421.2949, 15216.6986
Charge, Multiplicity	0, 1
Predicted log column density	11.262±4.880
Electronic energy	-132.63731

geom351



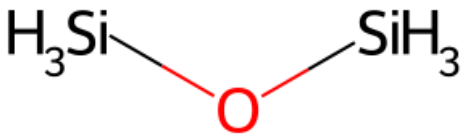
SMILES: `[SiH3][SiH2][SiH3]`

Nearest TMC-1 molecule (distance): `[C+]#C[O-]` (3.70)

Is DFT optimized?: True

Property	Value
Formula	H8Si3
Molecular weight	92.322
IUPAC name	disilylsilane
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	9269.3038, 1988.9569, 1736.1427
A_s, B_s, C_s	9242.4228, 1983.1890, 1731.1079
Charge, Multiplicity	0, 1
Predicted log column density	10.783±3.036
Electronic energy	-873.21574

geom352



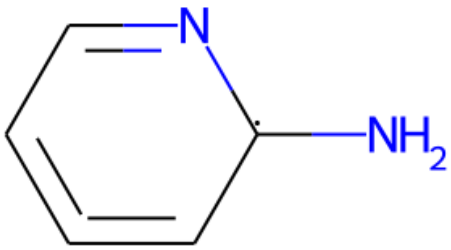
SMILES: [SiH3]O[SiH3]

Nearest TMC-1 molecule (distance): [C-]#[S+] (2.97)

Is DFT optimized?: True

Property	Value
Formula	H6OSi2
Molecular weight	78.219
IUPAC name	silyloxysilane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	42819.9770, 2745.3011, 2745.2928
A_s, B_s, C_s	42695.7991, 2737.3397, 2737.3314
Charge, Multiplicity	0, 1
Predicted log column density	11.163±2.739
Electronic energy	-657.81317

geom353



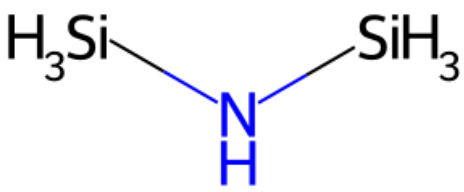
SMILES: N[C]1C=C=CC=N1

Nearest TMC-1 molecule (distance): C1=C=[C]1 (5.61)

Is DFT optimized?: True

Property	Value
Formula	C5H5N2
Molecular weight	93.109
IUPAC name	
$\mu_{a,b,c}$	1.0, 0.9, 0.9
A, B, C	6217.5633, 2774.2051, 1920.6951
A_s, B_s, C_s	6199.5324, 2766.1599, 1915.1251
Charge, Multiplicity	0, 2
Predicted log column density	12.544±4.632
Electronic energy	-302.86761

geom354



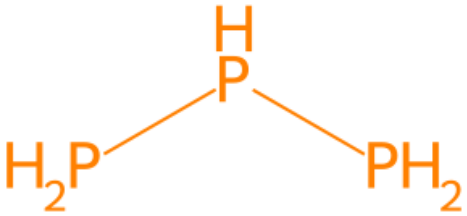
SMILES: [SiH3]N[SiH3]

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.93)

Is DFT optimized?: True

Property	Value
Formula	H7NSi2
Molecular weight	77.235
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.8, 0.1
A, B, C	24727.8319, 2988.9492, 2838.9596
A_s, B_s, C_s	24656.1212, 2980.2813, 2830.7266
Charge, Multiplicity	0, 1
Predicted log column density	11.062±2.697
Electronic energy	-637.91737

geom355



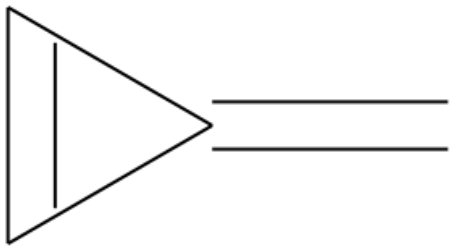
SMILES: PPP

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.72)

Is DFT optimized?: True

Property	Value
Formula	H5P3
Molecular weight	97.962
IUPAC name	bis(phosphanyl)phosphane
$\mu_{a,b,c}$	0.8, 0.5, 1.1
A, B, C	9832.2305, 2450.1412, 2053.2748
A_s, B_s, C_s	9803.7171, 2443.0358, 2047.3203
Charge, Multiplicity	0, 1
Predicted log column density	13.261±2.791
Electronic energy	-1026.98687

geom356



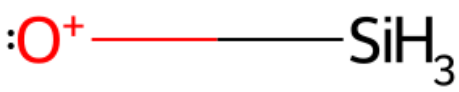
SMILES: C=C1C=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (3.73)

Is DFT optimized?: True

Property	Value
Formula	C4H4
Molecular weight	52.076
IUPAC name	3-methylidenecyclopropene
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	29439.6960, 7152.7742, 5754.6128
A_s, B_s, C_s	29354.3209, 7132.0312, 5737.9245
Charge, Multiplicity	0, 1
Predicted log column density	12.169±2.447
Electronic energy	-154.64794

geom357



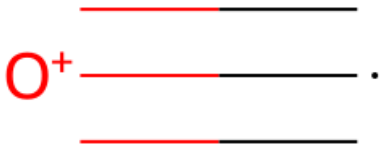
SMILES: [O+][SiH3]

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.56)

Is DFT optimized?: True

Property	Value
Formula	H3OSi+
Molecular weight	47.109
IUPAC name	
$\mu_{a,b,c}$	2.0, 0.0, 0.0
A, B, C	77304.2305, 13638.4693, 13638.2472
A_s, B_s, C_s	77080.0482, 13598.9178, 13598.6963
Charge, Multiplicity	1, 3
Predicted log column density	10.950±1.726
Electronic energy	-366.00232

geom358



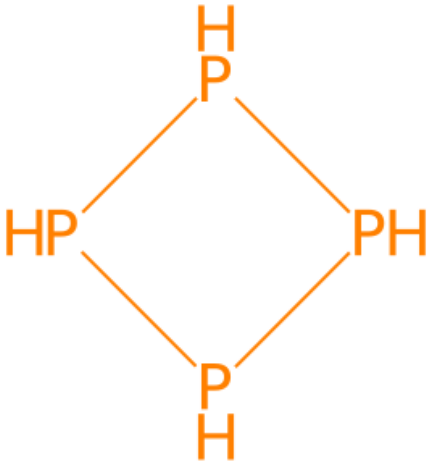
SMILES: [C]#[O+]

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.39)

Is DFT optimized?: False

Property	Value
Formula	CO+
Molecular weight	28.010
IUPAC name	methanone
$\mu_{a,b,c}$	2.7, 0.0, 0.0
A, B, C	∞, 65975.5774, 65975.5774
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	11.854±1.607
Electronic energy	-112.74646

geom359



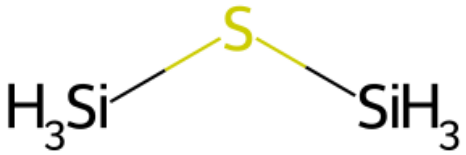
SMILES: P1PPP1

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (4.65)

Is DFT optimized?: True

Property	Value
Formula	H4P4
Molecular weight	127.928
IUPAC name	tetraphosphetane
$\mu_{a,b,c}$	0.0, 0.6, 1.3
A, B, C	3056.0510, 2873.8055, 1640.6864
A_s, B_s, C_s	3047.1884, 2865.4714, 1635.9284
Charge, Multiplicity	0, 1
Predicted log column density	13.283±4.320
Electronic energy	-1367.72104

geom360



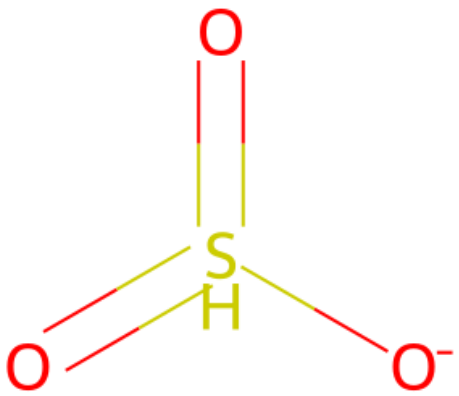
SMILES: [SiH3]S[SiH3]

Nearest TMC-1 molecule (distance): [C-]#[S+] (3.07)

Is DFT optimized?: True

Property	Value
Formula	H6SSi2
Molecular weight	94.287
IUPAC name	silylsulfanylsilane
$\mu_{a,b,c}$	0.0, 1.4, 0.0
A, B, C	9779.9034, 2726.6193, 2242.8867
A_s, B_s, C_s	9751.5417, 2718.7121, 2236.3823
Charge, Multiplicity	0, 1
Predicted log column density	11.048±3.061
Electronic energy	-980.76006

geom361



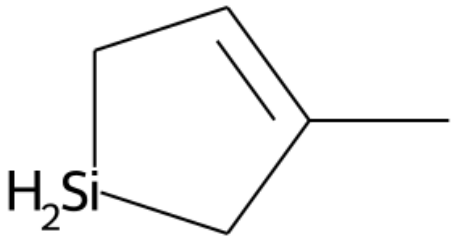
SMILES: O=[SH](=O)[O-]

Nearest TMC-1 molecule (distance): N (3.59)

Is DFT optimized?: True

Property	Value
Formula	HO3S-
Molecular weight	81.072
IUPAC name	sulfite
$\mu_{a,b,c}$	0.0, 0.0, 2.1
A, B, C	9307.9553, 9304.6524, 5113.5223
A_s, B_s, C_s	9280.9622, 9277.6689, 5098.6931
Charge, Multiplicity	-1, 1
Predicted log column density	10.982±3.109
Electronic energy	-624.39471

geom362



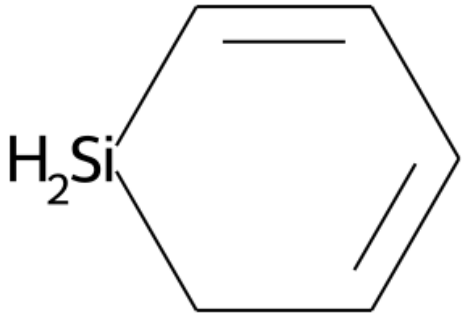
SMILES: CC1=CC[SiH2]C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.46)

Is DFT optimized?: True

Property	Value
Formula	C5H10Si
Molecular weight	98.221
IUPAC name	3-methyl-2,5-dihydro-1H-silole
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	5405.6597, 2220.2434, 1651.9421
A_s, B_s, C_s	5389.9833, 2213.8047, 1647.1515
Charge, Multiplicity	0, 1
Predicted log column density	11.382±3.376
Electronic energy	-485.95939

geom363



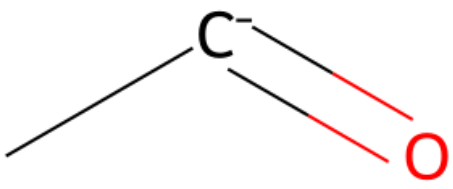
SMILES: C1=CC[SiH2]C=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.47)

Is DFT optimized?: True

Property	Value
Formula	C5H8Si
Molecular weight	96.205
IUPAC name	1,2-dihydrosiline
$\mu_{a,b,c}$	0.6, 0.5, 0.0
A, B, C	4181.1493, 3230.9758, 1882.7150
A_s, B_s, C_s	4169.0239, 3221.6060, 1877.2551
Charge, Multiplicity	0, 1
Predicted log column density	11.620±2.696
Electronic energy	-484.72546

geom364



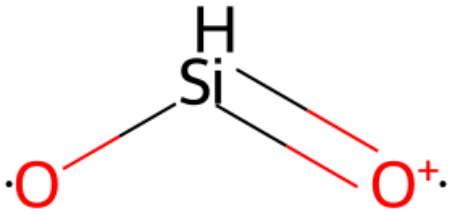
SMILES: C[C−]=O

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.87)

Is DFT optimized?: True

Property	Value
Formula	C2H3O-
Molecular weight	43.045
IUPAC name	ethanone
$\mu_{a,b,c}$	1.8, 2.1, 0.0
A, B, C	61479.5461, 10465.6828, 9472.8049
A_s, B_s, C_s	61301.2554, 10435.3323, 9445.3337
Charge, Multiplicity	-1, 1
Predicted log column density	12.508±2.564
Electronic energy	-153.14275

geom365



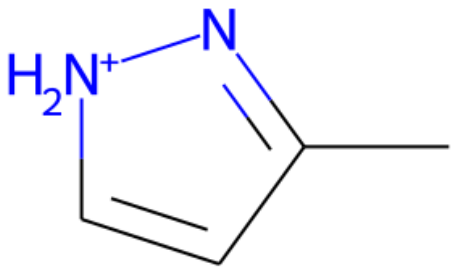
SMILES: [O][SiH]=[O+]

Nearest TMC-1 molecule (distance): [C-]#[S+] (1.59)

Is DFT optimized?: True

Property	Value
Formula	HO2Si+
Molecular weight	61.092
IUPAC name	
$\mu_{a,b,c}$	0.0, 3.2, 0.0
A, B, C	35991.3155, 8041.0274, 6572.6040
A_s, B_s, C_s	35886.9406, 8017.7085, 6553.5435
Charge, Multiplicity	1, 3
Predicted log column density	11.320±1.679
Electronic energy	-440.00816

geom366



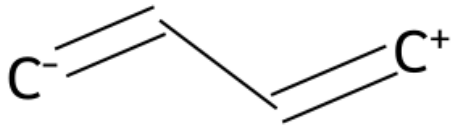
SMILES: CC1=N[NH2+]C=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.60)

Is DFT optimized?: True

Property	Value
Formula	C4H7N2+
Molecular weight	83.114
IUPAC name	3-methyl-1H-pyrazol-1-ium
$\mu_{a,b,c}$	3.8, 0.9, 0.0
A, B, C	8170.5869, 3384.9349, 2462.1791
A_s, B_s, C_s	8146.8922, 3375.1186, 2455.0388
Charge, Multiplicity	1, 1
Predicted log column density	10.966±4.726
Electronic energy	-265.75162

geom367



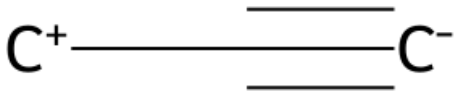
SMILES: [CH+]=CC=[CH−]

Nearest TMC-1 molecule (distance): [C+]#C[O−] (3.07)

Is DFT optimized?: True

Property	Value
Formula	C4H4
Molecular weight	52.076
IUPAC name	buta-1,3-diene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	41214.3789, 2022.4092, 1927.8110
A_s, B_s, C_s	41094.8572, 2016.5442, 1922.2203
Charge, Multiplicity	0, 1
Predicted log column density	12.113±2.242
Electronic energy	-154.59863

geom368



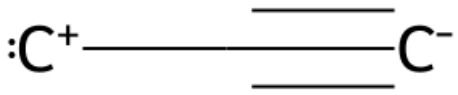
SMILES: [C−]#C[CH2+]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (0.64)

Is DFT optimized?: True

Property	Value
Formula	C3H2
Molecular weight	38.049
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	4.4, 0.0, 0.0
A, B, C	290557.7116, 10590.1322, 10217.7208
A_s, B_s, C_s	289715.0942, 10559.4208, 10188.0894
Charge, Multiplicity	0, 1
Predicted log column density	12.122±1.448
Electronic energy	-115.28837

geom369



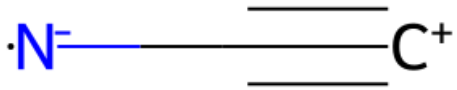
SMILES: [C+]C#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (0.74)

Is DFT optimized?: True

Property	Value
Formula	C3
Molecular weight	36.033
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 12502.2759, 12502.2759
A_s, B_s, C_s	∞, 12466.0193, 12466.0193
Charge, Multiplicity	0, 3
Predicted log column density	12.300±1.438
Electronic energy	-113.90839

geom370



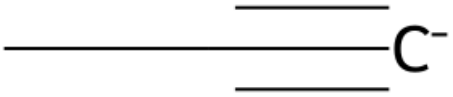
SMILES: [C+]#C[N−]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (2.18)

Is DFT optimized?: False

Property	Value
Formula	C2N
Molecular weight	38.029
IUPAC name	ethynylazanide
$\mu_{a,b,c}$	-, -, -
A, B, C	∞, 11067.2743, 11067.2743
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 2
Predicted log column density	13.155±2.170
Electronic energy	-

geom371



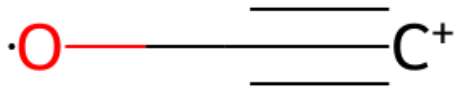
SMILES: [C−]#CC

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (2.30)

Is DFT optimized?: True

Property	Value
Formula	C3H3-
Molecular weight	39.057
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	7.0, 0.0, 0.0
A, B, C	160729.2470, 9153.8139, 9153.5790
A_s, B_s, C_s	160263.1322, 9127.2679, 9127.0336
Charge, Multiplicity	-1, 1
Predicted log column density	12.225±1.548
Electronic energy	-115.99320

geom372



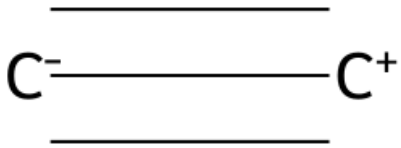
SMILES: [C+]#C[O]

Nearest TMC-1 molecule (distance): [C+]#C[O−] (1.22)

Is DFT optimized?: False

Property	Value
Formula	C2O+
Molecular weight	40.021
IUPAC name	ethynol
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	∞, 11104.6754, 11104.6754
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	12.241±1.507
Electronic energy	-150.65091

geom373



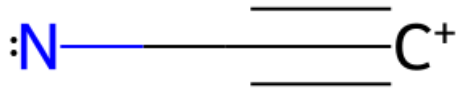
SMILES: [C+]#[C−]

Nearest TMC-1 molecule (distance): [C−]#[S+] (0.65)

Is DFT optimized?: True

Property	Value
Formula	C2
Molecular weight	24.022
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 53434.9733, 53434.9733
A_s, B_s, C_s	∞, 53280.0119, 53280.0119
Charge, Multiplicity	0, 1
Predicted log column density	13.171±1.249
Electronic energy	-75.84387

geom374



SMILES: [C+]#C[N]

Nearest TMC-1 molecule (distance): [C+]#C[O−] (1.83)

Is DFT optimized?: False

Property	Value
Formula	C2N+
Molecular weight	38.029
IUPAC name	ethynamine
$\mu_{a,b,c}$	-, -, -
A, B, C	∞, 11067.2743, 11067.2743
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 3
Predicted log column density	12.407±1.476
Electronic energy	-

geom375

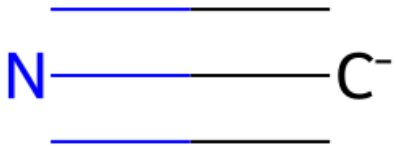
SMILES: N#[O+]

Nearest TMC-1 molecule (distance): NC#[O+] (1.85)

Is DFT optimized?: True

Property	Value
Formula	NO+
Molecular weight	30.006
IUPAC name	azanylidyneoxidanium
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	∞, 59317.1363, 59317.1363
A_s, B_s, C_s	∞, 59145.1166, 59145.1166
Charge, Multiplicity	1, 1
Predicted log column density	10.988±1.884
Electronic energy	-129.49268

geom376



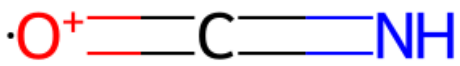
SMILES: [C−]#N

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (2.55)

Is DFT optimized?: True

Property	Value
Formula	CN-
Molecular weight	26.018
IUPAC name	cyanide
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	∞, 56101.4801, 56101.4801
A_s, B_s, C_s	∞, 55938.7858, 55938.7858
Charge, Multiplicity	-1, 1
Predicted log column density	12.460±2.010
Electronic energy	-92.82536

geom377



SMILES: N=C=[O+]

Nearest TMC-1 molecule (distance): NC#[O+] (2.39)

Is DFT optimized?: True

Property	Value
Formula	CHNO+
Molecular weight	43.025
IUPAC name	
$\mu_{a,b,c}$	2.9, 1.8, 0.0
A, B, C	781447.0831, 10808.5544, 10661.0959
A_s, B_s, C_s	779180.8866, 10777.2096, 10630.1787
Charge, Multiplicity	1, 2
Predicted log column density	12.728±1.921
Electronic energy	-168.19898

geom378

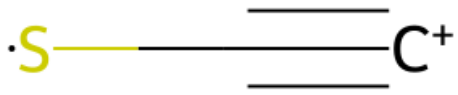
SMILES: [CH+]=C=[N−]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (2.64)

Is DFT optimized?: True

Property	Value
Formula	C2HN
Molecular weight	39.037
IUPAC name	ethenylideneazanide
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	90161163609.6067, 11014.2118, 11014.2105
A_s, B_s, C_s	89899696235.1388, 10982.2706, 10982.2693
Charge, Multiplicity	0, 1
Predicted log column density	13.322±2.862
Electronic energy	-131.32115

geom379



SMILES: [C+]#C[S]

Nearest TMC-1 molecule (distance): [C+]#C[O−] (1.69)

Is DFT optimized?: False

Property	Value
Formula	C2S+
Molecular weight	56.089
IUPAC name	ethynethiol
$\mu_{a,b,c}$	2.5, 0.0, 0.0
A, B, C	∞, 5970.6640, 5970.6640
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	13.660±1.718
Electronic energy	-473.71163

geom380

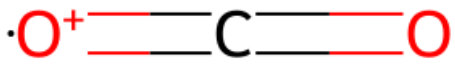
SMILES: [CH+]=C=[N]

Nearest TMC-1 molecule (distance): N#C[CH+] (1.90)

Is DFT optimized?: True

Property	Value
Formula	C2HN+
Molecular weight	39.037
IUPAC name	
$\mu_{a,b,c}$	4.8, 0.0, 0.0
A, B, C	19466655148.3246, 10991.4360, 10991.4351
A_s, B_s, C_s	19410201848.3944, 10959.5609, 10959.5599
Charge, Multiplicity	1, 2
Predicted log column density	12.869±1.507
Electronic energy	-130.97607

geom381



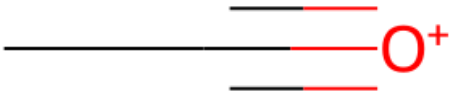
SMILES: O=C=[O+]

Nearest TMC-1 molecule (distance): O=C=[OH+] (2.38)

Is DFT optimized?: True

Property	Value
Formula	CO2+
Molecular weight	44.009
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 11427.9002, 11427.9002
A_s, B_s, C_s	∞, 11394.7592, 11394.7592
Charge, Multiplicity	1, 2
Predicted log column density	10.383±1.685
Electronic energy	-188.01671

geom382



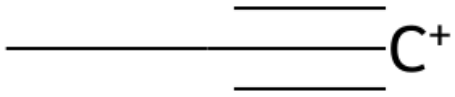
SMILES: CC#[O+]

Nearest TMC-1 molecule (distance): NC#[O+] (2.37)

Is DFT optimized?: True

Property	Value
Formula	C2H3O+
Molecular weight	43.045
IUPAC name	ethanone
$\mu_{a,b,c}$	3.3, 0.0, 0.0
A, B, C	153781.4764, 9121.9120, 9121.7723
A_s, B_s, C_s	153335.5101, 9095.4585, 9095.3192
Charge, Multiplicity	1, 1
Predicted log column density	11.534±1.662
Electronic energy	-152.87259

geom383



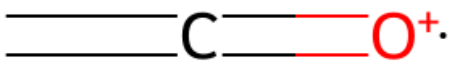
SMILES: [C+]#CC

Nearest TMC-1 molecule (distance): [C+]#C[O−] (2.39)

Is DFT optimized?: True

Property	Value
Formula	C3H3+
Molecular weight	39.057
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	153158.6939, 9462.3329, 9462.2555
A_s, B_s, C_s	152714.5336, 9434.8922, 9434.8149
Charge, Multiplicity	1, 1
Predicted log column density	12.957±1.537
Electronic energy	-115.39138

geom384



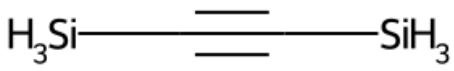
SMILES: C=C=[O+]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (2.89)

Is DFT optimized?: True

Property	Value
Formula	C2H2O+
Molecular weight	42.037
IUPAC name	ethenol
$\mu_{a,b,c}$	0.0, 3.7, 0.0
A, B, C	273370.5879, 9994.8956, 9642.3546
A_s, B_s, C_s	272577.8132, 9965.9104, 9614.3918
Charge, Multiplicity	1, 2
Predicted log column density	11.379±1.709
Electronic energy	-152.19835

geom385



SMILES: `[SiH3]C#C[SiH3]`

Nearest TMC-1 molecule (distance): `[CH+]=C=[C-]` (3.00)

Is DFT optimized?: True

Property	Value
Formula	C2H6Si2
Molecular weight	86.242
IUPAC name	2-silylethynylsilane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	42730.6578, 1259.4183, 1259.4171
A_s, B_s, C_s	42606.7389, 1255.7660, 1255.7648
Charge, Multiplicity	0, 1
Predicted log column density	10.291±2.802
Electronic energy	-658.67698

geom386

SMILES: [O+]=C=S

Nearest TMC-1 molecule (distance): NC#[O+] (2.81)

Is DFT optimized?: False

Property	Value
Formula	COS+
Molecular weight	60.077
IUPAC name	
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	∞, 5885.4348, 5885.4348
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	12.968±1.929
Electronic energy	-511.06050

geom387

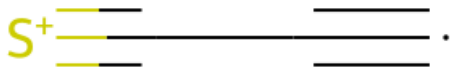
SMILES: [CH+]=C=S

Nearest TMC-1 molecule (distance): [C+]#C[O−] (2.54)

Is DFT optimized?: True

Property	Value
Formula	C2HS+
Molecular weight	57.097
IUPAC name	
$\mu_{a,b,c}$	3.0, 0.0, 0.0
A, B, C	1999595188.7920, 6006.5580, 6006.5405
A_s, B_s, C_s	1993796362.7445, 5989.1390, 5989.1215
Charge, Multiplicity	1, 1
Predicted log column density	14.426±1.733
Electronic energy	-474.47232

geom388



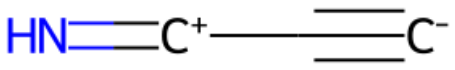
SMILES: [C]#CC#[S+]

Nearest TMC-1 molecule (distance): [C−]#CC#[S+] (2.54)

Is DFT optimized?: False

Property	Value
Formula	C3S+
Molecular weight	68.100
IUPAC name	prop-2-yne-1-thione
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	∞, 2719.4423, 2719.4423
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	12.684±1.513
Electronic energy	-511.86773

geom389



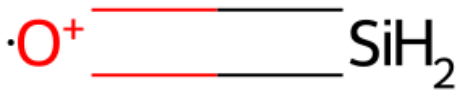
SMILES: [C−]#C[C+]=N

Nearest TMC-1 molecule (distance): [C−]#CC#[S+] (2.31)

Is DFT optimized?: True

Property	Value
Formula	C3HN
Molecular weight	51.048
IUPAC name	prop-2-yn-1-imine
$\mu_{a,b,c}$	5.6, 1.2, 0.0
A, B, C	1667074.3592, 4646.7623, 4633.8460
A_s, B_s, C_s	1662239.8436, 4633.2867, 4620.4079
Charge, Multiplicity	0, 1
Predicted log column density	13.468±2.009
Electronic energy	-169.43030

geom390



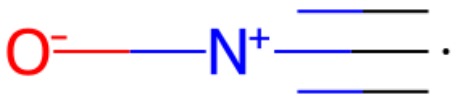
SMILES: [O+]=[SiH2]

Nearest TMC-1 molecule (distance): [C-]#[S+] (1.31)

Is DFT optimized?: True

Property	Value
Formula	H2OSi+
Molecular weight	46.101
IUPAC name	hydroxysilanylium
$\mu_{a,b,c}$	4.0, 0.0, 0.0
A, B, C	141092.3019, 17124.6469, 15271.1569
A_s, B_s, C_s	140683.1342, 17074.9854, 15226.8705
Charge, Multiplicity	1, 2
Predicted log column density	11.594±1.592
Electronic energy	-365.46644

geom391



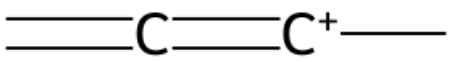
SMILES: [C]#[N+][O-]

Nearest TMC-1 molecule (distance): [C-]#[NH+] (2.85)

Is DFT optimized?: True

Property	Value
Formula	CNO
Molecular weight	42.017
IUPAC name	formonitrile oxide
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	∞, 12420.1479, 12420.1479
A_s, B_s, C_s	∞, 12384.1295, 12384.1295
Charge, Multiplicity	0, 2
Predicted log column density	12.348±2.533
Electronic energy	-167.84736

geom392



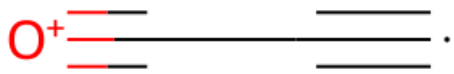
SMILES: C=C=[C+]C

Nearest TMC-1 molecule (distance): C=C=[C] (2.88)

Is DFT optimized?: True

Property	Value
Formula	C4H5+
Molecular weight	53.084
IUPAC name	but-2-yne
$\mu_{a,b,c}$	1.2, 0.0, 0.2
A, B, C	101312.1623, 3680.8109, 3631.1665
A_s, B_s, C_s	101018.3570, 3670.1366, 3620.6361
Charge, Multiplicity	1, 1
Predicted log column density	13.180±1.538
Electronic energy	-154.98273

geom393



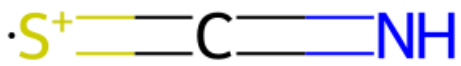
SMILES: [C]#CC#[O+]

Nearest TMC-1 molecule (distance): [C−]#CC#[S+] (1.45)

Is DFT optimized?: True

Property	Value
Formula	C3O+
Molecular weight	52.032
IUPAC name	prop-2-ynylidyneoxidanium
$\mu_{a,b,c}$	2.7, 0.0, 0.0
A, B, C	∞, 4826.0097, 4826.0097
A_s, B_s, C_s	∞, 4812.0143, 4812.0143
Charge, Multiplicity	1, 2
Predicted log column density	11.365±1.651
Electronic energy	-188.92085

geom394



SMILES: N=C=[S+]

Nearest TMC-1 molecule (distance): N=C=O (2.43)

Is DFT optimized?: False

Property	Value
Formula	CHNS+
Molecular weight	59.093
IUPAC name	
$\mu_{a,b,c}$	0.5, 1.7, 0.8
A, B, C	576138.9513, 6022.9945, 5960.6812
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	13.971±1.740
Electronic energy	-491.19675

geom395

SMILES: [C+]=C=C

Nearest TMC-1 molecule (distance): C=C=O (2.44)

Is DFT optimized?: True

Property	Value
Formula	C3H2+
Molecular weight	38.049
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	282378.3955, 10802.9659, 10404.9065
A_s, B_s, C_s	281559.4982, 10771.6373, 10374.7323
Charge, Multiplicity	1, 2
Predicted log column density	12.335±1.167
Electronic energy	-114.90613

geom396

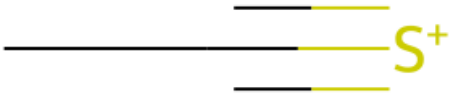
SMILES: C#[O+]

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.17)

Is DFT optimized?: False

Property	Value
Formula	CHO+
Molecular weight	29.018
IUPAC name	methanone
$\mu_{a,b,c}$	4.2, 0.0, 0.0
A, B, C	∞, 40701.3064, 40701.3064
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 1
Predicted log column density	11.992±1.625
Electronic energy	-113.49719

geom397



SMILES: CC#[S+]

Nearest TMC-1 molecule (distance): [C]#N (2.33)

Is DFT optimized?: True

Property	Value
Formula	C2H3S+
Molecular weight	59.113
IUPAC name	ethanethione
$\mu_{a,b,c}$	2.0, 0.0, 0.0
A, B, C	156182.3545, 5245.9339, 5245.8752
A_s, B_s, C_s	155729.4257, 5230.7207, 5230.6622
Charge, Multiplicity	1, 1
Predicted log column density	13.068±1.474
Electronic energy	-475.83261

geom398

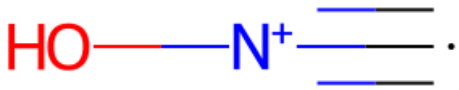
SMILES: [C]=C=C

Nearest TMC-1 molecule (distance): C=C=O (2.45)

Is DFT optimized?: True

Property	Value
Formula	C3H2
Molecular weight	38.049
IUPAC name	propa-1,2-diene
$\mu_{a,b,c}$	0.9, 0.0, 0.0
A, B, C	287090.2003, 10675.0180, 10292.3138
A_s, B_s, C_s	286257.6387, 10644.0605, 10262.4661
Charge, Multiplicity	0, 3
Predicted log column density	12.188±1.055
Electronic energy	-115.24235

geom399



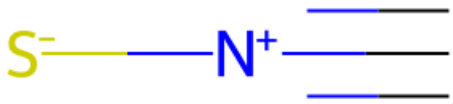
SMILES: [C]#[N+]O

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.43)

Is DFT optimized?: True

Property	Value
Formula	CHNO+
Molecular weight	43.025
IUPAC name	N-methylidenehydroxylamine
$\mu_{a,b,c}$	1.4, 1.9, 0.0
A, B, C	623770.5227, 11808.3749, 11588.9879
A_s, B_s, C_s	621961.5881, 11774.1306, 11555.3799
Charge, Multiplicity	1, 2
Predicted log column density	12.639±1.841
Electronic energy	-168.05255

geom400



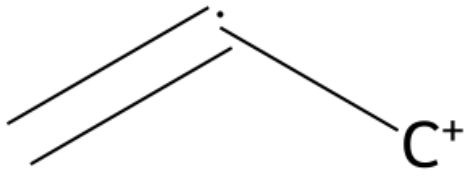
SMILES: C#[N+][S−]

Nearest TMC-1 molecule (distance): [C−]#[NH+] (3.41)

Is DFT optimized?: True

Property	Value
Formula	CHNS
Molecular weight	59.093
IUPAC name	methylidyne(sulfido)azanium
$\mu_{a,b,c}$	0.0, 4.2, 0.0
A, B, C	9257180757.1831, 6119.8831, 6119.8790
A_s, B_s, C_s	9230334932.9873, 6102.1354, 6102.1314
Charge, Multiplicity	0, 1
Predicted log column density	14.868±2.041
Electronic energy	-491.52045

geom401



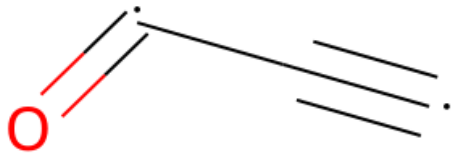
SMILES: C=[C][CH2+]

Nearest TMC-1 molecule (distance): C=C=O (2.52)

Is DFT optimized?: True

Property	Value
Formula	C3H4+
Molecular weight	40.065
IUPAC name	prop-1-ene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	142214.7455, 8940.8719, 8591.7410
A_s, B_s, C_s	141802.3228, 8914.9433, 8566.8250
Charge, Multiplicity	1, 2
Predicted log column density	12.137±1.205
Electronic energy	-116.26669

geom402



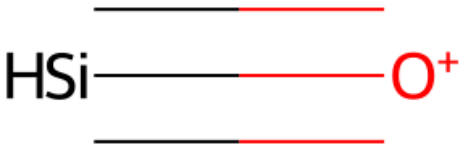
SMILES: [C]#C[C]=O

Nearest TMC-1 molecule (distance): C=C=C=O (2.97)

Is DFT optimized?: True

Property	Value
Formula	C3O
Molecular weight	52.032
IUPAC name	prop-2-ynal
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	31974999318.2229, 4737.2866, 4737.2859
A_s, B_s, C_s	31882271820.2001, 4723.5485, 4723.5478
Charge, Multiplicity	0, 3
Predicted log column density	11.699±1.062
Electronic energy	-189.21382

geom403



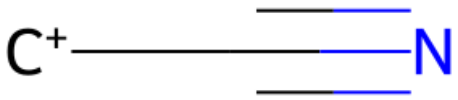
SMILES: [O+]#[SiH]

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.32)

Is DFT optimized?: False

Property	Value
Formula	HOSi+
Molecular weight	45.093
IUPAC name	oxosilanylium
$\mu_{a,b,c}$	0.0, 5.4, 0.1
A, B, C	277745.9541, 26341.8062, 24059.9296
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 1
Predicted log column density	11.711±1.607
Electronic energy	-364.79186

geom404



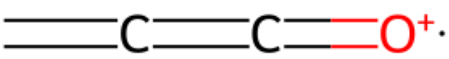
SMILES: [CH2+]C#N

Nearest TMC-1 molecule (distance): N#C[CH+] (0.46)

Is DFT optimized?: True

Property	Value
Formula	C2H2N+
Molecular weight	40.045
IUPAC name	acetonitrile
$\mu_{a,b,c}$	5.4, 0.0, 0.0
A, B, C	278952.2548, 10333.2465, 9964.1442
A_s, B_s, C_s	278143.2932, 10303.2800, 9935.2481
Charge, Multiplicity	1, 1
Predicted log column density	11.584±1.309
Electronic energy	-131.66791

geom405



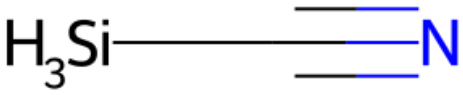
SMILES: C=C=C=[O+]

Nearest TMC-1 molecule (distance): C=C=C=O (3.10)

Is DFT optimized?: True

Property	Value
Formula	C3H2O+
Molecular weight	54.048
IUPAC name	propa-1,2-dien-1-ol
$\mu_{a,b,c}$	4.3, 0.0, 0.0
A, B, C	284624.9510, 4152.8368, 4093.1229
A_s, B_s, C_s	283799.5387, 4140.7936, 4081.2528
Charge, Multiplicity	1, 2
Predicted log column density	10.785±1.670
Electronic energy	-190.25793

geom406



SMILES: N#C[SiH3]

Nearest TMC-1 molecule (distance): N#C[CH+] (1.08)

Is DFT optimized?: True

Property	Value
Formula	CH3NSi
Molecular weight	57.128
IUPAC name	silylformonitrile
$\mu_{a,b,c}$	3.7, 0.0, 0.0
A, B, C	84233.6965, 4934.1399, 4934.1191
A_s, B_s, C_s	83989.4188, 4919.8309, 4919.8102
Charge, Multiplicity	0, 1
Predicted log column density	10.981±1.803
Electronic energy	-384.08065

geom407

SMILES: [O+]S

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.63)

Is DFT optimized?: False

Property	Value
Formula	HOS+
Molecular weight	49.074
IUPAC name	sulfanyloxidanium
$\mu_{a,b,c}$	0.0, 2.3, 1.4
A, B, C	295912.5667, 17717.9804, 16717.0357
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 3
Predicted log column density	12.676±2.129
Electronic energy	-473.49587

geom408

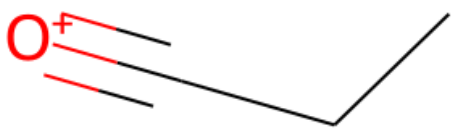
SMILES: N=[O+]

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.94)

Is DFT optimized?: True

Property	Value
Formula	HNO+
Molecular weight	31.014
IUPAC name	oxoazanium
$\mu_{a,b,c}$	0.0, 2.5, 1.5
A, B, C	750421.7071, 45999.7550, 43342.8986
A_s, B_s, C_s	748245.4841, 45866.3557, 43217.2042
Charge, Multiplicity	1, 2
Predicted log column density	12.564±1.866
Electronic energy	-130.05420

geom409



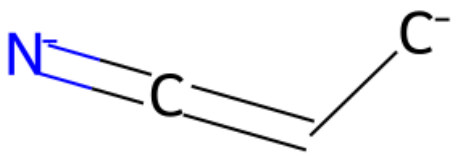
SMILES: CCC#[O+]

Nearest TMC-1 molecule (distance): NC#[O+] (3.44)

Is DFT optimized?: True

Property	Value
Formula	C3H5O+
Molecular weight	57.072
IUPAC name	propylidyneoxidanium
$\mu_{a,b,c}$	1.3, 1.5, 0.0
A, B, C	27092.0934, 4588.5504, 4129.9606
A_s, B_s, C_s	27013.5263, 4575.2436, 4117.9838
Charge, Multiplicity	1, 1
Predicted log column density	9.946±2.933
Electronic energy	-192.18415

geom410



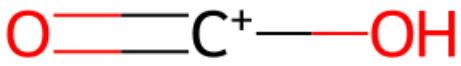
SMILES: [CH2−]C=C=[N−]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (3.67)

Is DFT optimized?: False

Property	Value
Formula	C3H3N-2
Molecular weight	53.064
IUPAC name	prop-1-enylideneazanide
$\mu_{a,b,c}$	0.8, 1.2, 4.4
A, B, C	45790.0258, 5002.3801, 4509.8328
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-2, 1
Predicted log column density	12.650±3.151
Electronic energy	-170.54955

geom411



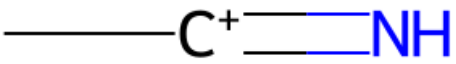
SMILES: O=[C+]O

Nearest TMC-1 molecule (distance): N#[NH+] (2.32)

Is DFT optimized?: True

Property	Value
Formula	CHO2+
Molecular weight	45.017
IUPAC name	
$\mu_{a,b,c}$	3.0, 1.9, 0.0
A, B, C	802772.2314, 10737.2012, 10595.4850
A_s, B_s, C_s	800444.1919, 10706.0633, 10564.7581
Charge, Multiplicity	1, 1
Predicted log column density	12.271±1.588
Electronic energy	-188.73395

geom412



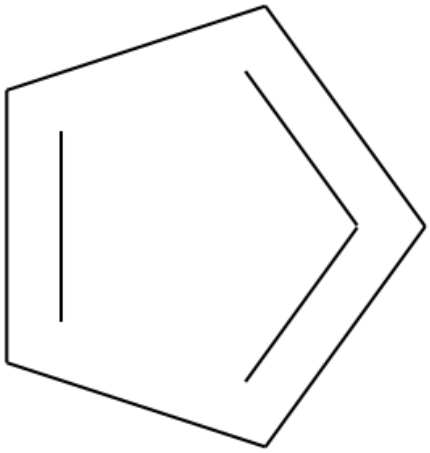
SMILES: C[C+]=N

Nearest TMC-1 molecule (distance): N#[NH+] (2.60)

Is DFT optimized?: True

Property	Value
Formula	C2H4N+
Molecular weight	42.061
IUPAC name	acetonitrilium
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	155797.7658, 8574.8129, 8574.7656
A_s, B_s, C_s	155345.9523, 8549.9459, 8549.8988
Charge, Multiplicity	1, 1
Predicted log column density	14.312±2.004
Electronic energy	-133.01612

geom413



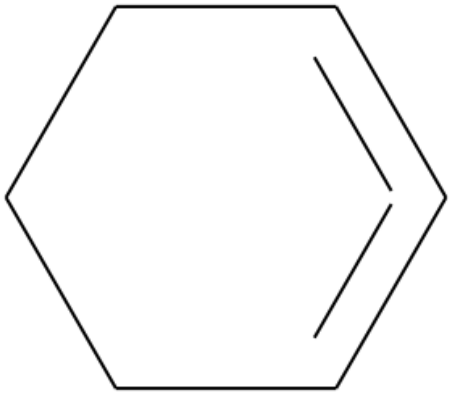
SMILES: C1=CC#CC=1

Nearest TMC-1 molecule (distance): C1C#C1 (4.55)

Is DFT optimized?: True

Property	Value
Formula	C5H2
Molecular weight	62.071
IUPAC name	
$\mu_{a,b,c}$	2.6, 0.7, 1.0
A, B, C	17005.8841, 7624.5008, 5567.0481
A_s, B_s, C_s	16956.5670, 7602.3898, 5550.9037
Charge, Multiplicity	0, 1
Predicted log column density	11.378±2.498
Electronic energy	-191.33755

geom414



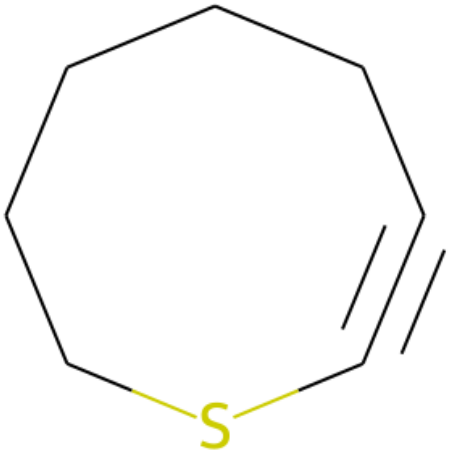
SMILES: C1=CCCCC=1

Nearest TMC-1 molecule (distance): C1=C=C1 (6.10)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	
$\mu_{a,b,c}$	0.1, 1.8, 0.1
A, B, C	5339.5195, 4750.7697, 2851.9937
A_s, B_s, C_s	5324.0349, 4736.9925, 2843.7229
Charge, Multiplicity	0, 1
Predicted log column density	11.476±4.414
Electronic energy	-233.27731

geom415



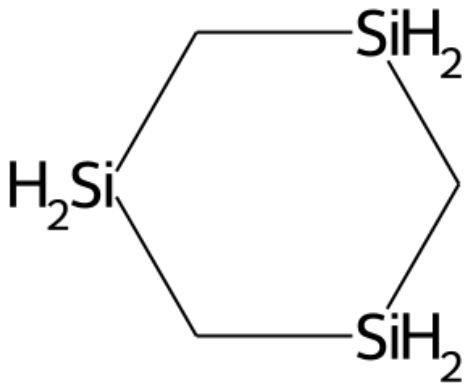
SMILES: C1#CSCCCCC1

Nearest TMC-1 molecule (distance): C1C#C1 (7.59)

Is DFT optimized?: True

Property	Value
Formula	C7H10S
Molecular weight	126.224
IUPAC name	1-thiacyclooct-7-yne
$\mu_{a,b,c}$	2.1, 2.4, 0.3
A, B, C	2824.0363, 1431.2096, 1010.8212
A_s, B_s, C_s	2815.8465, 1427.0591, 1007.8898
Charge, Multiplicity	0, 1
Predicted log column density	10.639±5.953
Electronic energy	-670.77481

geom416



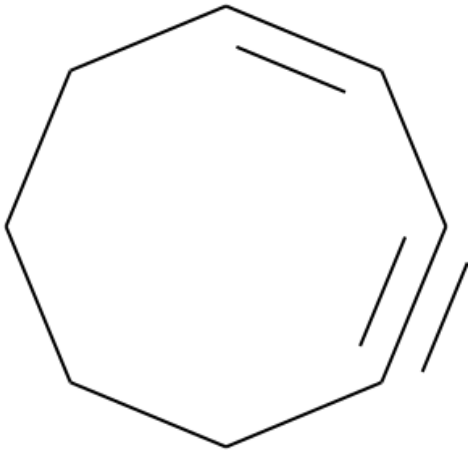
SMILES: C1[SiH2]C[SiH2]C[SiH2]1

Nearest TMC-1 molecule (distance): C1=C=[C]1 (6.05)

Is DFT optimized?: True

Property	Value
Formula	C3H12Si3
Molecular weight	132.387
IUPAC name	1,3,5-trisilinane
$\mu_{a,b,c}$	0.0, 0.0, 1.3
A, B, C	1967.3024, 1965.6483, 1082.1863
A_s, B_s, C_s	1961.5972, 1959.9480, 1079.0480
Charge, Multiplicity	0, 1
Predicted log column density	9.880±5.072
Electronic energy	-989.97457

geom417



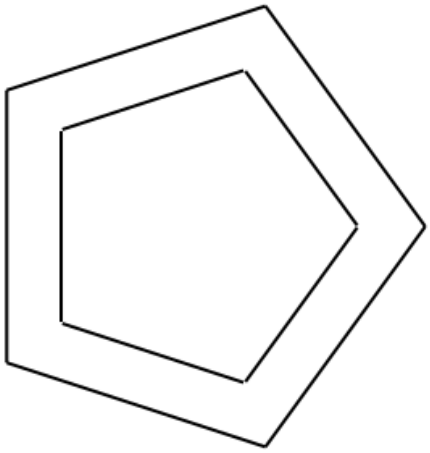
SMILES: C1#CCCCCC=C1

Nearest TMC-1 molecule (distance): C1C#C1 (7.98)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	cyclooct-1-en-3-yne
$\mu_{a,b,c}$	2.2, 1.1, 0.0
A, B, C	2933.0000, 2206.5289, 1300.6264
A_s, B_s, C_s	2924.4943, 2200.1299, 1296.8545
Charge, Multiplicity	0, 1
Predicted log column density	10.226±4.599
Electronic energy	-310.55862

geom418



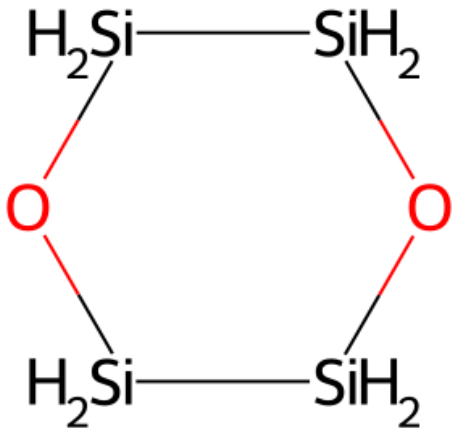
SMILES: C1=C=C=C=C=1

Nearest TMC-1 molecule (distance): C1C#C1 (8.19)

Is DFT optimized?: True

Property	Value
Formula	C5
Molecular weight	60.055
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.5, 0.0
A, B, C	17114.1045, 9239.4826, 6741.4511
A_s, B_s, C_s	17064.4736, 9212.6881, 6721.9009
Charge, Multiplicity	0, 1
Predicted log column density	12.339±2.898
Electronic energy	-190.01491

geom419



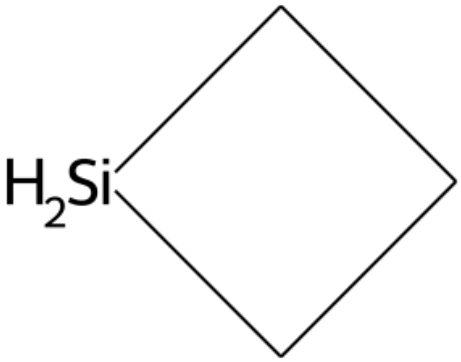
SMILES: `O1[SiH2][SiH2]O[SiH2][SiH2]1`

Nearest TMC-1 molecule (distance): `C1=C=[C]1` (6.53)

Is DFT optimized?: True

Property	Value
Formula	H8O2Si4
Molecular weight	152.406
IUPAC name	1,4,2,3,5,6-dioxatetrasilinane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	1792.0784, 1546.9910, 871.5113
A_s, B_s, C_s	1786.8814, 1542.5048, 868.9839
Charge, Multiplicity	0, 1
Predicted log column density	10.504±6.670
Electronic energy	-1313.25029

geom420



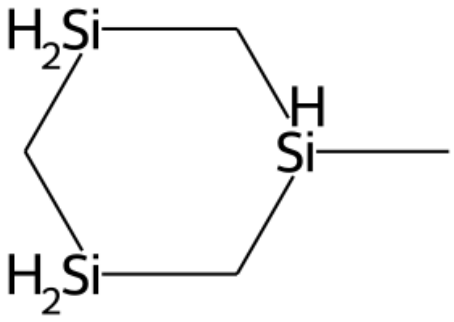
SMILES: C1C[SiH2]C1

Nearest TMC-1 molecule (distance): [C−]#[S+] (4.72)

Is DFT optimized?: True

Property	Value
Formula	C3H8Si
Molecular weight	72.183
IUPAC name	siletane
$\mu_{a,b,c}$	0.5, 0.0, 0.2
A, B, C	8819.3564, 6232.7339, 4203.3492
A_s, B_s, C_s	8793.7803, 6214.6590, 4191.1595
Charge, Multiplicity	0, 1
Predicted log column density	10.918±3.429
Electronic energy	-408.55111

geom421



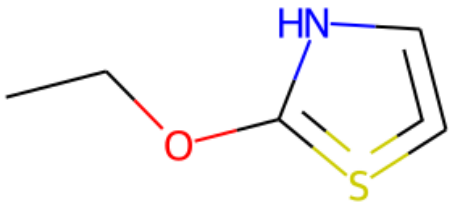
SMILES: C[SiH]1C[SiH2]C[SiH2]C1

Nearest TMC-1 molecule (distance): C1=C=[C]1 (6.64)

Is DFT optimized?: True

Property	Value
Formula	C4H14Si3
Molecular weight	146.414
IUPAC name	1-methyl-1,3,5-trisilinane
$\mu_{a,b,c}$	0.1, 0.0, 0.7
A, B, C	1666.5147, 1355.5391, 937.6534
A_s, B_s, C_s	1661.6818, 1351.6080, 934.9342
Charge, Multiplicity	0, 1
Predicted log column density	12.623±5.534
Electronic energy	-1029.29370

geom422



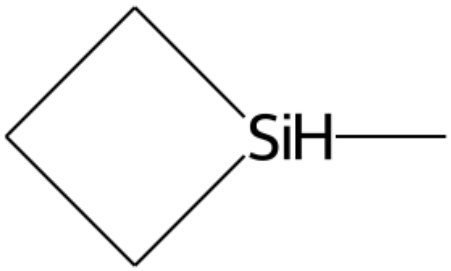
SMILES: CCOC1=S=C=CN1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (6.30)

Is DFT optimized?: True

Property	Value
Formula	C5H7NOS
Molecular weight	129.184
IUPAC name	2-ethoxy-1,3-thiazole
$\mu_{a,b,c}$	8.0, 3.1, 0.0
A, B, C	4824.4611, 1024.4367, 854.1775
A_s, B_s, C_s	4810.4701, 1021.4659, 851.7004
Charge, Multiplicity	0, 1
Predicted log column density	14.188±5.322
Electronic energy	-722.69341

geom423



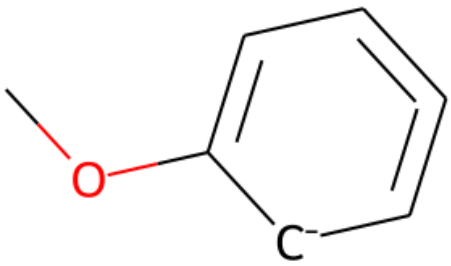
SMILES: C[SiH]1CCC1

Nearest TMC-1 molecule (distance): [C−]#[S+] (5.63)

Is DFT optimized?: True

Property	Value
Formula	C4H10Si
Molecular weight	86.210
IUPAC name	1-methylsiletane
$\mu_{a,b,c}$	0.4, 0.0, 0.5
A, B, C	7447.2190, 2858.7272, 2425.1350
A_s, B_s, C_s	7425.6221, 2850.4369, 2418.1021
Charge, Multiplicity	0, 1
Predicted log column density	13.335±4.163
Electronic energy	-447.87003

geom424



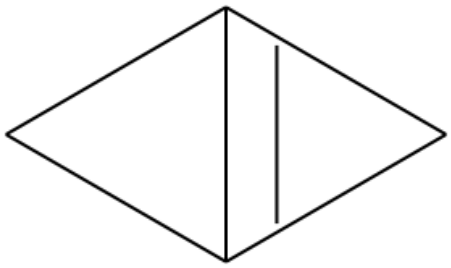
SMILES: COC1=CC=C=C[CH−]1

Nearest TMC-1 molecule (distance): C1=C=C1 (5.92)

Is DFT optimized?: True

Property	Value
Formula	C7H7O-
Molecular weight	107.132
IUPAC name	methoxybenzene
$\mu_{a,b,c}$	9.6, 0.2, 0.0
A, B, C	5173.6665, 1577.5865, 1218.3174
A_s, B_s, C_s	5158.6628, 1573.0115, 1214.7843
Charge, Multiplicity	-1, 1
Predicted log column density	15.622±3.967
Electronic energy	-346.00823

geom425



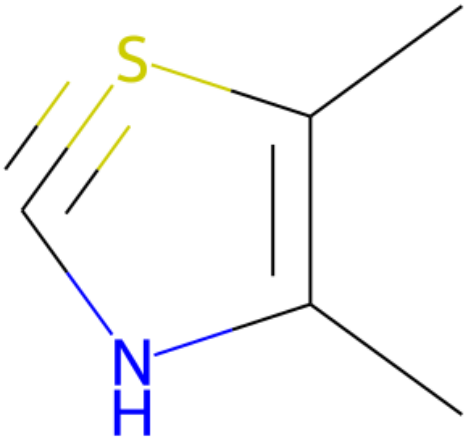
SMILES: C1C2=C1C2

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.98)

Is DFT optimized?: True

Property	Value
Formula	C4H4
Molecular weight	52.076
IUPAC name	bicyclo[1.1.0]but-1(3)-ene
$\mu_{a,b,c}$	0.0, 0.0, 0.9
A, B, C	28052.0966, 9026.2046, 8367.7890
A_s, B_s, C_s	27970.7455, 9000.0287, 8343.5224
Charge, Multiplicity	0, 1
Predicted log column density	10.673±4.563
Electronic energy	-154.57740

geom426



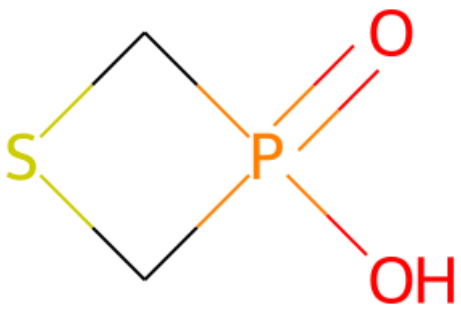
SMILES: CC1=C(C)S#CN1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (6.75)

Is DFT optimized?: True

Property	Value
Formula	C5H7NS
Molecular weight	113.185
IUPAC name	4,5-dimethyl-1,2-didehydro-3H-1,3-thiazole
$\mu_{a,b,c}$	4.7, 1.2, 0.0
A, B, C	3164.3661, 2440.5041, 1402.0119
A_s, B_s, C_s	3155.1894, 2433.4266, 1397.9461
Charge, Multiplicity	0, 1
Predicted log column density	13.437±5.675
Electronic energy	-647.54539

geom427



SMILES: O=P1(O)CSC1

Nearest TMC-1 molecule (distance): [C+]#C[O−] (7.77)

Is DFT optimized?: True

Property	Value
Formula	C2H5O2PS
Molecular weight	124.101
IUPAC name	3-hydroxy-1,3lambda5-thiaphosphetane 3-oxide
$\mu_{a,b,c}$	0.5, 1.4, 0.1
A, B, C	4497.0324, 1821.1800, 1783.8845
A_s, B_s, C_s	4483.9910, 1815.8986, 1778.7112
Charge, Multiplicity	0, 1
Predicted log column density	13.565±7.370
Electronic energy	-969.14493

geom428

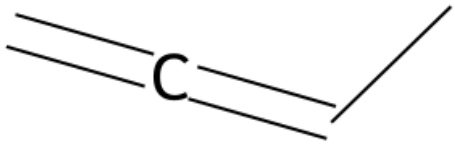
SMILES: [CH]=C=C

Nearest TMC-1 molecule (distance): C=C=[C] (2.93)

Is DFT optimized?: True

Property	Value
Formula	C3H3
Molecular weight	39.057
IUPAC name	propa-1,2-diene
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	288775.9870, 9501.0557, 9198.4174
A_s, B_s, C_s	287938.5367, 9473.5027, 9171.7420
Charge, Multiplicity	0, 2
Predicted log column density	12.600±1.495
Electronic energy	-115.95732

geom429



SMILES: C=C=CC

Nearest TMC-1 molecule (distance): C=C=[C] (3.07)

Is DFT optimized?: True

Property	Value
Formula	C4H6
Molecular weight	54.092
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.1, 0.0
A, B, C	34318.0973, 4185.5855, 3922.5612
A_s, B_s, C_s	34218.5748, 4173.4473, 3911.1858
Charge, Multiplicity	0, 1
Predicted log column density	13.197±1.907
Electronic energy	-155.92137

geom430

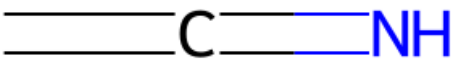
SMILES: C=C=[N]

Nearest TMC-1 molecule (distance): [CH2]C#N (2.19)

Is DFT optimized?: True

Property	Value
Formula	C2H2N
Molecular weight	40.045
IUPAC name	
$\mu_{a,b,c}$	0.0, 3.6, 0.0
A, B, C	284840.9473, 10238.1783, 9882.9505
A_s, B_s, C_s	284014.9086, 10208.4875, 9854.2900
Charge, Multiplicity	0, 2
Predicted log column density	12.567±1.496
Electronic energy	-132.04609

geom431



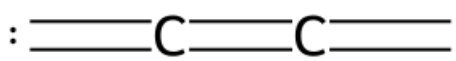
SMILES: C=C=N

Nearest TMC-1 molecule (distance): N=C=O (3.20)

Is DFT optimized?: True

Property	Value
Formula	C2H3N
Molecular weight	41.053
IUPAC name	
$\mu_{a,b,c}$	0.6, 0.0, 1.6
A, B, C	201658.1596, 9648.9958, 9463.7911
A_s, B_s, C_s	201073.3509, 9621.0137, 9436.3461
Charge, Multiplicity	0, 1
Predicted log column density	13.842±1.828
Electronic energy	-132.66532

geom432



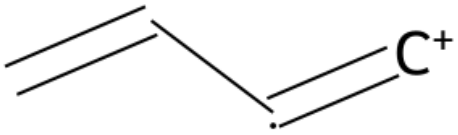
SMILES: [C]=C=C=C

Nearest TMC-1 molecule (distance): C=C=C=O (2.58)

Is DFT optimized?: True

Property	Value
Formula	C4H2
Molecular weight	50.060
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.0, 0.0
A, B, C	290389.3371, 4479.9853, 4411.9206
A_s, B_s, C_s	289547.2080, 4466.9933, 4399.1260
Charge, Multiplicity	0, 3
Predicted log column density	12.943±1.049
Electronic energy	-153.29467

geom433



SMILES: [CH+]=[C]C=C

Nearest TMC-1 molecule (distance): C=CC#N (3.38)

Is DFT optimized?: True

Property	Value
Formula	C4H4+
Molecular weight	52.076
IUPAC name	buta-1,3-diene
$\mu_{a,b,c}$	0.4, 0.5, 0.0
A, B, C	45455.3601, 4857.6911, 4388.6843
A_s, B_s, C_s	45323.5395, 4843.6038, 4375.9572
Charge, Multiplicity	1, 2
Predicted log column density	12.597±1.631
Electronic energy	-154.34038

geom434

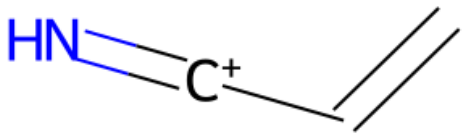
SMILES: C=C=S

Nearest TMC-1 molecule (distance): C=C=O (2.54)

Is DFT optimized?: True

Property	Value
Formula	C2H2S
Molecular weight	58.105
IUPAC name	
$\mu_{a,b,c}$	1.3, 0.0, 0.0
A, B, C	286392.1887, 5650.8141, 5541.4751
A_s, B_s, C_s	285561.6514, 5634.4267, 5525.4048
Charge, Multiplicity	0, 1
Predicted log column density	14.106±1.770
Electronic energy	-475.50243

geom435



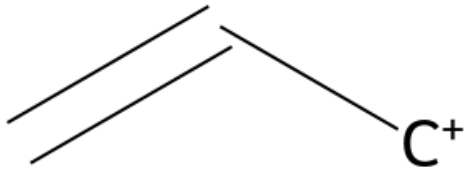
SMILES: C=C[C+]=N

Nearest TMC-1 molecule (distance): CC=C (3.64)

Is DFT optimized?: True

Property	Value
Formula	C3H4N+
Molecular weight	54.072
IUPAC name	prop-2-en-1-imine
$\mu_{a,b,c}$	1.6, 0.5, 0.0
A, B, C	46813.0616, 4761.1853, 4321.6464
A_s, B_s, C_s	46677.3037, 4747.3778, 4309.1137
Charge, Multiplicity	1, 1
Predicted log column density	13.490±2.228
Electronic energy	-171.08100

geom436



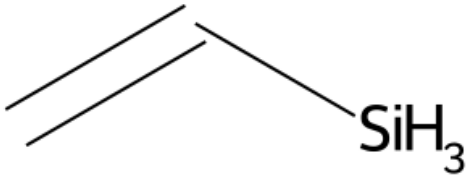
SMILES: C=C[CH2+]

Nearest TMC-1 molecule (distance): CC=C (2.30)

Is DFT optimized?: True

Property	Value
Formula	C3H5+
Molecular weight	41.073
IUPAC name	prop-1-ene
$\mu_{a,b,c}$	0.0, 0.7, 0.0
A, B, C	49847.0620, 11009.2200, 9017.6174
A_s, B_s, C_s	49702.5056, 10977.2932, 8991.4663
Charge, Multiplicity	1, 1
Predicted log column density	12.021±1.738
Electronic energy	-116.92551

geom437



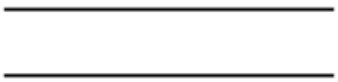
SMILES: C=C[SiH3]

Nearest TMC-1 molecule (distance): CC=C (2.33)

Is DFT optimized?: True

Property	Value
Formula	C2H6Si
Molecular weight	58.156
IUPAC name	ethenylsilane
$\mu_{a,b,c}$	0.7, 0.1, 0.0
A, B, C	34442.8954, 5164.0378, 4735.7839
A_s, B_s, C_s	34343.0110, 5149.0621, 4722.0501
Charge, Multiplicity	0, 1
Predicted log column density	11.270±1.809
Electronic energy	-369.23225

geom438



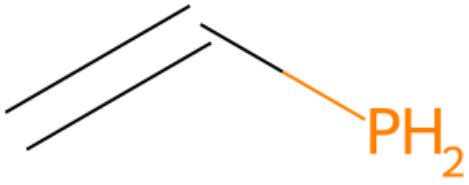
SMILES: C=C

Nearest TMC-1 molecule (distance): C=O (2.53)

Is DFT optimized?: True

Property	Value
Formula	C2H4
Molecular weight	28.054
IUPAC name	ethene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	146529.2358, 30089.3733, 24963.2408
A_s, B_s, C_s	146104.3010, 30002.1141, 24890.8474
Charge, Multiplicity	0, 1
Predicted log column density	11.766±1.684
Electronic energy	-78.56014

geom439



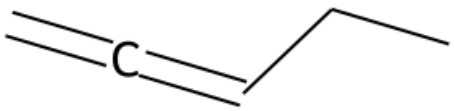
SMILES: C=CP

Nearest TMC-1 molecule (distance): CC=C (2.47)

Is DFT optimized?: True

Property	Value
Formula	C2H5P
Molecular weight	60.036
IUPAC name	ethenylphosphane
$\mu_{a,b,c}$	0.8, 0.1, 0.7
A, B, C	40776.1263, 5408.8886, 4939.5998
A_s, B_s, C_s	40657.8755, 5393.2029, 4925.2749
Charge, Multiplicity	0, 1
Predicted log column density	12.279±1.835
Electronic energy	-420.48484

geom440



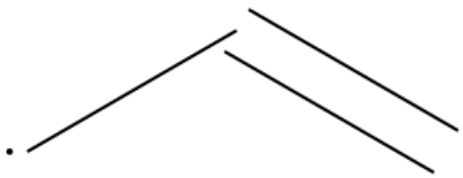
SMILES: C=C=CCC

Nearest TMC-1 molecule (distance): C=C=[C] (3.95)

Is DFT optimized?: True

Property	Value
Formula	C5H8
Molecular weight	68.119
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.0, 0.1
A, B, C	17710.2746, 2274.6741, 2235.9484
A_s, B_s, C_s	17658.9148, 2268.0775, 2229.4641
Charge, Multiplicity	0, 1
Predicted log column density	11.376±3.222
Electronic energy	-195.22486

geom441



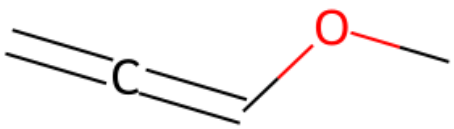
SMILES: [CH2]C=C

Nearest TMC-1 molecule (distance): CC=C (2.17)

Is DFT optimized?: True

Property	Value
Formula	C3H5
Molecular weight	41.073
IUPAC name	prop-1-ene
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	54495.4603, 10339.1727, 8690.3858
A_s, B_s, C_s	54337.4235, 10309.1890, 8665.1837
Charge, Multiplicity	0, 2
Predicted log column density	11.726±1.913
Electronic energy	-117.21922

geom442



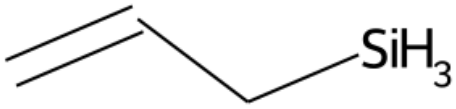
SMILES: C=C=COC

Nearest TMC-1 molecule (distance): C=C=[C] (4.07)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	
$\mu_{a,b,c}$	0.8, 1.2, 0.5
A, B, C	30294.7650, 2327.4039, 2281.7003
A_s, B_s, C_s	30206.9102, 2320.6544, 2275.0833
Charge, Multiplicity	0, 1
Predicted log column density	13.375±3.367
Electronic energy	-231.09604

geom443



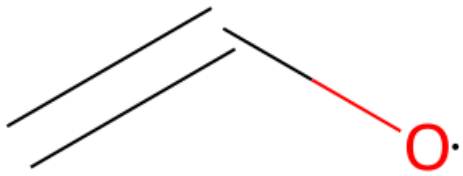
SMILES: C=CC[SiH3]

Nearest TMC-1 molecule (distance): CC=C (3.04)

Is DFT optimized?: True

Property	Value
Formula	C3H8Si
Molecular weight	72.183
IUPAC name	prop-2-enylsilane
$\mu_{a,b,c}$	0.1, 0.5, 0.0
A, B, C	15667.4149, 2752.1413, 2637.0424
A_s, B_s, C_s	15621.9794, 2744.1601, 2629.3950
Charge, Multiplicity	0, 1
Predicted log column density	9.953±2.644
Electronic energy	-408.54027

geom444



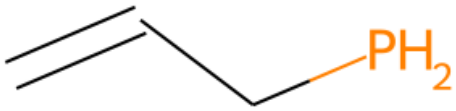
SMILES: C=C[O]

Nearest TMC-1 molecule (distance): CC=C (2.44)

Is DFT optimized?: True

Property	Value
Formula	C2H3O
Molecular weight	43.045
IUPAC name	ethenol
$\mu_{a,b,c}$	0.0, 3.1, 1.0
A, B, C	66992.0975, 11440.0077, 9771.3826
A_s, B_s, C_s	66797.8204, 11406.8317, 9743.0456
Charge, Multiplicity	0, 2
Predicted log column density	11.740±1.737
Electronic energy	-153.12433

geom445



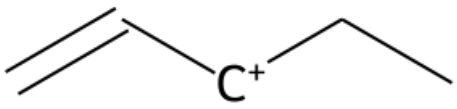
SMILES: C=CCP

Nearest TMC-1 molecule (distance): CC=C (3.29)

Is DFT optimized?: True

Property	Value
Formula	C3H7P
Molecular weight	74.063
IUPAC name	prop-2-enylphosphane
$\mu_{a,b,c}$	0.5, 0.7, 0.8
A, B, C	17534.9023, 2744.2175, 2641.9012
A_s, B_s, C_s	17484.0511, 2736.2592, 2634.2397
Charge, Multiplicity	0, 1
Predicted log column density	11.896±2.826
Electronic energy	-459.79019

geom446



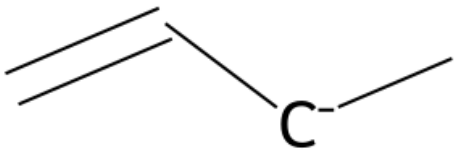
SMILES: C=C[CH+]CC

Nearest TMC-1 molecule (distance): CC=C (2.71)

Is DFT optimized?: True

Property	Value
Formula	C5H9+
Molecular weight	69.127
IUPAC name	pent-1-ene
$\mu_{a,b,c}$	2.4, 0.2, 0.7
A, B, C	15691.4878, 2366.2119, 2299.9267
A_s, B_s, C_s	15645.9824, 2359.3499, 2293.2569
Charge, Multiplicity	1, 1
Predicted log column density	10.981±2.568
Electronic energy	-195.56461

geom447



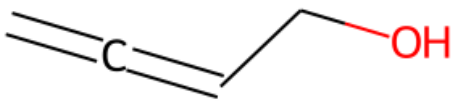
SMILES: C=C[CH−]C

Nearest TMC-1 molecule (distance): CC=C (3.16)

Is DFT optimized?: True

Property	Value
Formula	C4H7-
Molecular weight	55.100
IUPAC name	but-1-ene
$\mu_{a,b,c}$	3.6, 0.7, 0.0
A, B, C	38618.9792, 3864.6117, 3591.3706
A_s, B_s, C_s	38506.9842, 3853.4044, 3580.9556
Charge, Multiplicity	-1, 1
Predicted log column density	11.434±2.985
Electronic energy	-156.52905

geom448



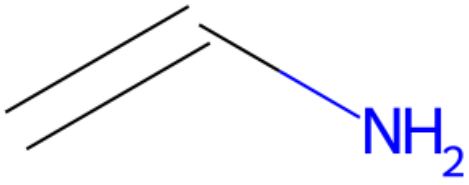
SMILES: C=C=CCO

Nearest TMC-1 molecule (distance): C=C=[C] (4.44)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	
$\mu_{a,b,c}$	1.7, 0.6, 0.2
A, B, C	19759.1811, 2310.9454, 2274.5696
A_s, B_s, C_s	19701.8795, 2304.2436, 2267.9734
Charge, Multiplicity	0, 1
Predicted log column density	10.788±3.200
Electronic energy	-231.11155

geom449



SMILES: C=CN

Nearest TMC-1 molecule (distance): CC=C (3.00)

Is DFT optimized?: True

Property	Value
Formula	C2H5N
Molecular weight	43.069
IUPAC name	ethenamine
$\mu_{a,b,c}$	1.8, 0.1, 0.0
A, B, C	58269.7298, 10006.0402, 8539.6219
A_s, B_s, C_s	58100.7476, 9977.0227, 8514.8570
Charge, Multiplicity	0, 1
Predicted log column density	12.732±2.853
Electronic energy	-133.90237

geom450

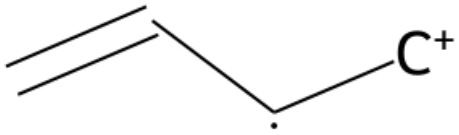
SMILES: C=CSO

Nearest TMC-1 molecule (distance): CC=C (3.30)

Is DFT optimized?: True

Property	Value
Formula	C2H4OS
Molecular weight	76.120
IUPAC name	hydroxysulfanylethene
$\mu_{a,b,c}$	0.6, 0.6, 1.7
A, B, C	19584.9435, 3590.1175, 3178.0540
A_s, B_s, C_s	19528.1471, 3579.7061, 3168.8377
Charge, Multiplicity	0, 1
Predicted log column density	12.085±3.432
Electronic energy	-551.90615

geom451



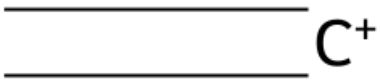
SMILES: C=C[CH][CH2+]

Nearest TMC-1 molecule (distance): CC=C (2.53)

Is DFT optimized?: True

Property	Value
Formula	C4H6+
Molecular weight	54.092
IUPAC name	but-1-ene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	40867.9167, 4454.4431, 4016.6541
A_s, B_s, C_s	40749.3997, 4441.5252, 4005.0058
Charge, Multiplicity	1, 2
Predicted log column density	12.202±2.470
Electronic energy	-155.62008

geom452



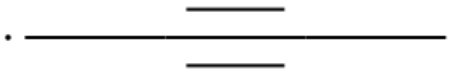
SMILES: [CH+]=C

Nearest TMC-1 molecule (distance): C=[OH+] (1.66)

Is DFT optimized?: True

Property	Value
Formula	C2H3+
Molecular weight	27.046
IUPAC name	ethene
$\mu_{a,b,c}$	0.5, 0.0, 0.0
A, B, C	282068.7092, 32830.7143, 29407.8570
A_s, B_s, C_s	281250.7099, 32735.5052, 29322.5742
Charge, Multiplicity	1, 1
Predicted log column density	12.466±1.404
Electronic energy	-77.55428

geom453



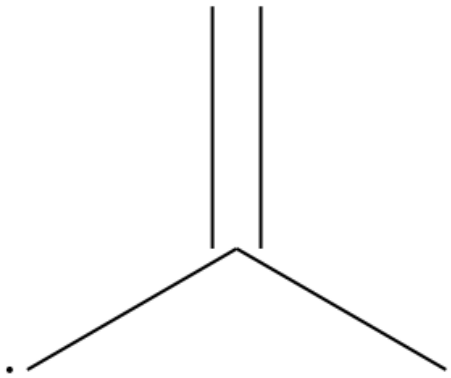
SMILES: [CH2]C#CC

Nearest TMC-1 molecule (distance): CC#C (3.21)

Is DFT optimized?: True

Property	Value
Formula	C4H5
Molecular weight	53.084
IUPAC name	but-2-yne
$\mu_{a,b,c}$	1.0, 0.0, 0.0
A, B, C	102841.8912, 3589.2238, 3544.9424
A_s, B_s, C_s	102543.6498, 3578.8151, 3534.6621
Charge, Multiplicity	0, 2
Predicted log column density	11.967±1.631
Electronic energy	-155.27121

geom454



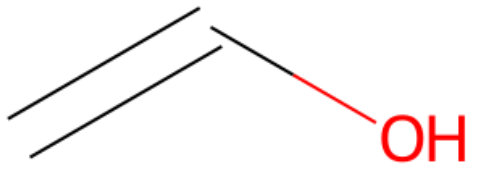
SMILES: [CH2]C(=C)C

Nearest TMC-1 molecule (distance): CC=C (3.54)

Is DFT optimized?: True

Property	Value
Formula	C4H7
Molecular weight	55.100
IUPAC name	2-methylprop-1-ene
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	9946.2743, 8801.3493, 4809.3815
A_s, B_s, C_s	9917.4301, 8775.8254, 4795.4343
Charge, Multiplicity	0, 2
Predicted log column density	11.076±3.237
Electronic energy	-156.52520

geom455



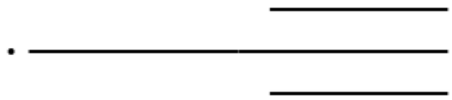
SMILES: C=CO

Nearest TMC-1 molecule (distance): CC=C (2.97)

Is DFT optimized?: True

Property	Value
Formula	C2H4O
Molecular weight	44.053
IUPAC name	ethenol
$\mu_{a,b,c}$	0.6, 0.9, 0.0
A, B, C	60462.3896, 10554.3963, 8985.8195
A_s, B_s, C_s	60287.0487, 10523.7886, 8959.7607
Charge, Multiplicity	0, 1
Predicted log column density	11.802±1.979
Electronic energy	-153.76219

geom456



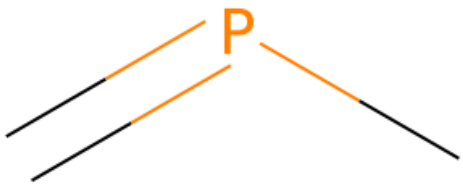
SMILES: C#C[CH2]

Nearest TMC-1 molecule (distance): CC#C (2.37)

Is DFT optimized?: True

Property	Value
Formula	C3H3
Molecular weight	39.057
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	288300.7842, 9505.5850, 9202.1794
A_s, B_s, C_s	287464.7120, 9478.0189, 9175.4930
Charge, Multiplicity	0, 2
Predicted log column density	12.375±1.587
Electronic energy	-115.95732

geom457



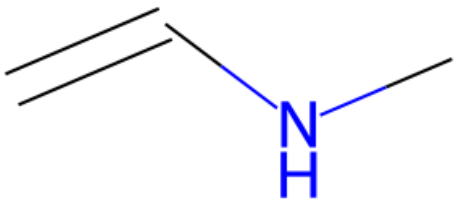
SMILES: C=PC

Nearest TMC-1 molecule (distance): C=[OH+] (2.23)

Is DFT optimized?: True

Property	Value
Formula	C2H5P
Molecular weight	60.036
IUPAC name	methyl(methylidene)phosphane
$\mu_{a,b,c}$	0.6, 1.3, 0.0
A, B, C	21412.3234, 7878.5515, 5976.3567
A_s, B_s, C_s	21350.2276, 7855.7037, 5959.0252
Charge, Multiplicity	0, 1
Predicted log column density	13.429±2.119
Electronic energy	-420.49183

geom458



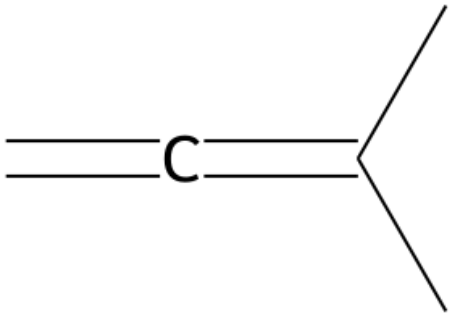
SMILES: C=CNC

Nearest TMC-1 molecule (distance): CC=C (3.38)

Is DFT optimized?: True

Property	Value
Formula	C3H7N
Molecular weight	57.096
IUPAC name	N-methylethenamine
$\mu_{a,b,c}$	2.0, 0.3, 0.0
A, B, C	38751.2043, 4145.5000, 3835.8973
A_s, B_s, C_s	38638.8258, 4133.4780, 3824.7732
Charge, Multiplicity	0, 1
Predicted log column density	13.825±3.455
Electronic energy	-173.19691

geom459



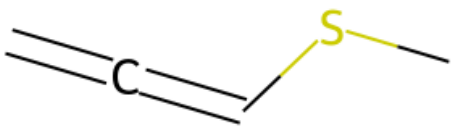
SMILES: C=C=C(C)C

Nearest TMC-1 molecule (distance): C=C=[C] (4.81)

Is DFT optimized?: True

Property	Value
Formula	C5H8
Molecular weight	68.119
IUPAC name	
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	8278.7480, 3606.0250, 2640.0669
A_s, B_s, C_s	8254.7397, 3595.5675, 2632.4107
Charge, Multiplicity	0, 1
Predicted log column density	10.995±4.227
Electronic energy	-195.22908

geom460



SMILES: C=C=CSC

Nearest TMC-1 molecule (distance): C=C=[C] (4.82)

Is DFT optimized?: True

Property	Value
Formula	C4H6S
Molecular weight	86.159
IUPAC name	
$\mu_{a,b,c}$	0.1, 1.5, 0.1
A, B, C	13624.3570, 1868.3003, 1772.4425
A_s, B_s, C_s	13584.8463, 1862.8822, 1767.3024
Charge, Multiplicity	0, 1
Predicted log column density	13.504±4.692
Electronic energy	-554.08648

geom461

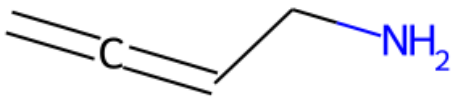
SMILES: C=[S+]

Nearest TMC-1 molecule (distance): C=S (1.50)

Is DFT optimized?: True

Property	Value
Formula	CH2S+
Molecular weight	46.094
IUPAC name	methylidenesulfanium
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	283592.3900, 18090.2957, 17005.5175
A_s, B_s, C_s	282769.9720, 18037.8338, 16956.2015
Charge, Multiplicity	1, 2
Predicted log column density	12.247±1.373
Electronic energy	-437.08326

geom462



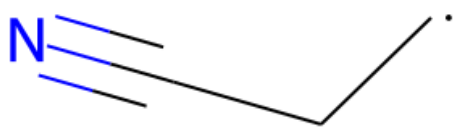
SMILES: C=C=CCN

Nearest TMC-1 molecule (distance): C=C=[C] (4.86)

Is DFT optimized?: True

Property	Value
Formula	C4H7N
Molecular weight	69.107
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.7, 1.3
A, B, C	19765.0211, 2279.6915, 2253.7505
A_s, B_s, C_s	19707.7025, 2273.0804, 2247.2147
Charge, Multiplicity	0, 1
Predicted log column density	9.744±3.242
Electronic energy	-211.25136

geom463



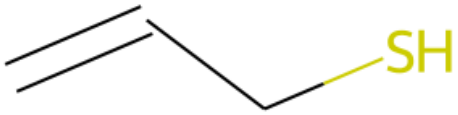
SMILES: [CH2]CC#N

Nearest TMC-1 molecule (distance): [CH2]C#N (2.74)

Is DFT optimized?: True

Property	Value
Formula	C3H4N
Molecular weight	54.072
IUPAC name	propanenitrile
$\mu_{a,b,c}$	3.8, 1.4, 0.1
A, B, C	32079.0129, 4894.7267, 4361.2772
A_s, B_s, C_s	31985.9838, 4880.5320, 4348.6295
Charge, Multiplicity	0, 2
Predicted log column density	10.784±2.652
Electronic energy	-171.33602

geom464



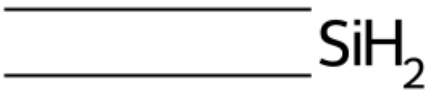
SMILES: C=CCS

Nearest TMC-1 molecule (distance): CC=C (3.79)

Is DFT optimized?: True

Property	Value
Formula	C3H6S
Molecular weight	74.148
IUPAC name	prop-2-ene-1-thiol
$\mu_{a,b,c}$	1.5, 0.1, 0.5
A, B, C	19572.8927, 2799.0812, 2699.9445
A_s, B_s, C_s	19516.1313, 2790.9639, 2692.1147
Charge, Multiplicity	0, 1
Predicted log column density	11.874±4.256
Electronic energy	-516.03529

geom465



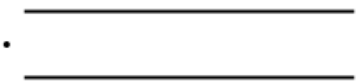
SMILES: C=[SiH2]

Nearest TMC-1 molecule (distance): C=S (1.38)

Is DFT optimized?: True

Property	Value
Formula	CH4Si
Molecular weight	44.129
IUPAC name	methylidenesilane
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	104907.4528, 14786.2821, 12959.6699
A_s, B_s, C_s	104603.2212, 14743.4019, 12922.0869
Charge, Multiplicity	0, 1
Predicted log column density	11.953±1.387
Electronic energy	-329.90197

geom466



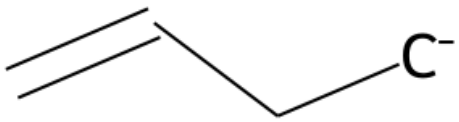
SMILES: [CH]=C

Nearest TMC-1 molecule (distance): C#[S+] (1.75)

Is DFT optimized?: True

Property	Value
Formula	C2H3
Molecular weight	27.046
IUPAC name	ethene
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	293464.2448, 31162.3519, 28170.9390
A_s, B_s, C_s	292613.1985, 31071.9811, 28089.2433
Charge, Multiplicity	0, 2
Predicted log column density	12.541±1.474
Electronic energy	-77.86490

geom467



SMILES: C=CC[CH2−]

Nearest TMC-1 molecule (distance): CC=C (3.84)

Is DFT optimized?: True

Property	Value
Formula	C4H7-
Molecular weight	55.100
IUPAC name	but-1-ene
$\mu_{a,b,c}$	5.5, 2.7, 1.0
A, B, C	23750.6684, 4335.1179, 4233.1799
A_s, B_s, C_s	23681.7915, 4322.5461, 4220.9036
Charge, Multiplicity	-1, 1
Predicted log column density	11.578±2.900
Electronic energy	-156.49438

geom468

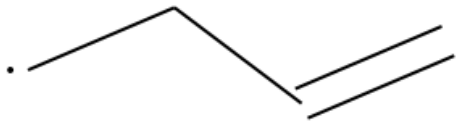
SMILES: C=[O+]

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.08)

Is DFT optimized?: True

Property	Value
Formula	CH2O+
Molecular weight	30.026
IUPAC name	methylideneoxidanium
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	265995.2793, 39911.2420, 34704.0721
A_s, B_s, C_s	265223.8930, 39795.4994, 34603.4303
Charge, Multiplicity	1, 2
Predicted log column density	11.348±1.644
Electronic energy	-114.06743

geom469



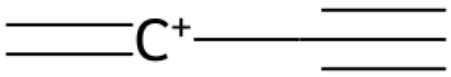
SMILES: [CH2]CC=C

Nearest TMC-1 molecule (distance): CC=C (4.06)

Is DFT optimized?: True

Property	Value
Formula	C4H7
Molecular weight	55.100
IUPAC name	but-1-ene
$\mu_{a,b,c}$	0.2, 0.3, 0.0
A, B, C	24298.0434, 4359.6912, 4245.4023
A_s, B_s, C_s	24227.5791, 4347.0481, 4233.0907
Charge, Multiplicity	0, 2
Predicted log column density	10.564±3.202
Electronic energy	-156.49757

geom470



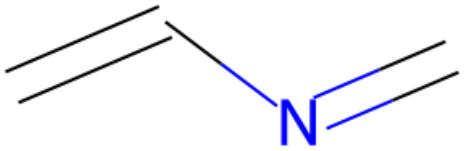
SMILES: C#C[C+]=C

Nearest TMC-1 molecule (distance): CC#C (3.29)

Is DFT optimized?: True

Property	Value
Formula	C4H3+
Molecular weight	51.068
IUPAC name	but-1-en-3-yne
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	283939.9798, 4213.1890, 4151.5864
A_s, B_s, C_s	283116.5538, 4200.9707, 4139.5468
Charge, Multiplicity	1, 1
Predicted log column density	13.021±1.678
Electronic energy	-153.71542

geom471



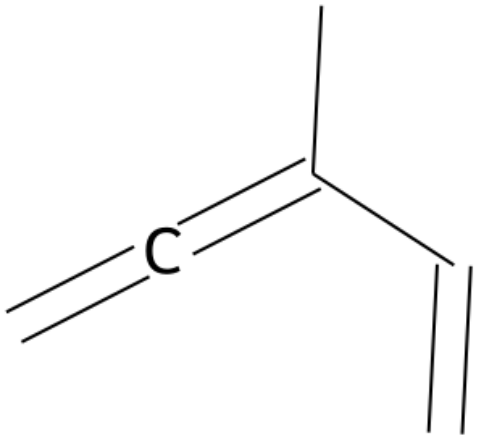
SMILES: C=CN=C

Nearest TMC-1 molecule (distance): CC=C (3.73)

Is DFT optimized?: True

Property	Value
Formula	C3H5N
Molecular weight	55.080
IUPAC name	N-ethenylmethanimine
$\mu_{a,b,c}$	0.5, 1.6, 0.0
A, B, C	47844.1151, 4886.1355, 4433.3934
A_s, B_s, C_s	47705.3672, 4871.9657, 4420.5365
Charge, Multiplicity	0, 1
Predicted log column density	10.235±2.638
Electronic energy	-171.96922

geom472



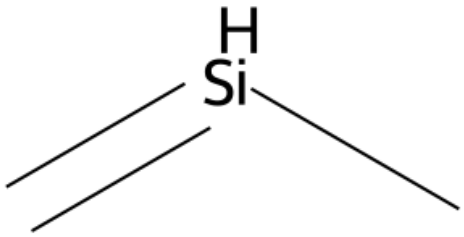
SMILES: C=C=C(C)C=C

Nearest TMC-1 molecule (distance): C=C=[C] (4.96)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.3, 0.0
A, B, C	6988.8103, 2298.5906, 1769.9308
A_s, B_s, C_s	6968.5428, 2291.9247, 1764.7980
Charge, Multiplicity	0, 1
Predicted log column density	10.716±3.165
Electronic energy	-233.29810

geom473



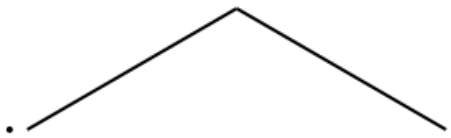
SMILES: C=[SiH]C

Nearest TMC-1 molecule (distance): C=S (1.61)

Is DFT optimized?: True

Property	Value
Formula	C2H6Si
Molecular weight	58.156
IUPAC name	methyl(methylidene)silane
$\mu_{a,b,c}$	1.7, 0.1, 0.0
A, B, C	27141.7149, 6085.8990, 5130.2151
A_s, B_s, C_s	27063.0039, 6068.2499, 5115.3374
Charge, Multiplicity	0, 1
Predicted log column density	12.352±1.538
Electronic energy	-369.22046

geom474



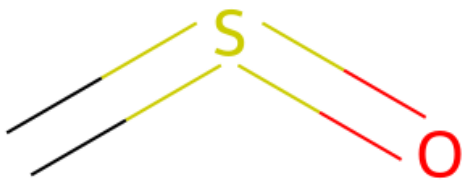
SMILES: [CH2]CC

Nearest TMC-1 molecule (distance): C=S (3.36)

Is DFT optimized?: True

Property	Value
Formula	C3H7
Molecular weight	43.089
IUPAC name	propane
$\mu_{a,b,c}$	0.2, 0.2, 0.1
A, B, C	32800.0843, 8976.2542, 7771.6288
A_s, B_s, C_s	32704.9641, 8950.2230, 7749.0911
Charge, Multiplicity	0, 2
Predicted log column density	11.354±3.050
Electronic energy	-118.43379

geom475



SMILES: C=S=O

Nearest TMC-1 molecule (distance): C=O (2.48)

Is DFT optimized?: False

Property	Value
Formula	CH2OS
Molecular weight	62.093
IUPAC name	sulfinylmethane
$\mu_{a,b,c}$	2.0, 1.6, 2.4
A, B, C	37569.8715, 9334.9296, 7477.1047
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.343±2.884
Electronic energy	-512.59734

geom476

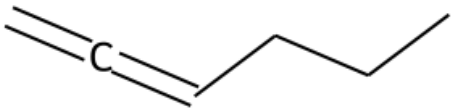
SMILES: [CH2]S

Nearest TMC-1 molecule (distance): C=S (1.49)

Is DFT optimized?: True

Property	Value
Formula	CH3S
Molecular weight	47.102
IUPAC name	methanethiol
$\mu_{a,b,c}$	0.4, 1.1, 0.0
A, B, C	144378.6034, 15429.3610, 13939.7044
A_s, B_s, C_s	143959.9054, 15384.6159, 13899.2793
Charge, Multiplicity	0, 2
Predicted log column density	13.242±2.095
Electronic energy	-438.00164

geom477



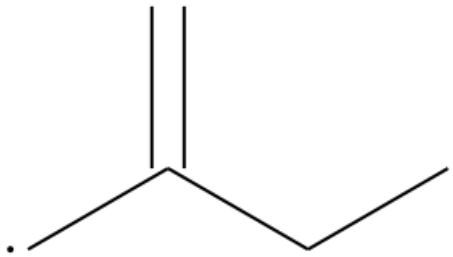
SMILES: C=C=CCCC

Nearest TMC-1 molecule (distance): C=C=[C] (5.18)

Is DFT optimized?: True

Property	Value
Formula	C6H10
Molecular weight	82.146
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.0, 0.0
A, B, C	12938.8082, 1334.8570, 1307.2692
A_s, B_s, C_s	12901.2857, 1330.9859, 1303.4781
Charge, Multiplicity	0, 1
Predicted log column density	10.022±3.752
Electronic energy	-234.52871

geom478



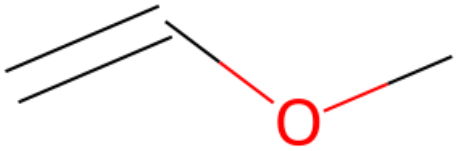
SMILES: [CH2]C(=C)CC

Nearest TMC-1 molecule (distance): CC=C (4.38)

Is DFT optimized?: True

Property	Value
Formula	C5H9
Molecular weight	69.127
IUPAC name	2-methylbut-1-ene
$\mu_{a,b,c}$	0.4, 0.3, 0.0
A, B, C	8956.2561, 3733.4743, 2723.9839
A_s, B_s, C_s	8930.2830, 3722.6472, 2716.0843
Charge, Multiplicity	0, 2
Predicted log column density	10.327±3.842
Electronic energy	-195.82744

geom479



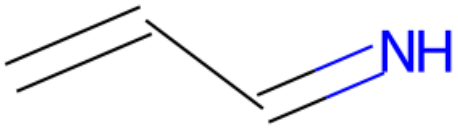
SMILES: C=COC

Nearest TMC-1 molecule (distance): CC=C (3.55)

Is DFT optimized?: True

Property	Value
Formula	C3H6O
Molecular weight	58.080
IUPAC name	methoxyethene
$\mu_{a,b,c}$	1.3, 1.4, 0.0
A, B, C	40305.0894, 4522.6889, 4175.2651
A_s, B_s, C_s	40188.2047, 4509.5731, 4163.1569
Charge, Multiplicity	0, 1
Predicted log column density	13.925±3.946
Electronic energy	-193.05183

geom480



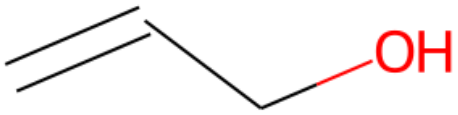
SMILES: C=CC=N

Nearest TMC-1 molecule (distance): CC=C (3.65)

Is DFT optimized?: True

Property	Value
Formula	C3H5N
Molecular weight	55.080
IUPAC name	prop-2-en-1-imine
$\mu_{a,b,c}$	2.8, 0.9, 0.0
A, B, C	44118.5490, 4557.7724, 4131.0086
A_s, B_s, C_s	43990.6052, 4544.5548, 4119.0287
Charge, Multiplicity	0, 1
Predicted log column density	13.547±3.354
Electronic energy	-171.97727

geom481



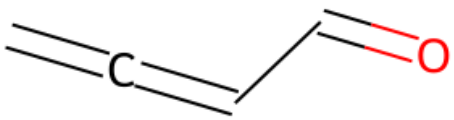
SMILES: C=CCO

Nearest TMC-1 molecule (distance): CC=C (3.68)

Is DFT optimized?: True

Property	Value
Formula	C3H6O
Molecular weight	58.080
IUPAC name	prop-2-en-1-ol
$\mu_{a,b,c}$	1.6, 0.1, 0.8
A, B, C	25778.3492, 4318.7488, 4223.5829
A_s, B_s, C_s	25703.5920, 4306.2244, 4211.3346
Charge, Multiplicity	0, 1
Predicted log column density	10.385±3.463
Electronic energy	-193.05785

geom482



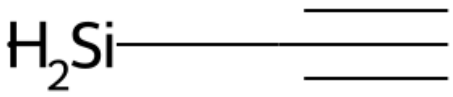
SMILES: C=C=CC=O

Nearest TMC-1 molecule (distance): C=C=[C] (5.26)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	
$\mu_{a,b,c}$	3.9, 0.5, 0.0
A, B, C	35560.1867, 2395.3961, 2279.6456
A_s, B_s, C_s	35457.0621, 2388.4494, 2273.0346
Charge, Multiplicity	0, 1
Predicted log column density	11.360±2.445
Electronic energy	-229.90733

geom483



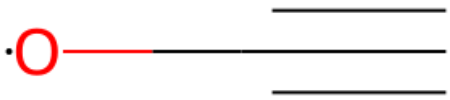
SMILES: C#C[SiH2]

Nearest TMC-1 molecule (distance): CC#C (2.00)

Is DFT optimized?: True

Property	Value
Formula	C2H3Si
Molecular weight	55.132
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.0, 0.1
A, B, C	133889.7625, 5062.4223, 4947.2101
A_s, B_s, C_s	133501.4822, 5047.7413, 4932.8632
Charge, Multiplicity	0, 2
Predicted log column density	12.725±1.490
Electronic energy	-367.33706

geom484



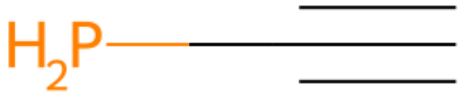
SMILES: C#C[O]

Nearest TMC-1 molecule (distance): CC#C (2.01)

Is DFT optimized?: True

Property	Value
Formula	C2HO
Molecular weight	41.029
IUPAC name	ethynol
$\mu_{a,b,c}$	2.3, 0.0, 0.0
A, B, C	∞, 10729.6013, 10729.6013
A_s, B_s, C_s	∞, 10698.4854, 10698.4854
Charge, Multiplicity	0, 2
Predicted log column density	12.627±1.486
Electronic energy	-151.86990

geom485



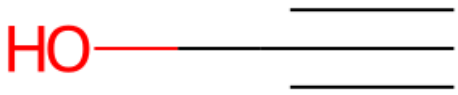
SMILES: C#CP

Nearest TMC-1 molecule (distance): CC#C (2.07)

Is DFT optimized?: True

Property	Value
Formula	C2H3P
Molecular weight	58.020
IUPAC name	ethynylphosphane
$\mu_{a,b,c}$	0.2, 0.0, 0.8
A, B, C	130981.7717, 5083.0635, 5057.5147
A_s, B_s, C_s	130601.9246, 5068.3226, 5042.8479
Charge, Multiplicity	0, 1
Predicted log column density	13.021±1.695
Electronic energy	-419.23133

geom486



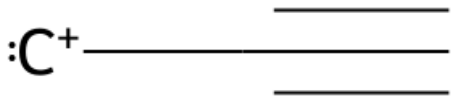
SMILES: C#CO

Nearest TMC-1 molecule (distance): CC#C (2.14)

Is DFT optimized?: True

Property	Value
Formula	C2H2O
Molecular weight	42.037
IUPAC name	ethynol
$\mu_{a,b,c}$	0.6, 1.7, 0.0
A, B, C	673635.8806, 9705.4138, 9567.5690
A_s, B_s, C_s	671682.3365, 9677.2681, 9539.8230
Charge, Multiplicity	0, 1
Predicted log column density	12.617±1.582
Electronic energy	-152.48603

geom487



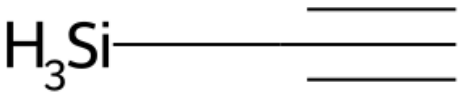
SMILES: [C+]C#C

Nearest TMC-1 molecule (distance): CC#C (2.29)

Is DFT optimized?: True

Property	Value
Formula	C3H+
Molecular weight	37.041
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	1.0, 0.0, 0.0
A, B, C	∞, 11464.5984, 11464.5984
A_s, B_s, C_s	∞, 11431.3511, 11431.3511
Charge, Multiplicity	1, 3
Predicted log column density	13.038±1.507
Electronic energy	-114.23757

geom488



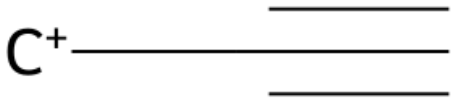
SMILES: C#C[SiH3]

Nearest TMC-1 molecule (distance): CC#C (2.31)

Is DFT optimized?: True

Property	Value
Formula	C2H4Si
Molecular weight	56.140
IUPAC name	ethynylsilane
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	85486.2297, 4793.7135, 4793.6782
A_s, B_s, C_s	85238.3196, 4779.8118, 4779.7765
Charge, Multiplicity	0, 1
Predicted log column density	11.966±1.829
Electronic energy	-367.98766

geom489



SMILES: C#C[CH2+]

Nearest TMC-1 molecule (distance): CC#C (2.31)

Is DFT optimized?: True

Property	Value
Formula	C3H3+
Molecular weight	39.057
IUPAC name	prop-1-yne
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	284250.8238, 9658.1886, 9340.8107
A_s, B_s, C_s	283426.4964, 9630.1799, 9313.7224
Charge, Multiplicity	1, 1
Predicted log column density	12.882±1.492
Electronic energy	-115.64048

geom490

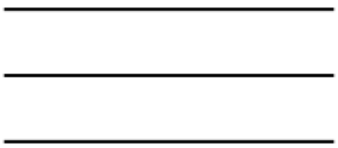
SMILES: C#COC

Nearest TMC-1 molecule (distance): CC#C (2.55)

Is DFT optimized?: True

Property	Value
Formula	C3H4O
Molecular weight	56.064
IUPAC name	methoxyethyne
$\mu_{a,b,c}$	1.5, 1.4, 0.0
A, B, C	39446.1241, 5068.4615, 4624.8205
A_s, B_s, C_s	39331.7304, 5053.7629, 4611.4086
Charge, Multiplicity	0, 1
Predicted log column density	12.907±2.454
Electronic energy	-191.77958

geom491



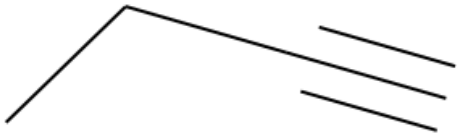
SMILES: C#C

Nearest TMC-1 molecule (distance): C#[S+] (1.97)

Is DFT optimized?: True

Property	Value
Formula	C2H2
Molecular weight	26.038
IUPAC name	acetylene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 35265.4582, 35265.4582
A_s, B_s, C_s	∞, 35163.1883, 35163.1883
Charge, Multiplicity	0, 1
Predicted log column density	13.337±1.515
Electronic energy	-77.29814

geom492



SMILES: C#CCC

Nearest TMC-1 molecule (distance): CC#C (2.96)

Is DFT optimized?: True

Property	Value
Formula	C4H6
Molecular weight	54.092
IUPAC name	but-1-yne
$\mu_{a,b,c}$	0.8, 0.2, 0.0
A, B, C	27464.0507, 4509.3489, 4069.0539
A_s, B_s, C_s	27384.4050, 4496.2718, 4057.2536
Charge, Multiplicity	0, 1
Predicted log column density	12.489±2.984
Electronic energy	-155.91556

geom493

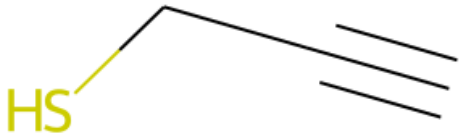
SMILES: C#CSO

Nearest TMC-1 molecule (distance): CC#C (3.03)

Is DFT optimized?: True

Property	Value
Formula	C2H2OS
Molecular weight	74.104
IUPAC name	hydroxysulfanylethyne
$\mu_{a,b,c}$	0.8, 0.5, 1.6
A, B, C	19673.3234, 3946.8877, 3320.8200
A_s, B_s, C_s	19616.2708, 3935.4417, 3311.1896
Charge, Multiplicity	0, 1
Predicted log column density	12.253±2.964
Electronic energy	-550.64365

geom494



SMILES: C#CCS

Nearest TMC-1 molecule (distance): CC#C (3.28)

Is DFT optimized?: True

Property	Value
Formula	C3H4S
Molecular weight	72.132
IUPAC name	prop-2-yne-1-thiol
$\mu_{a,b,c}$	0.9, 0.5, 0.8
A, B, C	22274.8386, 3020.0856, 2738.7481
A_s, B_s, C_s	22210.2416, 3011.3273, 2730.8057
Charge, Multiplicity	0, 1
Predicted log column density	13.742±3.416
Electronic energy	-514.77436

geom495

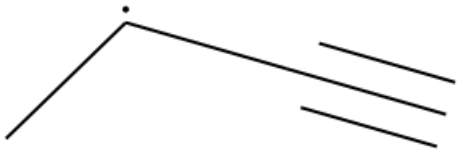
SMILES: C#CSC

Nearest TMC-1 molecule (distance): CC#C (3.49)

Is DFT optimized?: True

Property	Value
Formula	C3H4S
Molecular weight	72.132
IUPAC name	methylsulfanylethyne
$\mu_{a,b,c}$	0.7, 1.6, 0.0
A, B, C	15926.8936, 3948.4149, 3229.4312
A_s, B_s, C_s	15880.7056, 3936.9645, 3220.0658
Charge, Multiplicity	0, 1
Predicted log column density	12.888±3.789
Electronic energy	-514.77446

geom496



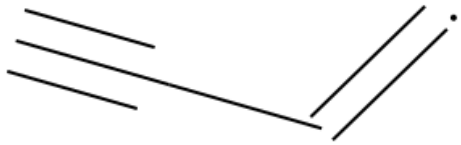
SMILES: C#C[CH]C

Nearest TMC-1 molecule (distance): [C]#C[C]=O (2.24)

Is DFT optimized?: True

Property	Value
Formula	C4H5
Molecular weight	53.084
IUPAC name	but-1-yne
$\mu_{a,b,c}$	0.6, 0.1, 0.0
A, B, C	38581.9328, 4414.5331, 4061.0331
A_s, B_s, C_s	38470.0452, 4401.7310, 4049.2561
Charge, Multiplicity	0, 2
Predicted log column density	13.017±1.861
Electronic energy	-155.26567

geom497



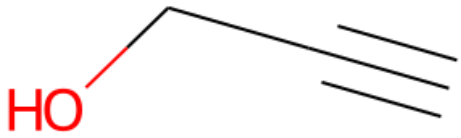
SMILES: [CH]=CC#C

Nearest TMC-1 molecule (distance): [C]#C[C]=O (2.60)

Is DFT optimized?: True

Property	Value
Formula	C4H3
Molecular weight	51.068
IUPAC name	but-1-en-3-yne
$\mu_{a,b,c}$	0.3, 0.4, 0.0
A, B, C	49704.5235, 5101.8670, 4626.9398
A_s, B_s, C_s	49560.3804, 5087.0716, 4613.5217
Charge, Multiplicity	0, 2
Predicted log column density	12.362±1.700
Electronic energy	-153.98745

geom498



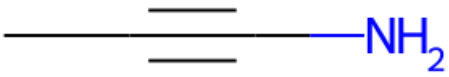
SMILES: C#CCO

Nearest TMC-1 molecule (distance): CC#C (3.52)

Is DFT optimized?: True

Property	Value
Formula	C3H4O
Molecular weight	56.064
IUPAC name	prop-2-yn-1-ol
$\mu_{a,b,c}$	1.1, 0.2, 1.3
A, B, C	33282.6162, 4641.4106, 4213.1093
A_s, B_s, C_s	33186.0966, 4627.9505, 4200.8912
Charge, Multiplicity	0, 1
Predicted log column density	12.389±3.105
Electronic energy	-191.79723

geom499



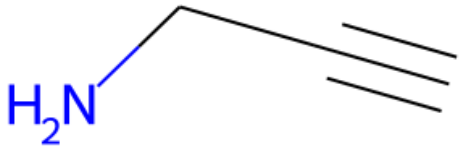
SMILES: CC#CN

Nearest TMC-1 molecule (distance): CC#N (2.96)

Is DFT optimized?: True

Property	Value
Formula	C3H5N
Molecular weight	55.080
IUPAC name	prop-1-yn-1-amine
$\mu_{a,b,c}$	0.6, 0.0, 1.3
A, B, C	104948.5368, 3462.8031, 3436.0287
A_s, B_s, C_s	104644.1861, 3452.7610, 3426.0642
Charge, Multiplicity	0, 1
Predicted log column density	12.350±1.803
Electronic energy	-171.94856

geom500



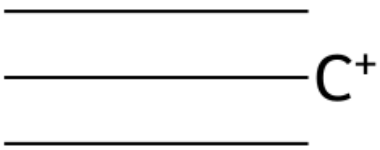
SMILES: C#CCN

Nearest TMC-1 molecule (distance): CC#C (3.70)

Is DFT optimized?: True

Property	Value
Formula	C3H5N
Molecular weight	55.080
IUPAC name	prop-2-yn-1-amine
$\mu_{a,b,c}$	0.8, 0.8, 1.3
A, B, C	31565.4390, 4592.9528, 4150.9300
A_s, B_s, C_s	31473.8992, 4579.6333, 4138.8923
Charge, Multiplicity	0, 1
Predicted log column density	11.648±2.759
Electronic energy	-171.93762

geom501



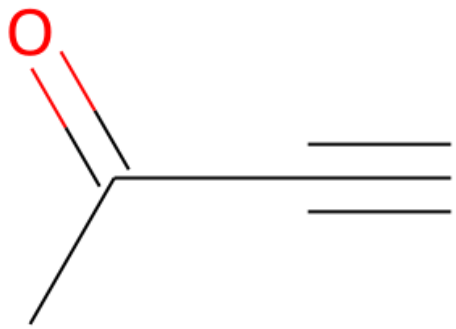
SMILES: [C+]#C

Nearest TMC-1 molecule (distance): C#[S+] (0.64)

Is DFT optimized?: False

Property	Value
Formula	C2H+
Molecular weight	25.030
IUPAC name	ethyne
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	∞, 45148.7718, 45148.7718
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 1
Predicted log column density	13.028±1.263
Electronic energy	-76.04522

geom502



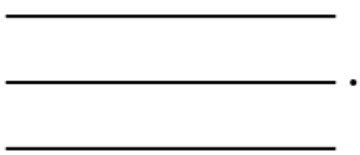
SMILES: C#CC(C)=O

Nearest TMC-1 molecule (distance): CC#C (3.98)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	but-3-yn-2-one
$\mu_{a,b,c}$	1.4, 2.9, 0.0
A, B, C	10336.4646, 3984.6658, 2928.3872
A_s, B_s, C_s	10306.4888, 3973.1103, 2919.8949
Charge, Multiplicity	0, 1
Predicted log column density	11.071±3.678
Electronic energy	-229.89860

geom503



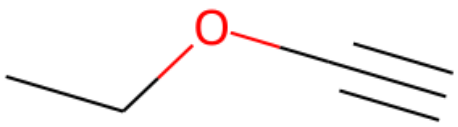
SMILES: [C]#C

Nearest TMC-1 molecule (distance): C#[S+] (0.42)

Is DFT optimized?: True

Property	Value
Formula	C2H
Molecular weight	25.030
IUPAC name	acetylene
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	∞, 44028.2496, 44028.2496
A_s, B_s, C_s	∞, 43900.5677, 43900.5677
Charge, Multiplicity	0, 2
Predicted log column density	12.946±1.148
Electronic energy	-76.57591

geom504



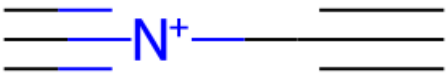
SMILES: C#COCC

Nearest TMC-1 molecule (distance): CC#C (4.00)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	ethynoxyethane
$\mu_{a,b,c}$	1.8, 1.4, 0.0
A, B, C	30693.6097, 2484.3953, 2367.1254
A_s, B_s, C_s	30604.5982, 2477.1906, 2360.2607
Charge, Multiplicity	0, 1
Predicted log column density	11.973±4.004
Electronic energy	-231.08871

geom505



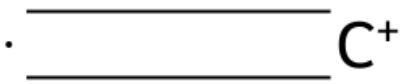
SMILES: C#C[N+]#C

Nearest TMC-1 molecule (distance): C#CC#[NH+] (3.82)

Is DFT optimized?: True

Property	Value
Formula	C3H2N+
Molecular weight	52.056
IUPAC name	ethynyl(methylidyne)azanium
$\mu_{a,b,c}$	2.7, 0.0, 0.0
A, B, C	∞, 4654.5881, 4654.5881
A_s, B_s, C_s	∞, 4641.0897, 4641.0897
Charge, Multiplicity	1, 1
Predicted log column density	13.117±2.021
Electronic energy	-169.77491

geom506



SMILES: [CH]=[CH+]

Nearest TMC-1 molecule (distance): C#[S+] (0.44)

Is DFT optimized?: True

Property	Value
Formula	C2H2+
Molecular weight	26.038
IUPAC name	ethene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 33183.5264, 33183.5264
A_s, B_s, C_s	∞, 33087.2942, 33087.2942
Charge, Multiplicity	1, 2
Predicted log column density	13.055±1.162
Electronic energy	-76.88948

geom507

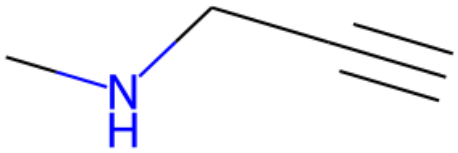
SMILES: CC#[N+]C

Nearest TMC-1 molecule (distance): [C]#N (3.36)

Is DFT optimized?: True

Property	Value
Formula	C3H6N+
Molecular weight	56.088
IUPAC name	N-methylacetonitrilium
$\mu_{a,b,c}$	0.5, 0.0, 0.0
A, B, C	78004.7791, 3538.7304, 3538.7130
A_s, B_s, C_s	77778.5652, 3528.4681, 3528.4507
Charge, Multiplicity	1, 1
Predicted log column density	13.162±1.984
Electronic energy	-172.34048

geom508



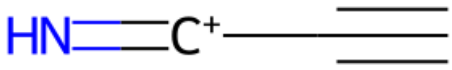
SMILES: C#CCNC

Nearest TMC-1 molecule (distance): CC#C (4.10)

Is DFT optimized?: True

Property	Value
Formula	C4H7N
Molecular weight	69.107
IUPAC name	N-methylprop-2-yn-1-amine
$\mu_{a,b,c}$	0.7, 0.4, 1.1
A, B, C	26684.8593, 2335.4399, 2216.9758
A_s, B_s, C_s	26607.4732, 2328.6671, 2210.5466
Charge, Multiplicity	0, 1
Predicted log column density	14.139±4.338
Electronic energy	-211.23430

geom509



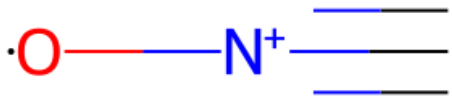
SMILES: C#C[C+]=N

Nearest TMC-1 molecule (distance): C#CC#[NH+] (3.03)

Is DFT optimized?: True

Property	Value
Formula	C3H2N+
Molecular weight	52.056
IUPAC name	prop-2-ynenitrilium
$\mu_{a,b,c}$	1.2, 0.0, 0.0
A, B, C	50321862011.2794, 4313.1276, 4313.1273
A_s, B_s, C_s	50175928611.4467, 4300.6196, 4300.6193
Charge, Multiplicity	1, 1
Predicted log column density	14.446±2.057
Electronic energy	-169.80304

geom510



SMILES: C#[N+][O]

Nearest TMC-1 molecule (distance): C#[S+] (2.68)

Is DFT optimized?: True

Property	Value
Formula	CHNO+
Molecular weight	43.025
IUPAC name	N-methylidenehydroxylamine
$\mu_{a,b,c}$	4.4, 0.0, 0.0
A, B, C	∞, 11417.7918, 11417.7918
A_s, B_s, C_s	∞, 11384.6802, 11384.6802
Charge, Multiplicity	1, 2
Predicted log column density	12.685±1.947
Electronic energy	-168.12298

geom511

SMILES: C#[SH]

Nearest TMC-1 molecule (distance): C#[S+] (1.35)

Is DFT optimized?: True

Property	Value
Formula	CH2S
Molecular weight	46.094
IUPAC name	
$\mu_{a,b,c}$	1.6, 2.7, 0.0
A, B, C	193180.2162, 18680.4819, 17033.3656
A_s, B_s, C_s	192619.9936, 18626.3085, 16983.9688
Charge, Multiplicity	0, 1
Predicted log column density	13.839±2.052
Electronic energy	-437.34246

geom512

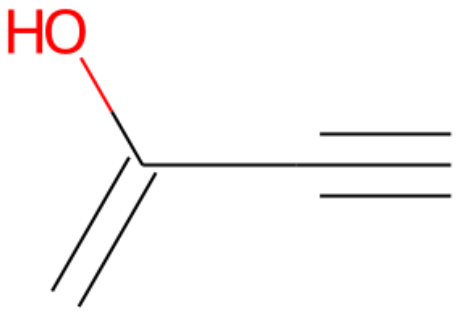
SMILES: [CH]=O

Nearest TMC-1 molecule (distance): C#[S+] (1.29)

Is DFT optimized?: True

Property	Value
Formula	CHO
Molecular weight	29.018
IUPAC name	formaldehyde
$\mu_{a,b,c}$	0.0, 1.6, 0.9
A, B, C	711651.5829, 44696.1720, 42054.8635
A_s, B_s, C_s	709587.7933, 44566.5531, 41932.9044
Charge, Multiplicity	0, 2
Predicted log column density	12.391±1.372
Electronic energy	-113.81536

geom513



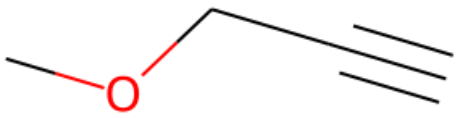
SMILES: C#CC(=C)O

Nearest TMC-1 molecule (distance): CC#C (4.40)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	but-1-en-3-yn-2-ol
$\mu_{a,b,c}$	1.8, 0.4, 0.0
A, B, C	10544.7276, 4116.2056, 2960.5392
A_s, B_s, C_s	10514.1479, 4104.2687, 2951.9536
Charge, Multiplicity	0, 1
Predicted log column density	10.590±3.238
Electronic energy	-229.87611

geom514



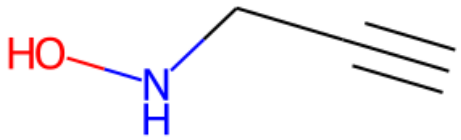
SMILES: C#CCOC

Nearest TMC-1 molecule (distance): CC#C (4.42)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	3-methoxyprop-1-yne
$\mu_{a,b,c}$	0.9, 1.5, 0.0
A, B, C	29339.0943, 2421.5991, 2302.2731
A_s, B_s, C_s	29254.0109, 2414.5765, 2295.5965
Charge, Multiplicity	0, 1
Predicted log column density	14.368±3.848
Electronic energy	-231.08866

geom515



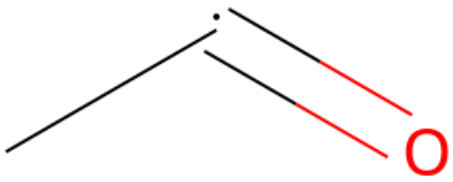
SMILES: C#CCNO

Nearest TMC-1 molecule (distance): CC#C (4.42)

Is DFT optimized?: True

Property	Value
Formula	C3H5NO
Molecular weight	71.079
IUPAC name	N-prop-2-ynylhydroxylamine
$\mu_{a,b,c}$	0.2, 0.1, 0.2
A, B, C	29349.4741, 2361.7651, 2243.2501
A_s, B_s, C_s	29264.3606, 2354.9160, 2236.7446
Charge, Multiplicity	0, 1
Predicted log column density	11.460±4.233
Electronic energy	-247.08500

geom516



SMILES: C[C]=O

Nearest TMC-1 molecule (distance): O=C=[OH+] (2.47)

Is DFT optimized?: True

Property	Value
Formula	C2H3O
Molecular weight	43.045
IUPAC name	acetaldehyde
$\mu_{a,b,c}$	2.7, 0.2, 0.0
A, B, C	83722.8600, 9954.3091, 9416.1335
A_s, B_s, C_s	83480.0637, 9925.4416, 9388.8267
Charge, Multiplicity	0, 2
Predicted log column density	11.894±1.524
Electronic energy	-153.13390

geom517

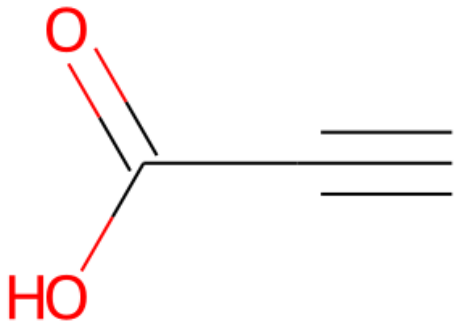
SMILES: [CH]=S

Nearest TMC-1 molecule (distance): C#[S+] (1.49)

Is DFT optimized?: True

Property	Value
Formula	CHS
Molecular weight	45.086
IUPAC name	methanethione
$\mu_{a,b,c}$	1.2, 0.0, 0.0
A, B, C	∞, 19682.7795, 19682.7795
A_s, B_s, C_s	∞, 19625.6995, 19625.6995
Charge, Multiplicity	0, 2
Predicted log column density	14.051±1.546
Electronic energy	-436.75395

geom518



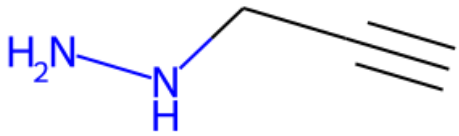
SMILES: C#CC(=O)O

Nearest TMC-1 molecule (distance): C#[C]=O (4.45)

Is DFT optimized?: True

Property	Value
Formula	C3H2O2
Molecular weight	70.047
IUPAC name	prop-2-ynoic acid
$\mu_{a,b,c}$	3.8, 2.9, 0.0
A, B, C	11733.0043, 4181.9006, 3083.0381
A_s, B_s, C_s	11698.9786, 4169.7731, 3074.0973
Charge, Multiplicity	0, 1
Predicted log column density	10.204±3.460
Electronic energy	-265.80866

geom519



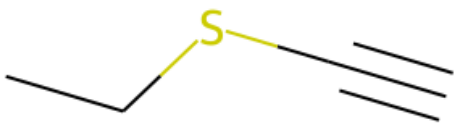
SMILES: C#CCNN

Nearest TMC-1 molecule (distance): CC#C (4.57)

Is DFT optimized?: True

Property	Value
Formula	C3H6N2
Molecular weight	70.095
IUPAC name	prop-2-ynylhydrazine
$\mu_{a,b,c}$	0.3, 1.8, 0.6
A, B, C	28018.2590, 2350.7811, 2233.2327
A_s, B_s, C_s	27937.0060, 2343.9638, 2226.7563
Charge, Multiplicity	0, 1
Predicted log column density	12.727±4.706
Electronic energy	-227.24058

geom520



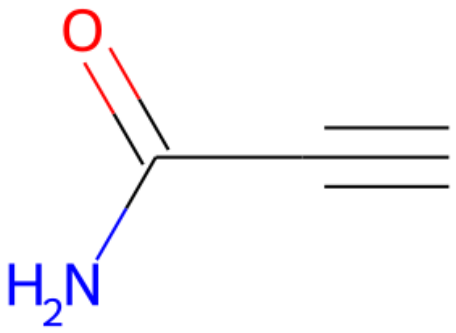
SMILES: C#CSCC

Nearest TMC-1 molecule (distance): CC#C (4.59)

Is DFT optimized?: True

Property	Value
Formula	C4H6S
Molecular weight	86.159
IUPAC name	ethynylsulfanylethane
$\mu_{a,b,c}$	1.2, 1.5, 0.0
A, B, C	13619.7505, 2051.1411, 1823.5486
A_s, B_s, C_s	13580.2532, 2045.1928, 1818.2603
Charge, Multiplicity	0, 1
Predicted log column density	11.334±4.516
Electronic energy	-554.07901

geom521



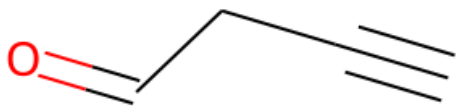
SMILES: C#CC(N)=O

Nearest TMC-1 molecule (distance): C#[C]=O (4.56)

Is DFT optimized?: True

Property	Value
Formula	C3H3NO
Molecular weight	69.063
IUPAC name	prop-2-ynamide
$\mu_{a,b,c}$	1.2, 4.0, 0.0
A, B, C	11405.4584, 4121.9234, 3027.7111
A_s, B_s, C_s	11372.3826, 4109.9698, 3018.9307
Charge, Multiplicity	0, 1
Predicted log column density	11.494±3.371
Electronic energy	-245.95551

geom522



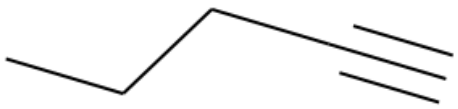
SMILES: C#CCC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (2.80)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	but-3-ynal
$\mu_{a,b,c}$	2.3, 0.0, 0.4
A, B, C	29198.6494, 2473.1569, 2318.5668
A_s, B_s, C_s	29113.9733, 2465.9848, 2311.8430
Charge, Multiplicity	0, 1
Predicted log column density	9.741±2.398
Electronic energy	-229.89294

geom523



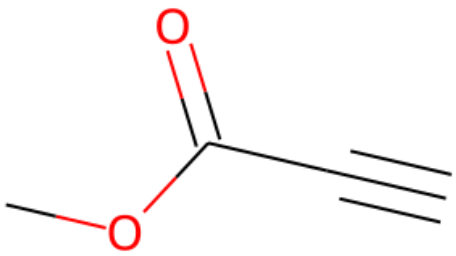
SMILES: C#CCCC

Nearest TMC-1 molecule (distance): CC#C (4.82)

Is DFT optimized?: True

Property	Value
Formula	C5H8
Molecular weight	68.119
IUPAC name	pent-1-yne
$\mu_{a,b,c}$	-, -, -
A, B, C	23524.4911, 2220.6892, 2108.6823
A_s, B_s, C_s	23456.2701, 2214.2492, 2102.5672
Charge, Multiplicity	0, 1
Predicted log column density	11.915±3.552
Electronic energy	-

geom524



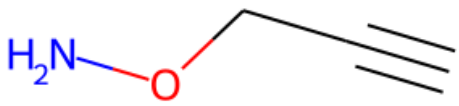
SMILES: C#CC(=O)OC

Nearest TMC-1 molecule (distance): CC#C (4.84)

Is DFT optimized?: True

Property	Value
Formula	C4H4O2
Molecular weight	84.074
IUPAC name	methyl prop-2-ynoate
$\mu_{a,b,c}$	0.2, 2.0, 0.0
A, B, C	9545.8459, 2431.6548, 1962.1058
A_s, B_s, C_s	9518.1629, 2424.6030, 1956.4157
Charge, Multiplicity	0, 1
Predicted log column density	12.146±4.321
Electronic energy	-305.10782

geom525



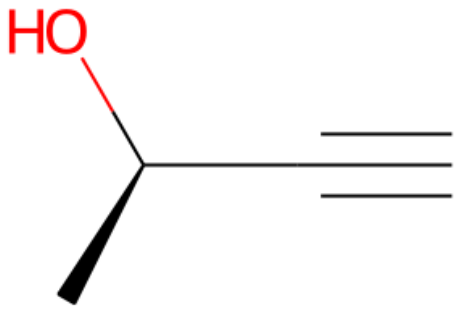
SMILES: C#CCON

Nearest TMC-1 molecule (distance): CC#C (4.87)

Is DFT optimized?: True

Property	Value
Formula	C3H5NO
Molecular weight	71.079
IUPAC name	O-prop-2-ynylhydroxylamine
$\mu_{a,b,c}$	0.9, 0.0, 0.0
A, B, C	31191.9567, 2409.1772, 2296.0258
A_s, B_s, C_s	31101.5001, 2402.1905, 2289.3674
Charge, Multiplicity	0, 1
Predicted log column density	12.195±4.287
Electronic energy	-247.07823

geom526



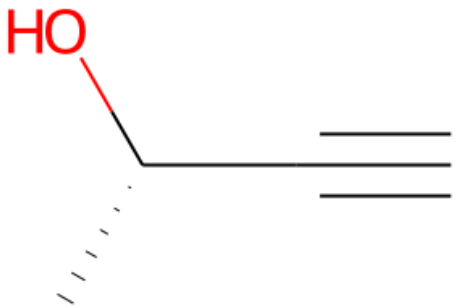
SMILES: C#C[C@@H](C)O

Nearest TMC-1 molecule (distance): CC#C (4.92)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	(2R)-but-3-yn-2-ol
$\mu_{a,b,c}$	1.0, 0.1, 1.0
A, B, C	8835.2658, 3855.1466, 2897.9734
A_s, B_s, C_s	8809.6435, 3843.9667, 2889.5692
Charge, Multiplicity	0, 1
Predicted log column density	11.926±4.509
Electronic energy	-231.10625

geom527



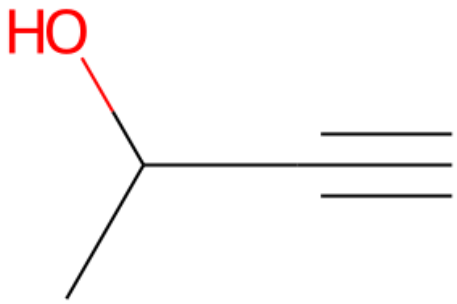
SMILES: C#C[C@H](C)O

Nearest TMC-1 molecule (distance): CC#C (4.92)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	(2S)-but-3-yn-2-ol
$\mu_{a,b,c}$	1.3, 1.5, 1.0
A, B, C	8742.1982, 3888.8454, 2904.4965
A_s, B_s, C_s	8716.8458, 3877.5677, 2896.0735
Charge, Multiplicity	0, 1
Predicted log column density	11.926±4.509
Electronic energy	-231.10303

geom528



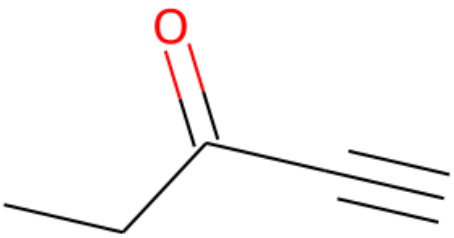
SMILES: C#CC(C)O

Nearest TMC-1 molecule (distance): CC#C (4.92)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	but-3-yn-2-ol
$\mu_{a,b,c}$	0.6, 1.3, 0.9
A, B, C	8599.9596, 3879.5932, 2911.1726
A_s, B_s, C_s	8575.0197, 3868.3423, 2902.7302
Charge, Multiplicity	0, 1
Predicted log column density	11.926±4.509
Electronic energy	-231.10600

geom529



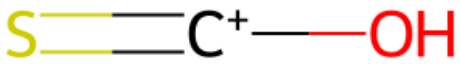
SMILES: C#CC(=O)CC

Nearest TMC-1 molecule (distance): CC#C (4.93)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	pent-1-yn-3-one
$\mu_{a,b,c}$	0.7, 3.1, 0.0
A, B, C	8665.5694, 2208.5402, 1798.9069
A_s, B_s, C_s	8640.4392, 2202.1354, 1793.6901
Charge, Multiplicity	0, 1
Predicted log column density	10.903±3.944
Electronic energy	-269.20421

geom530



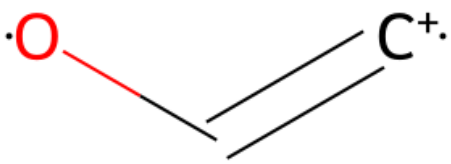
SMILES: O[C+]=S

Nearest TMC-1 molecule (distance): S=O (2.56)

Is DFT optimized?: True

Property	Value
Formula	CHOS+
Molecular weight	61.085
IUPAC name	
$\mu_{a,b,c}$	1.9, 1.8, 0.0
A, B, C	795509.6397, 5748.3736, 5707.1337
A_s, B_s, C_s	793202.6617, 5731.7033, 5690.5830
Charge, Multiplicity	1, 1
Predicted log column density	13.857±1.765
Electronic energy	-511.71053

geom531



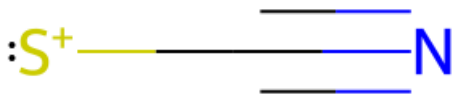
SMILES: [C+]=C[O]

Nearest TMC-1 molecule (distance): N#[NH+] (2.29)

Is DFT optimized?: True

Property	Value
Formula	C2HO+
Molecular weight	41.029
IUPAC name	ethenol
$\mu_{a,b,c}$	2.1, 2.2, 0.0
A, B, C	79799.7172, 13318.3708, 11413.4885
A_s, B_s, C_s	79568.2980, 13279.7476, 11380.3894
Charge, Multiplicity	1, 3
Predicted log column density	12.440±1.604
Electronic energy	-151.37934

geom532



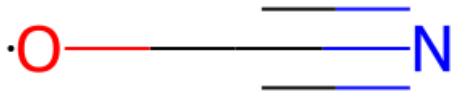
SMILES: N#C[S+]

Nearest TMC-1 molecule (distance): N#C[CH+] (0.49)

Is DFT optimized?: False

Property	Value
Formula	CNS+
Molecular weight	58.085
IUPAC name	cyanosulfanium
$\mu_{a,b,c}$	3.3, 0.0, 0.0
A, B, C	∞, 5598.7258, 5598.7258
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 3
Predicted log column density	11.647±1.250
Electronic energy	-490.52121

geom533



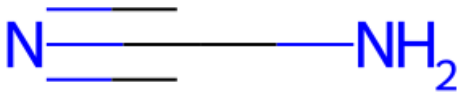
SMILES: N#C[O]

Nearest TMC-1 molecule (distance): OC#N (1.44)

Is DFT optimized?: True

Property	Value
Formula	CNO
Molecular weight	42.017
IUPAC name	cyanic acid
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	∞, 11663.8397, 11663.8397
A_s, B_s, C_s	∞, 11630.0146, 11630.0146
Charge, Multiplicity	0, 2
Predicted log column density	11.411±1.445
Electronic energy	-167.94518

geom534



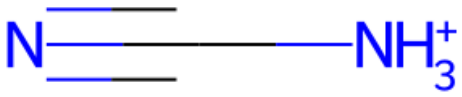
SMILES: N#CN

Nearest TMC-1 molecule (distance): N#C[CH+] (1.72)

Is DFT optimized?: True

Property	Value
Formula	CH2N2
Molecular weight	42.041
IUPAC name	cyanamide
$\mu_{a,b,c}$	4.9, 0.0, 0.0
A, B, C	332992.2824, 10161.5524, 9860.6461
A_s, B_s, C_s	332026.6048, 10132.0839, 9832.0502
Charge, Multiplicity	0, 1
Predicted log column density	11.718±1.729
Electronic energy	-148.73316

geom535



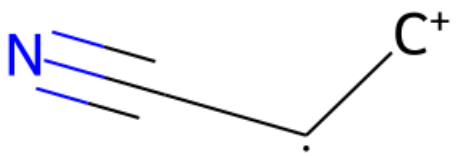
SMILES: N#C[NH3+]

Nearest TMC-1 molecule (distance): N#C[CH+] (1.72)

Is DFT optimized?: True

Property	Value
Formula	CH3N2+
Molecular weight	43.049
IUPAC name	cyanoazanium
$\mu_{a,b,c}$	7.9, 0.0, 0.0
A, B, C	179023.0901, 9115.2820, 9115.1738
A_s, B_s, C_s	178503.9231, 9088.8476, 9088.7398
Charge, Multiplicity	1, 1
Predicted log column density	9.422±2.276
Electronic energy	-149.01003

geom536



SMILES: [CH2+][CH]C#N

Nearest TMC-1 molecule (distance): N#C[CH+] (2.77)

Is DFT optimized?: True

Property	Value
Formula	C3H3N+
Molecular weight	53.064
IUPAC name	propanenitrile
$\mu_{a,b,c}$	5.5, 0.5, 0.0
A, B, C	45038.4543, 5039.9284, 4532.7068
A_s, B_s, C_s	44907.8428, 5025.3126, 4519.5619
Charge, Multiplicity	1, 2
Predicted log column density	12.024±1.656
Electronic energy	-170.38172

geom537

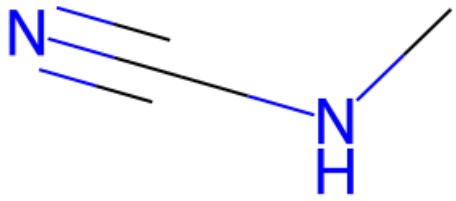
SMILES: COC#N

Nearest TMC-1 molecule (distance): CC#N (2.95)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO
Molecular weight	57.052
IUPAC name	methyl cyanate
$\mu_{a,b,c}$	4.7, 0.6, 0.0
A, B, C	40962.6506, 5238.5746, 4787.9964
A_s, B_s, C_s	40843.8589, 5223.3828, 4774.1113
Charge, Multiplicity	0, 1
Predicted log column density	12.911±2.647
Electronic energy	-207.87496

geom538



SMILES: CNC#N

Nearest TMC-1 molecule (distance): OC#N (3.08)

Is DFT optimized?: True

Property	Value
Formula	C2H4N2
Molecular weight	56.068
IUPAC name	methylcyanamide
$\mu_{a,b,c}$	5.0, 1.5, 0.0
A, B, C	38204.5293, 4856.1876, 4429.8344
A_s, B_s, C_s	38093.7362, 4842.1046, 4416.9879
Charge, Multiplicity	0, 1
Predicted log column density	12.343±3.439
Electronic energy	-188.02916

geom539

SMILES: N#CS[O-]

Nearest TMC-1 molecule (distance): N#C[CH+] (2.66)

Is DFT optimized?: True

Property	Value
Formula	CNOS-
Molecular weight	74.084
IUPAC name	oxido thiocyanate
$\mu_{a,b,c}$	0.2, 2.4, 0.0
A, B, C	27455.4343, 3888.6262, 3406.1931
A_s, B_s, C_s	27375.8135, 3877.3492, 3396.3151
Charge, Multiplicity	-1, 1
Predicted log column density	11.252±3.355
Electronic energy	-566.19227

geom540

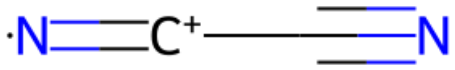
SMILES: N#CSO

Nearest TMC-1 molecule (distance): OC#N (2.72)

Is DFT optimized?: True

Property	Value
Formula	CHNOS
Molecular weight	75.092
IUPAC name	hydroxy thiocyanate
$\mu_{a,b,c}$	4.3, 1.6, 0.0
A, B, C	19184.8613, 4193.4056, 3441.2276
A_s, B_s, C_s	19129.2252, 4181.2447, 3431.2480
Charge, Multiplicity	0, 1
Predicted log column density	11.095±3.571
Electronic energy	-566.72298

geom541



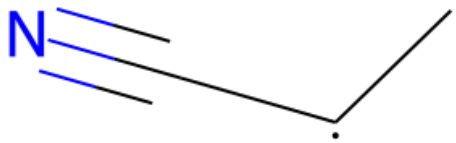
SMILES: [N]=[C+]C#N

Nearest TMC-1 molecule (distance): N#C[CH+] (2.40)

Is DFT optimized?: True

Property	Value
Formula	C2N2+
Molecular weight	52.036
IUPAC name	2-iminoacetonitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 4661.9658, 4661.9658
A_s, B_s, C_s	∞, 4648.4461, 4648.4461
Charge, Multiplicity	1, 2
Predicted log column density	12.450±1.613
Electronic energy	-185.10128

geom542



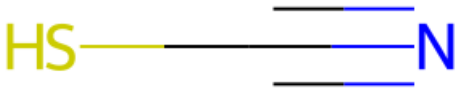
SMILES: C[CH]C#N

Nearest TMC-1 molecule (distance): [CH2]C#N (3.48)

Is DFT optimized?: True

Property	Value
Formula	C3H4N
Molecular weight	54.072
IUPAC name	propanenitrile
$\mu_{a,b,c}$	4.1, 0.9, 0.0
A, B, C	39068.9447, 4574.6337, 4201.7954
A_s, B_s, C_s	38955.6448, 4561.3672, 4189.6102
Charge, Multiplicity	0, 2
Predicted log column density	12.991±1.814
Electronic energy	-171.35631

geom543



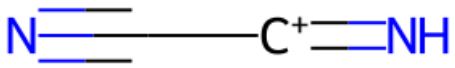
SMILES: N#CS

Nearest TMC-1 molecule (distance): N#C[CH+] (2.95)

Is DFT optimized?: True

Property	Value
Formula	CHNS
Molecular weight	59.093
IUPAC name	thiocyanic acid
$\mu_{a,b,c}$	3.4, 1.1, 0.0
A, B, C	289847.1155, 5759.1418, 5646.9394
A_s, B_s, C_s	289006.5588, 5742.4403, 5630.5633
Charge, Multiplicity	0, 1
Predicted log column density	13.270±3.054
Electronic energy	-491.55986

geom544



SMILES: N#C[C+]=N

Nearest TMC-1 molecule (distance): N#C[CH+] (2.83)

Is DFT optimized?: True

Property	Value
Formula	C2HN2+
Molecular weight	53.044
IUPAC name	2-iminoacetonitrile
$\mu_{a,b,c}$	6.1, 0.0, 0.0
A, B, C	5235190999.3664, 4426.7991, 4426.7958
A_s, B_s, C_s	5220008945.4682, 4413.9614, 4413.9581
Charge, Multiplicity	1, 1
Predicted log column density	13.648±1.995
Electronic energy	-185.84061

geom545

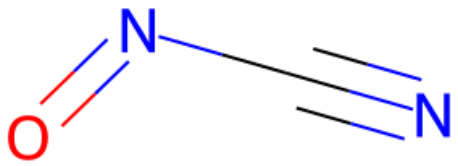
SMILES: N#CC=O

Nearest TMC-1 molecule (distance): N#C[CH+] (3.79)

Is DFT optimized?: True

Property	Value
Formula	C2HNO
Molecular weight	55.036
IUPAC name	formyl cyanide
$\mu_{a,b,c}$	1.1, 2.3, 0.0
A, B, C	66802.3357, 5005.5126, 4656.5935
A_s, B_s, C_s	66608.6089, 4990.9966, 4643.0893
Charge, Multiplicity	0, 1
Predicted log column density	11.281±1.815
Electronic energy	-206.66762

geom546



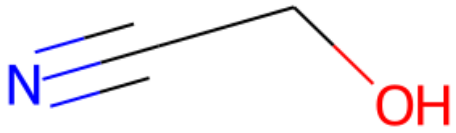
SMILES: N#CN=O

Nearest TMC-1 molecule (distance): [C]#NC#N (2.47)

Is DFT optimized?: True

Property	Value
Formula	CN2O
Molecular weight	56.024
IUPAC name	oxocyanamide
$\mu_{a,b,c}$	1.1, 0.3, 0.0
A, B, C	83463.7618, 5388.2479, 5061.4907
A_s, B_s, C_s	83221.7169, 5372.6220, 5046.8124
Charge, Multiplicity	0, 1
Predicted log column density	11.461±2.291
Electronic energy	-222.61324

geom547



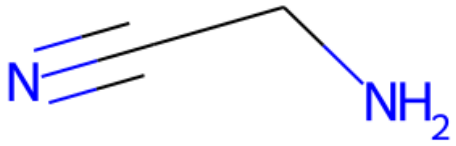
SMILES: N#CCO

Nearest TMC-1 molecule (distance): OC#N (3.24)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO
Molecular weight	57.052
IUPAC name	2-hydroxyacetonitrile
$\mu_{a,b,c}$	2.4, 1.4, 1.4
A, B, C	34004.7616, 4807.2915, 4368.7560
A_s, B_s, C_s	33906.1478, 4793.3503, 4356.0866
Charge, Multiplicity	0, 1
Predicted log column density	11.093±2.909
Electronic energy	-207.89047

geom548



SMILES: N#CCN

Nearest TMC-1 molecule (distance): OC#N (3.67)

Is DFT optimized?: True

Property	Value
Formula	C2H4N2
Molecular weight	56.068
IUPAC name	2-aminoacetonitrile
$\mu_{a,b,c}$	4.2, 2.0, 1.3
A, B, C	32334.5478, 4752.4228, 4301.7765
A_s, B_s, C_s	32240.7776, 4738.6408, 4289.3014
Charge, Multiplicity	0, 1
Predicted log column density	10.328±2.851
Electronic energy	-188.03286

geom549

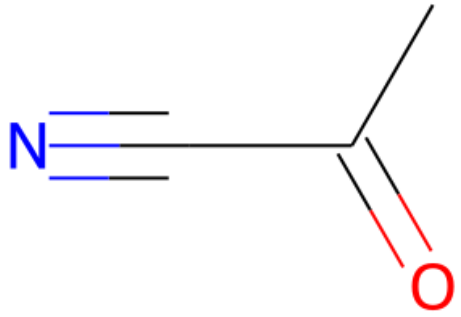
SMILES: CSC#N

Nearest TMC-1 molecule (distance): N#C[CH+] (3.65)

Is DFT optimized?: True

Property	Value
Formula	C2H3NS
Molecular weight	73.120
IUPAC name	methyl thiocyanate
$\mu_{a,b,c}$	4.2, 0.6, 0.0
A, B, C	15725.7870, 4107.7118, 3326.5365
A_s, B_s, C_s	15680.1822, 4095.7994, 3316.8895
Charge, Multiplicity	0, 1
Predicted log column density	11.746±4.282
Electronic energy	-530.86739

geom550



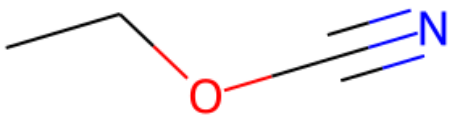
SMILES: CC(=O)C#N

Nearest TMC-1 molecule (distance): CC#N (4.25)

Is DFT optimized?: True

Property	Value
Formula	C3H3NO
Molecular weight	69.063
IUPAC name	acetyl cyanide
$\mu_{a,b,c}$	2.4, 2.7, 0.0
A, B, C	10142.8851, 4152.3833, 3001.1181
A_s, B_s, C_s	10113.4708, 4140.3414, 2992.4149
Charge, Multiplicity	0, 1
Predicted log column density	10.551±3.537
Electronic energy	-245.98699

geom551



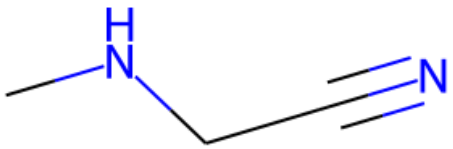
SMILES: CCOC#N

Nearest TMC-1 molecule (distance): CCC#N (3.12)

Is DFT optimized?: True

Property	Value
Formula	C3H5NO
Molecular weight	71.079
IUPAC name	ethyl cyanate
$\mu_{a,b,c}$	5.0, 0.8, 0.0
A, B, C	31091.2519, 2523.7750, 2405.4927
A_s, B_s, C_s	31001.0872, 2516.4561, 2398.5168
Charge, Multiplicity	0, 1
Predicted log column density	12.076±4.174
Electronic energy	-247.18463

geom552



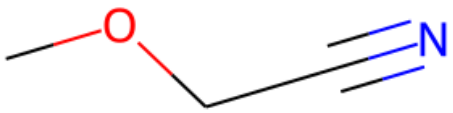
SMILES: CNCC#N

Nearest TMC-1 molecule (distance): CCC#N (3.99)

Is DFT optimized?: True

Property	Value
Formula	C3H6N2
Molecular weight	70.095
IUPAC name	2-(methylamino)acetonitrile
$\mu_{a,b,c}$	4.1, 1.5, 1.1
A, B, C	27106.1951, 2373.1849, 2254.3004
A_s, B_s, C_s	27027.5872, 2366.3027, 2247.7629
Charge, Multiplicity	0, 1
Predicted log column density	12.873±4.249
Electronic energy	-227.32942

geom553



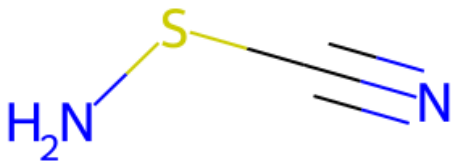
SMILES: COCC#N

Nearest TMC-1 molecule (distance): CCC#N (3.47)

Is DFT optimized?: True

Property	Value
Formula	C3H5NO
Molecular weight	71.079
IUPAC name	2-methoxyacetonitrile
$\mu_{a,b,c}$	4.3, 2.6, 0.0
A, B, C	29898.7443, 2461.6472, 2342.2092
A_s, B_s, C_s	29812.0379, 2454.5084, 2335.4168
Charge, Multiplicity	0, 1
Predicted log column density	13.087±3.699
Electronic energy	-247.18216

geom554



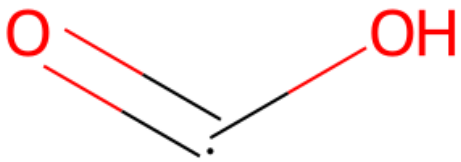
SMILES: N#CSN

Nearest TMC-1 molecule (distance): N#C[CH+] (3.57)

Is DFT optimized?: True

Property	Value
Formula	CH2N2S
Molecular weight	74.108
IUPAC name	amino thiocyanate
$\mu_{a,b,c}$	5.0, 0.3, 0.0
A, B, C	18985.6296, 3994.6372, 3362.8715
A_s, B_s, C_s	18930.5712, 3983.0528, 3353.1191
Charge, Multiplicity	0, 1
Predicted log column density	11.715±3.938
Electronic energy	-546.88361

geom555



SMILES: O=[C]O

Nearest TMC-1 molecule (distance): O=C=[OH+] (2.01)

Is DFT optimized?: True

Property	Value
Formula	CHO2
Molecular weight	45.017
IUPAC name	formic acid
$\mu_{a,b,c}$	1.5, 1.4, 0.0
A, B, C	139721.8787, 11809.5634, 10889.1881
A_s, B_s, C_s	139316.6852, 11775.3156, 10857.6095
Charge, Multiplicity	0, 2
Predicted log column density	11.250±1.576
Electronic energy	-189.03575

geom556

SMILES: N=C=S

Nearest TMC-1 molecule (distance): N=C=O (2.82)

Is DFT optimized?: False

Property	Value
Formula	CHNS
Molecular weight	59.093
IUPAC name	
$\mu_{a,b,c}$	0.6, 1.5, 1.1
A, B, C	576130.0547, 6023.0017, 5960.6873
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	15.894±2.168
Electronic energy	-491.56824

geom557

SMILES: C[N+]=C=O

Nearest TMC-1 molecule (distance): O=C=[OH+] (2.47)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO+
Molecular weight	57.052
IUPAC name	
$\mu_{a,b,c}$	3.4, 1.1, 0.0
A, B, C	79215.4392, 4358.5243, 4238.4943
A_s, B_s, C_s	78985.7145, 4345.8846, 4226.2027
Charge, Multiplicity	1, 2
Predicted log column density	11.831±1.860
Electronic energy	-207.53494

geom558

SMILES: N=C=N

Nearest TMC-1 molecule (distance): N=C=O (3.41)

Is DFT optimized?: True

Property	Value
Formula	CH2N2
Molecular weight	42.041
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 2.4
A, B, C	375057.6522, 10343.5255, 10343.0595
A_s, B_s, C_s	373969.9851, 10313.5293, 10313.0646
Charge, Multiplicity	0, 1
Predicted log column density	15.123±2.497
Electronic energy	-148.72938

geom559

SMILES: O=C=O

Nearest TMC-1 molecule (distance): O=C=S (2.60)

Is DFT optimized?: True

Property	Value
Formula	CO2
Molecular weight	44.009
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 11644.2095, 11644.2095
A_s, B_s, C_s	∞, 11610.4413, 11610.4413
Charge, Multiplicity	0, 1
Predicted log column density	10.452±1.702
Electronic energy	-188.52686

geom560

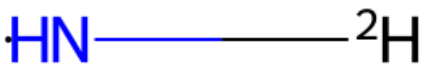
SMILES: [N−]=C=O

Nearest TMC-1 molecule (distance): O=C=[OH+] (3.55)

Is DFT optimized?: True

Property	Value
Formula	CNO-
Molecular weight	42.017
IUPAC name	isocyanate
$\mu_{a,b,c}$	1.7, 0.0, 0.0
A, B, C	∞, 11508.9489, 11508.9489
A_s, B_s, C_s	∞, 11475.5730, 11475.5730
Charge, Multiplicity	-1, 1
Predicted log column density	11.825±3.029
Electronic energy	-168.07620

geom561



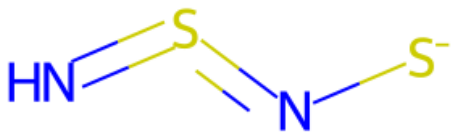
SMILES: [2H][NH]

Nearest TMC-1 molecule (distance): C=[N] (1.98)

Is DFT optimized?: True

Property	Value
Formula	H2N
Molecular weight	17.029
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 2.2
A, B, C	713445.7499, 381601.6947, 248621.2891
A_s, B_s, C_s	711376.7573, 380495.0498, 247900.2873
Charge, Multiplicity	0, 2
Predicted log column density	13.494±2.046
Electronic energy	-55.85550

geom562



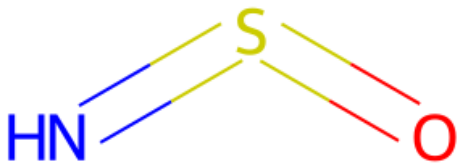
SMILES: N=S=N[S-]

Nearest TMC-1 molecule (distance): C=[N] (3.49)

Is DFT optimized?: True

Property	Value
Formula	HN2S2-
Molecular weight	93.156
IUPAC name	imino(sulfidoimino)-lambda4-sulfane
$\mu_{a,b,c}$	2.7, 3.1, 0.0
A, B, C	39822.2377, 2266.5891, 2144.5276
A_s, B_s, C_s	39706.7533, 2260.0160, 2138.3085
Charge, Multiplicity	-1, 1
Predicted log column density	14.473±2.823
Electronic energy	-906.36437

geom563



SMILES: N=S=O

Nearest TMC-1 molecule (distance): C=[N] (3.05)

Is DFT optimized?: False

Property	Value
Formula	HNOS
Molecular weight	63.081
IUPAC name	
$\mu_{a,b,c}$	0.4, 4.3, 0.9
A, B, C	45063.5096, 9387.7690, 7769.2541
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.800±3.285
Electronic energy	-528.62705

geom564

SMILES: N=O

Nearest TMC-1 molecule (distance): C=[N] (1.77)

Is DFT optimized?: True

Property	Value
Formula	HNO
Molecular weight	31.014
IUPAC name	nitroxyl
$\mu_{a,b,c}$	0.0, 1.1, 1.5
A, B, C	561624.6085, 42854.7631, 39816.5607
A_s, B_s, C_s	559995.8972, 42730.4843, 39701.0926
Charge, Multiplicity	0, 1
Predicted log column density	13.264±1.835
Electronic energy	-130.43180

geom565

SMILES: O=[O+]

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.61)

Is DFT optimized?: True

Property	Value
Formula	O2+
Molecular weight	31.998
IUPAC name	oxooxidanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 50939.9648, 50939.9648
A_s, B_s, C_s	∞, 50792.2389, 50792.2389
Charge, Multiplicity	1, 2
Predicted log column density	11.385±1.649
Electronic energy	-149.81410

geom566

SMILES: [O+]O

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.67)

Is DFT optimized?: True

Property	Value
Formula	HO2+
Molecular weight	33.006
IUPAC name	hydroxyoxidanium
$\mu_{a,b,c}$	0.0, 1.7, 2.1
A, B, C	656029.9719, 38511.2922, 36375.8976
A_s, B_s, C_s	654127.4850, 38399.6094, 36270.4075
Charge, Multiplicity	1, 3
Predicted log column density	11.346±1.618
Electronic energy	-150.43977

geom567

SMILES: N[O+]

Nearest TMC-1 molecule (distance): [C−]#[S+] (1.70)

Is DFT optimized?: True

Property	Value
Formula	H2NO+
Molecular weight	32.022
IUPAC name	aminooxidanium
$\mu_{a,b,c}$	0.0, 3.1, 0.5
A, B, C	295362.8319, 35052.3739, 31476.8772
A_s, B_s, C_s	294506.2797, 34950.7221, 31385.5943
Charge, Multiplicity	1, 3
Predicted log column density	11.622±1.546
Electronic energy	-130.65372

geom568

SMILES: [O+]=S

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.02)

Is DFT optimized?: False

Property	Value
Formula	OS+
Molecular weight	48.066
IUPAC name	oxosulfanium
$\mu_{a,b,c}$	2.5, 0.0, 0.0
A, B, C	∞, 19236.6458, 19236.6458
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	12.818±1.730
Electronic energy	-472.90044

geom569

SMILES: PP

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.31)

Is DFT optimized?: True

Property	Value
Formula	H4P2
Molecular weight	65.980
IUPAC name	phosphanylphosphane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	64978.7646, 5756.6261, 5706.0539
A_s, B_s, C_s	64790.3262, 5739.9319, 5689.5064
Charge, Multiplicity	0, 1
Predicted log column density	13.057±2.185
Electronic energy	-685.04988

geom570

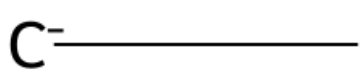
SMILES: [O−2]

Nearest TMC-1 molecule (distance): N (1.86)

Is DFT optimized?: False

Property	Value
Formula	O-2
Molecular weight	15.999
IUPAC name	oxygen(2-)
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-2, 1
Predicted log column density	12.223±1.825
Electronic energy	-74.82824

geom571



SMILES: [CH2−]C

Nearest TMC-1 molecule (distance): C=[OH+] (2.32)

Is DFT optimized?: True

Property	Value
Formula	C2H5-
Molecular weight	29.062
IUPAC name	ethane
$\mu_{a,b,c}$	4.0, 0.0, 2.2
A, B, C	97444.1546, 21732.1148, 20724.8614
A_s, B_s, C_s	97161.5666, 21669.0917, 20664.7593
Charge, Multiplicity	-1, 1
Predicted log column density	13.075±2.206
Electronic energy	-79.11393

geom572

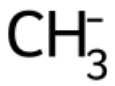
SMILES: [N−]=O

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.47)

Is DFT optimized?: True

Property	Value
Formula	NO-
Molecular weight	30.006
IUPAC name	nitroxyl anion
$\mu_{a,b,c}$	1.6, 0.0, 0.0
A, B, C	∞, 43575.0533, 43575.0533
A_s, B_s, C_s	∞, 43448.6857, 43448.6857
Charge, Multiplicity	-1, 1
Predicted log column density	12.916±2.260
Electronic energy	-129.81339

geom573



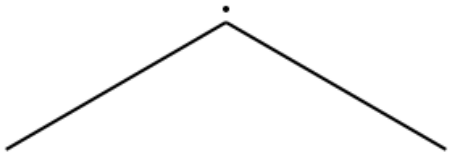
SMILES: [CH3−]

Nearest TMC-1 molecule (distance): [CH] (1.62)

Is DFT optimized?: True

Property	Value
Formula	CH3-
Molecular weight	15.035
IUPAC name	carbanide
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	282769.0859, 282664.4159, 141358.3707
A_s, B_s, C_s	281949.0555, 281844.6891, 140948.4314
Charge, Multiplicity	-1, 1
Predicted log column density	12.201±1.714
Electronic energy	-39.81528

geom574



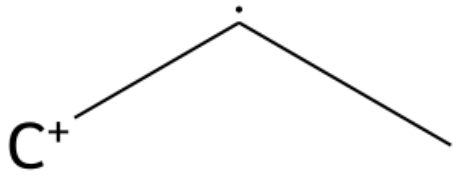
SMILES: C[CH]C

Nearest TMC-1 molecule (distance): CC=O (2.01)

Is DFT optimized?: True

Property	Value
Formula	C3H7
Molecular weight	43.089
IUPAC name	propane
$\mu_{a,b,c}$	0.0, 0.1, 0.2
A, B, C	37092.9285, 8359.4670, 7458.1712
A_s, B_s, C_s	36985.3590, 8335.2245, 7436.5425
Charge, Multiplicity	0, 2
Predicted log column density	14.449±2.146
Electronic energy	-118.43976

geom575



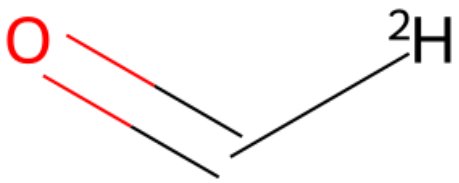
SMILES: [CH2+][CH]C

Nearest TMC-1 molecule (distance): CC=O (2.14)

Is DFT optimized?: True

Property	Value
Formula	C3H6+
Molecular weight	42.081
IUPAC name	propane
$\mu_{a,b,c}$	0.9, 0.4, 0.0
A, B, C	45616.3568, 9176.7756, 8000.2915
A_s, B_s, C_s	45484.0693, 9150.1629, 7977.0906
Charge, Multiplicity	1, 2
Predicted log column density	13.509±1.734
Electronic energy	-117.52108

geom576



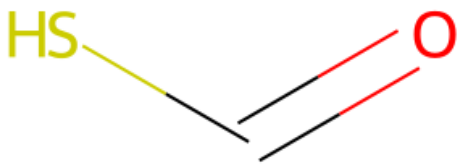
SMILES: [2H]C=O

Nearest TMC-1 molecule (distance): CC=O (2.24)

Is DFT optimized?: True

Property	Value
Formula	CH2O
Molecular weight	31.032
IUPAC name	deuterioformaldehyde
$\mu_{a,b,c}$	2.6, 0.0, 0.0
A, B, C	283499.5036, 38883.8753, 34193.9452
A_s, B_s, C_s	282677.3550, 38771.1121, 34094.7828
Charge, Multiplicity	0, 1
Predicted log column density	11.731±1.736
Electronic energy	-114.46701

geom577



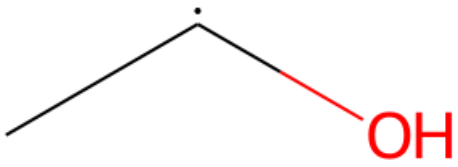
SMILES: O=CS

Nearest TMC-1 molecule (distance): CC=O (2.33)

Is DFT optimized?: True

Property	Value
Formula	CH2OS
Molecular weight	62.093
IUPAC name	methanethioic S-acid
$\mu_{a,b,c}$	1.4, 0.7, 0.0
A, B, C	61857.5519, 6117.6850, 5567.1141
A_s, B_s, C_s	61678.1649, 6099.9437, 5550.9694
Charge, Multiplicity	0, 1
Predicted log column density	13.010±2.365
Electronic energy	-512.65641

geom578



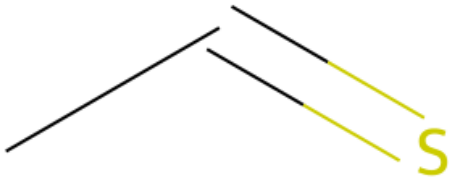
SMILES: C[CH]O

Nearest TMC-1 molecule (distance): CC=O (2.34)

Is DFT optimized?: True

Property	Value
Formula	C2H5O
Molecular weight	45.061
IUPAC name	ethanol
$\mu_{a,b,c}$	1.4, 1.2, 0.1
A, B, C	44119.6044, 9441.6961, 8252.2247
A_s, B_s, C_s	43991.6575, 9414.3152, 8228.2932
Charge, Multiplicity	0, 2
Predicted log column density	13.221±2.167
Electronic energy	-154.33298

geom579



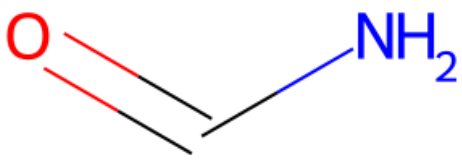
SMILES: CC=S

Nearest TMC-1 molecule (distance): CC=O (2.44)

Is DFT optimized?: True

Property	Value
Formula	C2H4S
Molecular weight	60.121
IUPAC name	ethanethial
$\mu_{a,b,c}$	2.6, 0.5, 0.0
A, B, C	47960.7212, 5755.2417, 5306.7439
A_s, B_s, C_s	47821.6351, 5738.5515, 5291.3544
Charge, Multiplicity	0, 1
Predicted log column density	15.450±2.280
Electronic energy	-476.73846

geom580



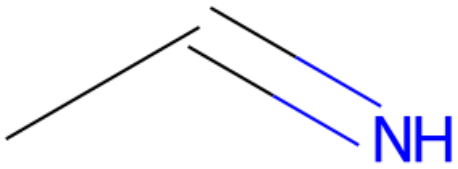
SMILES: NC=O

Nearest TMC-1 molecule (distance): CC=O (2.72)

Is DFT optimized?: True

Property	Value
Formula	CH3NO
Molecular weight	45.041
IUPAC name	formamide
$\mu_{a,b,c}$	4.1, 0.9, 0.0
A, B, C	73201.8947, 11350.7031, 9826.9679
A_s, B_s, C_s	72989.6092, 11317.7861, 9798.4697
Charge, Multiplicity	0, 1
Predicted log column density	12.349±2.607
Electronic energy	-169.84439

geom581



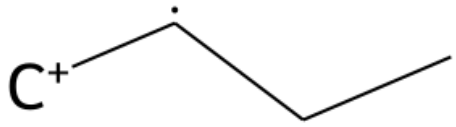
SMILES: CC=N

Nearest TMC-1 molecule (distance): CC=O (2.82)

Is DFT optimized?: True

Property	Value
Formula	C2H5N
Molecular weight	43.069
IUPAC name	ethanimine
$\mu_{a,b,c}$	2.7, 0.6, 0.0
A, B, C	49531.0608, 9846.9446, 8658.5144
A_s, B_s, C_s	49387.4207, 9818.3884, 8633.4047
Charge, Multiplicity	0, 1
Predicted log column density	14.635±2.542
Electronic energy	-133.90776

geom582



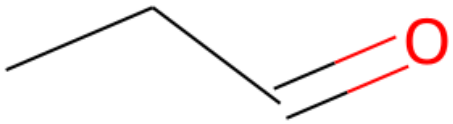
SMILES: [CH2+][CH]CC

Nearest TMC-1 molecule (distance): CC=O (2.94)

Is DFT optimized?: True

Property	Value
Formula	C4H8+
Molecular weight	56.108
IUPAC name	butane
$\mu_{a,b,c}$	3.1, 0.0, 0.4
A, B, C	28051.2315, 3927.8786, 3698.3412
A_s, B_s, C_s	27969.8830, 3916.4877, 3687.6161
Charge, Multiplicity	1, 2
Predicted log column density	11.464±3.094
Electronic energy	-156.82891

geom583



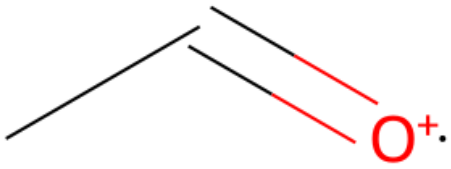
SMILES: CCC=O

Nearest TMC-1 molecule (distance): CC=O (3.00)

Is DFT optimized?: True

Property	Value
Formula	C3H6O
Molecular weight	58.080
IUPAC name	propanal
$\mu_{a,b,c}$	1.8, 2.3, 0.0
A, B, C	16761.0230, 5854.4016, 4583.0801
A_s, B_s, C_s	16712.4160, 5837.4239, 4569.7892
Charge, Multiplicity	0, 1
Predicted log column density	9.350±3.220
Electronic energy	-193.08929

geom584



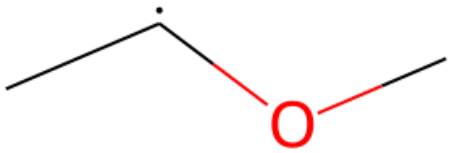
SMILES: CC=[O+]

Nearest TMC-1 molecule (distance): CC=O (3.05)

Is DFT optimized?: True

Property	Value
Formula	C2H4O+
Molecular weight	44.053
IUPAC name	ethylideneoxidanium
$\mu_{a,b,c}$	1.9, 1.9, 0.0
A, B, C	56248.9174, 10226.5378, 9154.3168
A_s, B_s, C_s	56085.7955, 10196.8808, 9127.7693
Charge, Multiplicity	1, 2
Predicted log column density	12.529±1.886
Electronic energy	-153.41123

geom585



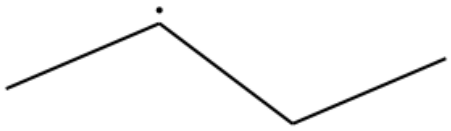
SMILES: C[CH]OC

Nearest TMC-1 molecule (distance): CC=O (3.11)

Is DFT optimized?: True

Property	Value
Formula	C3H7O
Molecular weight	59.088
IUPAC name	methoxyethane
$\mu_{a,b,c}$	0.7, 0.9, 0.4
A, B, C	34313.0254, 4174.6676, 3917.1972
A_s, B_s, C_s	34213.5176, 4162.5610, 3905.8373
Charge, Multiplicity	0, 2
Predicted log column density	14.444±3.411
Electronic energy	-193.62718

geom586



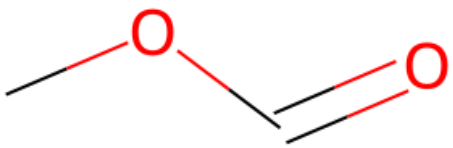
SMILES: C[CH]CC

Nearest TMC-1 molecule (distance): CC=O (3.17)

Is DFT optimized?: True

Property	Value
Formula	C4H9
Molecular weight	57.116
IUPAC name	butane
$\mu_{a,b,c}$	0.1, 0.2, 0.2
A, B, C	26658.3007, 3641.5430, 3416.8113
A_s, B_s, C_s	26580.9916, 3630.9825, 3406.9026
Charge, Multiplicity	0, 2
Predicted log column density	12.320±3.337
Electronic energy	-157.74290

geom587



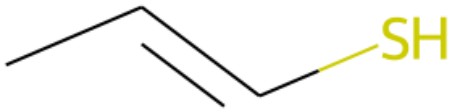
SMILES: COC=O

Nearest TMC-1 molecule (distance): CC=O (3.33)

Is DFT optimized?: True

Property	Value
Formula	C2H4O2
Molecular weight	60.052
IUPAC name	methyl formate
$\mu_{a,b,c}$	1.9, 0.7, 0.0
A, B, C	20253.7275, 6867.0850, 5300.6636
A_s, B_s, C_s	20194.9917, 6847.1704, 5285.2917
Charge, Multiplicity	0, 1
Predicted log column density	10.988±3.635
Electronic energy	-228.99860

geom588



SMILES: CC=CS

Nearest TMC-1 molecule (distance): CC=O (3.40)

Is DFT optimized?: True

Property	Value
Formula	C3H6S
Molecular weight	74.148
IUPAC name	prop-1-ene-1-thiol
$\mu_{a,b,c}$	1.4, 0.6, 0.0
A, B, C	37291.6852, 2400.1247, 2287.1904
A_s, B_s, C_s	37183.5393, 2393.1644, 2280.5576
Charge, Multiplicity	0, 1
Predicted log column density	15.184±2.913
Electronic energy	-516.03570

geom589

SMILES: [O][S+]=O

Nearest TMC-1 molecule (distance): S=O (1.64)

Is DFT optimized?: False

Property	Value
Formula	O2S+
Molecular weight	64.065
IUPAC name	hydroxy(oxo)sulfanium
$\mu_{a,b,c}$	0.0, 1.1, 1.7
A, B, C	42102.1504, 9219.7412, 7563.4572
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	12.131±1.663
Electronic energy	-548.03894

geom590

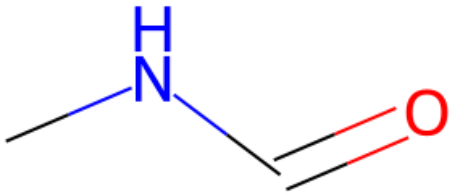
SMILES: [CH2]C

Nearest TMC-1 molecule (distance): C=S (1.65)

Is DFT optimized?: True

Property	Value
Formula	C2H5
Molecular weight	29.062
IUPAC name	ethane
$\mu_{a,b,c}$	0.3, 0.0, 0.2
A, B, C	103201.5792, 22702.0171, 21037.1896
A_s, B_s, C_s	102902.2946, 22636.1812, 20976.1818
Charge, Multiplicity	0, 2
Predicted log column density	12.348±1.500
Electronic energy	-79.13081

geom591



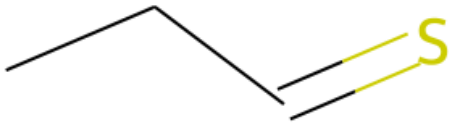
SMILES: CNC=O

Nearest TMC-1 molecule (distance): CC=O (3.46)

Is DFT optimized?: True

Property	Value
Formula	C2H5NO
Molecular weight	59.068
IUPAC name	N-methylformamide
$\mu_{a,b,c}$	3.3, 2.7, 0.0
A, B, C	19496.9187, 6283.0741, 4897.6934
A_s, B_s, C_s	19440.3776, 6264.8532, 4883.4901
Charge, Multiplicity	0, 1
Predicted log column density	13.284±3.879
Electronic energy	-209.14252

geom592



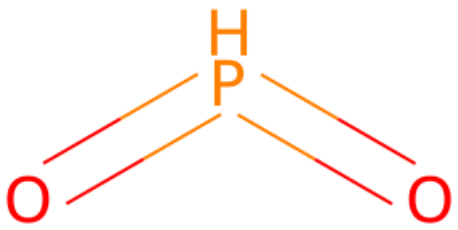
SMILES: CCC=S

Nearest TMC-1 molecule (distance): CC=O (3.50)

Is DFT optimized?: True

Property	Value
Formula	C3H6S
Molecular weight	74.148
IUPAC name	propanethial
$\mu_{a,b,c}$	2.7, 0.4, 0.7
A, B, C	22023.4209, 2701.1211, 2662.9951
A_s, B_s, C_s	21959.5530, 2693.2878, 2655.2724
Charge, Multiplicity	0, 1
Predicted log column density	13.214±3.600
Electronic energy	-516.04401

geom593



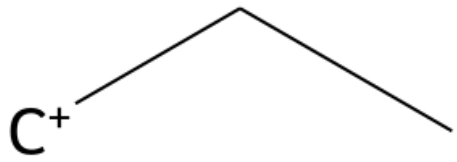
SMILES: O=[PH]=O

Nearest TMC-1 molecule (distance): S=O (2.00)

Is DFT optimized?: True

Property	Value
Formula	HO2P
Molecular weight	63.980
IUPAC name	dioxophosphanium
$\mu_{a,b,c}$	0.0, 2.9, 0.0
A, B, C	64918.9600, 8621.7994, 7610.9939
A_s, B_s, C_s	64730.6950, 8596.7962, 7588.9220
Charge, Multiplicity	0, 1
Predicted log column density	12.224±1.941
Electronic energy	-492.33908

geom594



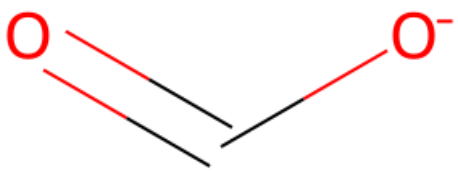
SMILES: [CH2+]CC

Nearest TMC-1 molecule (distance): S=O (2.69)

Is DFT optimized?: True

Property	Value
Formula	C3H7+
Molecular weight	43.089
IUPAC name	propane
$\mu_{a,b,c}$	0.0, 0.8, 0.0
A, B, C	40697.8760, 8543.9249, 7708.5756
A_s, B_s, C_s	40579.8522, 8519.1475, 7686.2207
Charge, Multiplicity	1, 1
Predicted log column density	12.147±2.403
Electronic energy	-118.17003

geom595



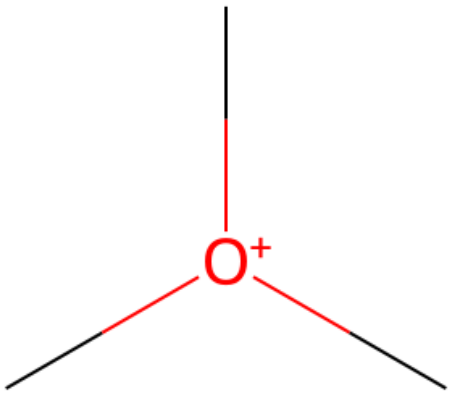
SMILES: O=C[O-]

Nearest TMC-1 molecule (distance): CC=O (3.57)

Is DFT optimized?: True

Property	Value
Formula	CHO2-
Molecular weight	45.017
IUPAC name	formate
$\mu_{a,b,c}$	0.0, 1.5, 0.0
A, B, C	107826.5266, 12212.6457, 10970.1454
A_s, B_s, C_s	107513.8296, 12177.2290, 10938.3319
Charge, Multiplicity	-1, 1
Predicted log column density	9.460±3.321
Electronic energy	-189.15212

geom596



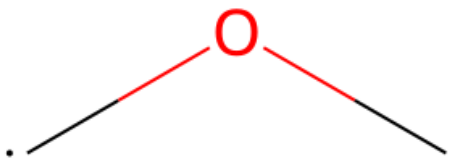
SMILES: C[O+](C)C

Nearest TMC-1 molecule (distance): CO (2.47)

Is DFT optimized?: True

Property	Value
Formula	C3H9O+
Molecular weight	61.104
IUPAC name	trimethyloxidanium
$\mu_{a,b,c}$	0.0, 0.0, 0.7
A, B, C	8522.4479, 8520.5872, 4784.1330
A_s, B_s, C_s	8497.7328, 8495.8775, 4770.2590
Charge, Multiplicity	1, 1
Predicted log column density	13.035±2.292
Electronic energy	-194.59650

geom597



SMILES: [CH2]OC

Nearest TMC-1 molecule (distance): C=S (2.71)

Is DFT optimized?: True

Property	Value
Formula	C2H5O
Molecular weight	45.061
IUPAC name	methoxymethane
$\mu_{a,b,c}$	0.9, 1.1, 0.4
A, B, C	47649.8400, 10711.0935, 9314.0901
A_s, B_s, C_s	47511.6555, 10680.0313, 9287.0792
Charge, Multiplicity	0, 2
Predicted log column density	13.333±2.411
Electronic energy	-154.31594

geom598

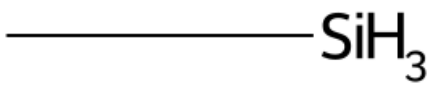
SMILES: O=O

Nearest TMC-1 molecule (distance): S=O (1.49)

Is DFT optimized?: True

Property	Value
Formula	O2
Molecular weight	31.998
IUPAC name	molecular oxygen
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 43546.6785, 43546.6785
A_s, B_s, C_s	∞, 43420.3932, 43420.3932
Charge, Multiplicity	0, 1
Predicted log column density	11.969±1.614
Electronic energy	-150.21578

geom599



SMILES: C[SiH3]

Nearest TMC-1 molecule (distance): [CH] (1.69)

Is DFT optimized?: True

Property	Value
Formula	CH6Si
Molecular weight	46.145
IUPAC name	methylsilane
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	56084.3175, 10841.0512, 10840.9458
A_s, B_s, C_s	55921.6729, 10809.6121, 10809.5070
Charge, Multiplicity	0, 1
Predicted log column density	12.155±1.788
Electronic energy	-331.17447

geom600

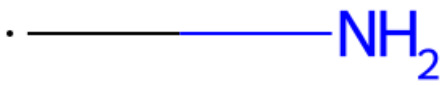
SMILES: [CH2]O

Nearest TMC-1 molecule (distance): C=S (1.68)

Is DFT optimized?: True

Property	Value
Formula	CH3O
Molecular weight	31.034
IUPAC name	methanol
$\mu_{a,b,c}$	0.2, 1.7, 0.0
A, B, C	195109.2958, 30031.9820, 26025.9643
A_s, B_s, C_s	194543.4788, 29944.8893, 25950.4890
Charge, Multiplicity	0, 2
Predicted log column density	11.809±1.531
Electronic energy	-115.02112

geom601



SMILES: [CH2]N

Nearest TMC-1 molecule (distance): C=O (1.68)

Is DFT optimized?: True

Property	Value
Formula	CH4N
Molecular weight	30.050
IUPAC name	methanamine
$\mu_{a,b,c}$	1.0, 0.0, 0.5
A, B, C	145790.1130, 27443.9087, 23784.3501
A_s, B_s, C_s	145367.3216, 27364.3214, 23715.3755
Charge, Multiplicity	0, 2
Predicted log column density	12.292±1.695
Electronic energy	-95.16949

geom602

SMILES: [S]S

Nearest TMC-1 molecule (distance): S=O (1.46)

Is DFT optimized?: True

Property	Value
Formula	HS2
Molecular weight	65.142
IUPAC name	
$\mu_{a,b,c}$	0.0, 1.4, 1.1
A, B, C	298846.6804, 7783.2199, 7585.6576
A_s, B_s, C_s	297980.0251, 7760.6486, 7563.6592
Charge, Multiplicity	0, 2
Predicted log column density	14.772±2.203
Electronic energy	-796.91180

geom603

SMILES: S=S

Nearest TMC-1 molecule (distance): S=O (1.42)

Is DFT optimized?: True

Property	Value
Formula	S2
Molecular weight	64.134
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 8725.9301, 8725.9301
A_s, B_s, C_s	∞, 8700.6249, 8700.6249
Charge, Multiplicity	0, 1
Predicted log column density	14.921±1.928
Electronic energy	-796.28089

geom604

SMILES: N=S

Nearest TMC-1 molecule (distance): S=O (1.86)

Is DFT optimized?: True

Property	Value
Formula	HNS
Molecular weight	47.082
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.1, 1.7
A, B, C	594397.0060, 19434.7851, 18819.4523
A_s, B_s, C_s	592673.2547, 19378.4243, 18764.8759
Charge, Multiplicity	0, 1
Predicted log column density	14.712±1.901
Electronic energy	-453.42478

geom605

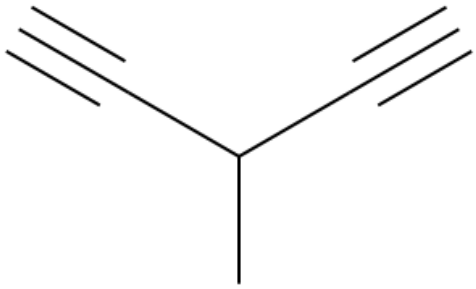
SMILES: [PH2−]

Nearest TMC-1 molecule (distance): [CH] (0.19)

Is DFT optimized?: True

Property	Value
Formula	H2P-
Molecular weight	32.990
IUPAC name	phosphanide
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	268960.3247, 233203.9234, 124904.5570
A_s, B_s, C_s	268180.3398, 232527.6321, 124542.3338
Charge, Multiplicity	-1, 1
Predicted log column density	12.608±1.442
Electronic energy	-342.52260

geom606



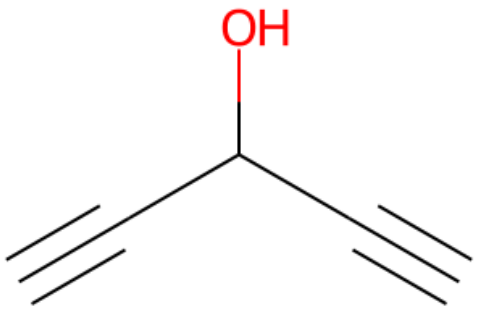
SMILES: C#CC(C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (4.72)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	3-methylpenta-1,4-diyne
$\mu_{a,b,c}$	0.0, 0.7, 0.1
A, B, C	5447.4589, 2758.5095, 1952.8905
A_s, B_s, C_s	5431.6613, 2750.5098, 1947.2271
Charge, Multiplicity	0, 1
Predicted log column density	10.495±4.351
Electronic energy	-232.02130

geom607



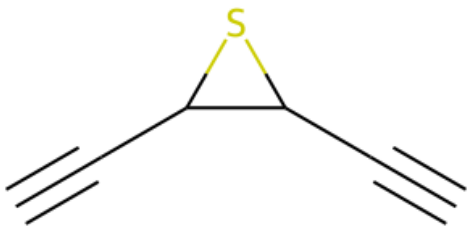
SMILES: C#CC(O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (4.87)

Is DFT optimized?: True

Property	Value
Formula	C5H4O
Molecular weight	80.086
IUPAC name	penta-1,4-diyn-3-ol
$\mu_{a,b,c}$	0.0, 1.4, 0.8
A, B, C	5652.3945, 2823.0892, 1996.9324
A_s, B_s, C_s	5636.0026, 2814.9022, 1991.1413
Charge, Multiplicity	0, 1
Predicted log column density	10.607±4.498
Electronic energy	-267.90303

geom608



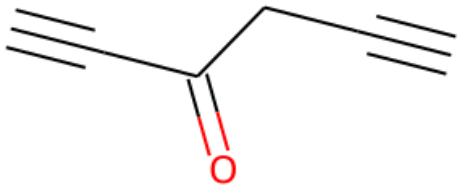
SMILES: C#CC1SC1C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (4.94)

Is DFT optimized?: True

Property	Value
Formula	C6H4S
Molecular weight	108.165
IUPAC name	2,3-diethynylthiirane
$\mu_{a,b,c}$	0.0, 1.5, 0.0
A, B, C	4118.2452, 1460.2333, 1137.9019
A_s, B_s, C_s	4106.3023, 1455.9987, 1134.6020
Charge, Multiplicity	0, 1
Predicted log column density	10.876±4.337
Electronic energy	-628.96243

geom609



SMILES: C#CCC(=O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (5.02)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	hexa-1,5-diyn-3-one
$\mu_{a,b,c}$	1.6, 2.2, 1.2
A, B, C	3750.2895, 2204.4637, 1477.6768
A_s, B_s, C_s	3739.4137, 2198.0707, 1473.3915
Charge, Multiplicity	0, 1
Predicted log column density	12.517±4.032
Electronic energy	-306.00596

geom610

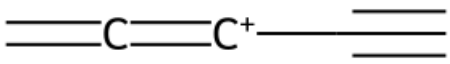
SMILES: C#CCCC#C

Nearest TMC-1 molecule (distance): [C]#CC#C (5.33)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	hexa-1,5-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	25240.8019, 1452.9129, 1397.5401
A_s, B_s, C_s	25167.6035, 1448.6994, 1393.4873
Charge, Multiplicity	0, 1
Predicted log column density	12.415±2.753
Electronic energy	-232.02675

geom611



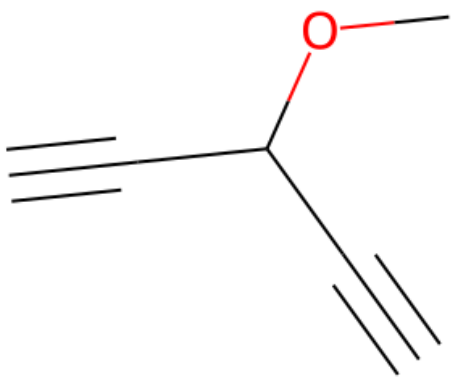
SMILES: C#C[C+]=C=C

Nearest TMC-1 molecule (distance): C#CC#[NH+] (3.69)

Is DFT optimized?: True

Property	Value
Formula	C5H3+
Molecular weight	63.079
IUPAC name	penta-1,3-diyne
$\mu_{a,b,c}$	1.4, 0.0, 0.0
A, B, C	285721.7514, 2187.3866, 2170.7685
A_s, B_s, C_s	284893.1584, 2181.0432, 2164.4732
Charge, Multiplicity	1, 1
Predicted log column density	12.927±1.800
Electronic energy	-191.78740

geom612



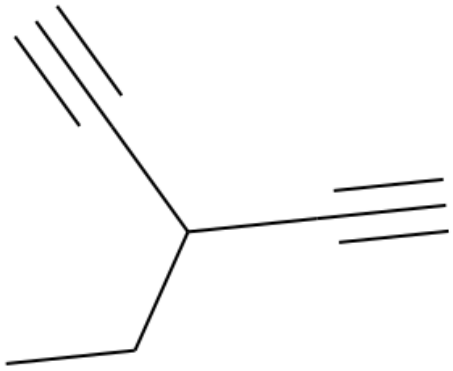
SMILES: C#CC(C#C)OC

Nearest TMC-1 molecule (distance): [C]#CC#C (5.75)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	
$\mu_{a,b,c}$	1.0, 0.6, 1.0
A, B, C	3342.9462, 2319.6426, 1433.0091
A_s, B_s, C_s	3333.2517, 2312.9156, 1428.8533
Charge, Multiplicity	0, 1
Predicted log column density	11.261±4.938
Electronic energy	-307.19397

geom613



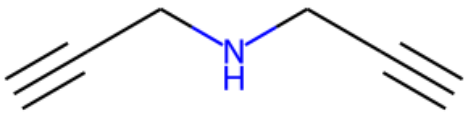
SMILES: C#CC(C#C)CC

Nearest TMC-1 molecule (distance): [C]#CC#C (5.76)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	3-ethylpenta-1,4-diyne
$\mu_{a,b,c}$	0.6, 0.6, 0.0
A, B, C	3257.5775, 2143.3570, 1364.5083
A_s, B_s, C_s	3248.1305, 2137.1412, 1360.5512
Charge, Multiplicity	0, 1
Predicted log column density	9.033±5.274
Electronic energy	-271.32565

geom614



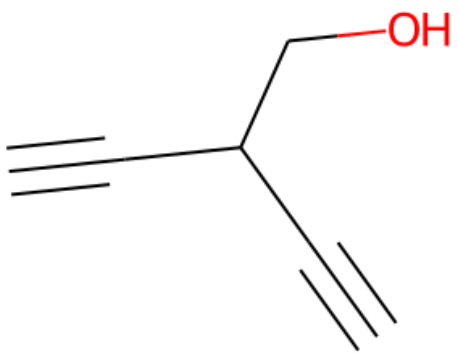
SMILES: C#CCNCC#C

Nearest TMC-1 molecule (distance): [C]#CC#C (5.83)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	N-prop-2-ynylprop-2-yn-1-amine
$\mu_{a,b,c}$	0.0, 0.8, 1.1
A, B, C	11502.5913, 1012.2702, 943.1961
A_s, B_s, C_s	11469.2338, 1009.3346, 940.4609
Charge, Multiplicity	0, 1
Predicted log column density	13.931±4.827
Electronic energy	-287.34364

geom615



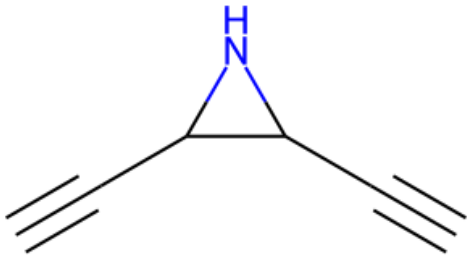
SMILES: C#CC(C#C)CO

Nearest TMC-1 molecule (distance): [C]#CC#C (5.83)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	2-ethynylbut-3-yn-1-ol
$\mu_{a,b,c}$	0.6, 1.0, 0.7
A, B, C	3392.2601, 2169.2543, 1389.2403
A_s, B_s, C_s	3382.4226, 2162.9634, 1385.2115
Charge, Multiplicity	0, 1
Predicted log column density	8.598±4.826
Electronic energy	-307.21354

geom616



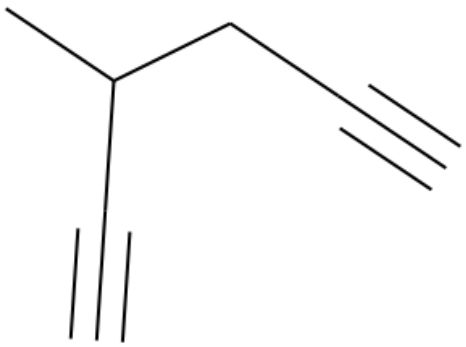
SMILES: C#CC1NC1C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (5.88)

Is DFT optimized?: True

Property	Value
Formula	C6H5N
Molecular weight	91.113
IUPAC name	2,3-diethynylaziridine
$\mu_{a,b,c}$	1.0, 0.9, 1.0
A, B, C	9267.0359, 1418.1006, 1312.8717
A_s, B_s, C_s	9240.1615, 1413.9881, 1309.0644
Charge, Multiplicity	0, 1
Predicted log column density	9.842±5.986
Electronic energy	-286.10907

geom617



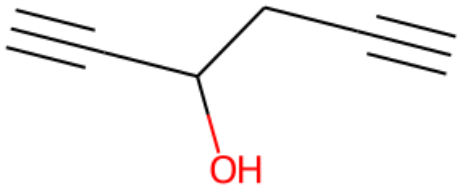
SMILES: C#CCC(C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (5.88)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	3-methylhexa-1,5-diyne
$\mu_{a,b,c}$	0.0, 0.2, 0.0
A, B, C	6682.8030, 1421.3006, 1227.6185
A_s, B_s, C_s	6663.4229, 1417.1789, 1224.0584
Charge, Multiplicity	0, 1
Predicted log column density	12.461±4.512
Electronic energy	-271.33178

geom618



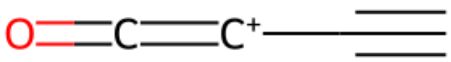
SMILES: C#CCC(O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (5.88)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hexa-1,5-diyn-3-ol
$\mu_{a,b,c}$	0.5, 1.3, 0.7
A, B, C	3606.2475, 2081.0634, 1671.7953
A_s, B_s, C_s	3595.7894, 2075.0283, 1666.9471
Charge, Multiplicity	0, 1
Predicted log column density	11.520±4.675
Electronic energy	-307.21729

geom619



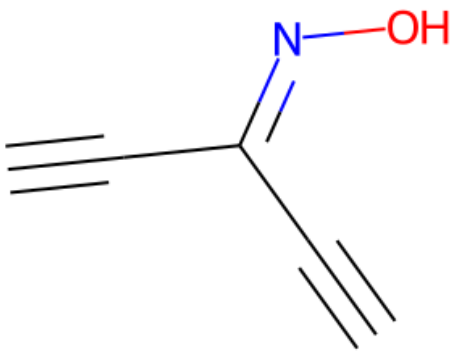
SMILES: C#C[C+]=C=O

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (3.04)

Is DFT optimized?: True

Property	Value
Formula	C4HO+
Molecular weight	65.051
IUPAC name	
$\mu_{a,b,c}$	4.8, 0.0, 0.0
A, B, C	1824814020.7529, 2225.1692, 2225.1666
A_s, B_s, C_s	1819522060.0928, 2218.7162, 2218.7136
Charge, Multiplicity	1, 1
Predicted log column density	12.084±1.720
Electronic energy	-227.64991

geom620



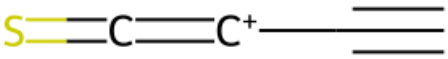
SMILES: C#CC(C#C)=NO

Nearest TMC-1 molecule (distance): [C]#CC#C (5.89)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	0.3, 0.3, 0.0
A, B, C	3806.9268, 2319.9424, 1441.4950
A_s, B_s, C_s	3795.8867, 2313.2145, 1437.3146
Charge, Multiplicity	0, 1
Predicted log column density	8.416±5.636
Electronic energy	-321.98530

geom621



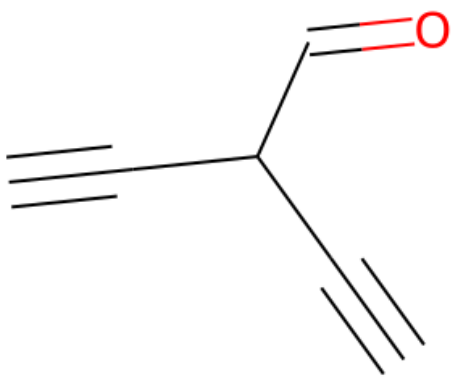
SMILES: C#C[C+]=C=S

Nearest TMC-1 molecule (distance): C#CC#[NH+] (3.35)

Is DFT optimized?: True

Property	Value
Formula	C4HS+
Molecular weight	81.119
IUPAC name	
$\mu_{a,b,c}$	3.6, 0.0, 0.0
A, B, C	1805924959.5014, 1451.9209, 1451.9198
A_s, B_s, C_s	1800687777.1188, 1447.7104, 1447.7092
Charge, Multiplicity	1, 1
Predicted log column density	14.673±2.055
Electronic energy	-550.63798

geom622



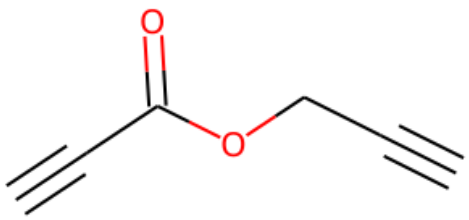
SMILES: C#CC(C#C)C=O

Nearest TMC-1 molecule (distance): [C]#CC#C (6.04)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	
$\mu_{a,b,c}$	2.3, 0.3, 0.8
A, B, C	2729.9938, 2689.6225, 1432.4999
A_s, B_s, C_s	2722.0768, 2681.8226, 1428.3457
Charge, Multiplicity	0, 1
Predicted log column density	8.250±4.420
Electronic energy	-305.99573

geom623



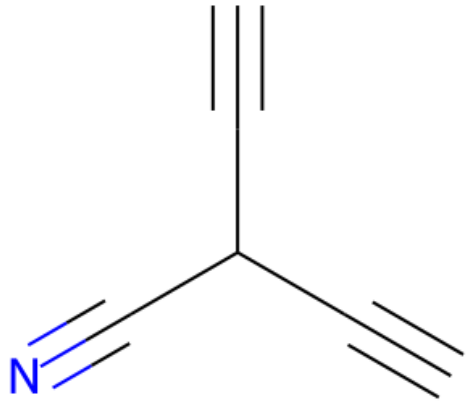
SMILES: C#CCOC(=O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (6.14)

Is DFT optimized?: True

Property	Value
Formula	C6H4O2
Molecular weight	108.096
IUPAC name	prop-2-ynyl prop-2-ynoate
$\mu_{a,b,c}$	0.1, 1.8, 0.2
A, B, C	5142.9711, 1108.3029, 1093.1841
A_s, B_s, C_s	5128.0564, 1105.0889, 1090.0138
Charge, Multiplicity	0, 1
Predicted log column density	11.615±4.704
Electronic energy	-381.21421

geom624



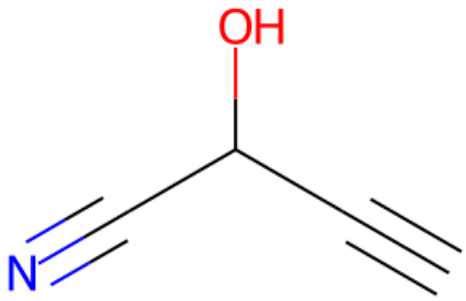
SMILES: C#CC(C#C)C#N

Nearest TMC-1 molecule (distance): [C]#CC#C (6.14)

Is DFT optimized?: True

Property	Value
Formula	C6H3N
Molecular weight	89.097
IUPAC name	
$\mu_{a,b,c}$	0.0, 3.6, 1.1
A, B, C	2838.1142, 2752.7950, 1474.5009
A_s, B_s, C_s	2829.8837, 2744.8119, 1470.2249
Charge, Multiplicity	0, 1
Predicted log column density	9.646±4.343
Electronic energy	-284.90752

geom625



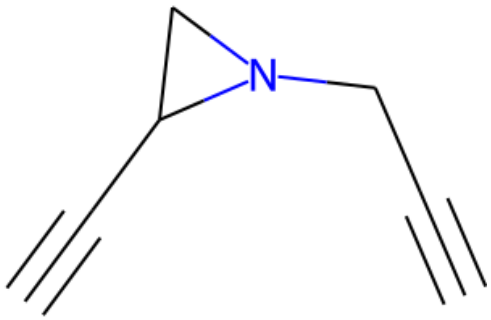
SMILES: C#CC(O)C#N

Nearest TMC-1 molecule (distance): [C]#CC#N (4.60)

Is DFT optimized?: True

Property	Value
Formula	C4H3NO
Molecular weight	81.074
IUPAC name	2-hydroxybut-3-ynenitrile
$\mu_{a,b,c}$	3.4, 0.4, 0.2
A, B, C	5720.1511, 2870.3047, 2025.5946
A_s, B_s, C_s	5703.5627, 2861.9808, 2019.7204
Charge, Multiplicity	0, 1
Predicted log column density	10.638±4.272
Electronic energy	-283.99441

geom626



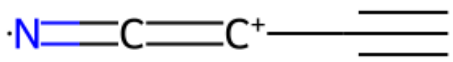
SMILES: C#CCN1CC1C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (6.20)

Is DFT optimized?: True

Property	Value
Formula	C7H7N
Molecular weight	105.140
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.6, 1.5
A, B, C	8170.2632, 933.9631, 908.1422
A_s, B_s, C_s	8146.5694, 931.2546, 905.5086
Charge, Multiplicity	0, 1
Predicted log column density	11.950±5.457
Electronic energy	-325.40364

geom627



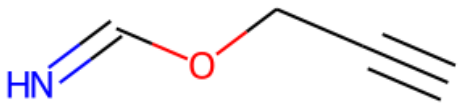
SMILES: C#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (3.22)

Is DFT optimized?: True

Property	Value
Formula	C4HN+
Molecular weight	63.059
IUPAC name	
$\mu_{a,b,c}$	6.3, 0.0, 0.0
A, B, C	567545086201.4253, 2305.4247, 2305.4247
A_s, B_s, C_s	565899205451.4412, 2298.7389, 2298.7389
Charge, Multiplicity	1, 2
Predicted log column density	13.160±1.832
Electronic energy	-207.16140

geom628



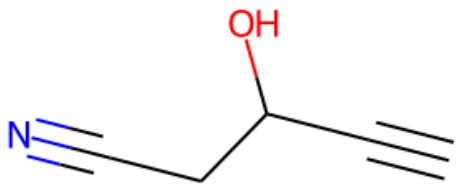
SMILES: C#CCOC=N

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.25)

Is DFT optimized?: True

Property	Value
Formula	C4H5NO
Molecular weight	83.090
IUPAC name	prop-2-ynyl methanimidate
$\mu_{a,b,c}$	2.9, 1.3, 0.0
A, B, C	21229.7290, 1555.3283, 1462.5654
A_s, B_s, C_s	21168.1628, 1550.8179, 1458.3240
Charge, Multiplicity	0, 1
Predicted log column density	15.001±4.692
Electronic energy	-285.21253

geom629



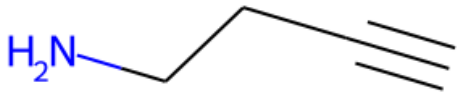
SMILES: C#CC(O)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.78)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	3-hydroxypent-4-ynenitrile
$\mu_{a,b,c}$	3.0, 0.5, 1.9
A, B, C	3808.3814, 2013.9725, 1392.1380
A_s, B_s, C_s	3797.3371, 2008.1320, 1388.1008
Charge, Multiplicity	0, 1
Predicted log column density	10.319±4.626
Electronic energy	-323.31031

geom630



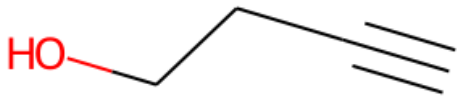
SMILES: C#CCCN

Nearest TMC-1 molecule (distance): CC#C (5.21)

Is DFT optimized?: True

Property	Value
Formula	C4H7N
Molecular weight	69.107
IUPAC name	but-3-yn-1-amine
$\mu_{a,b,c}$	0.8, 0.8, 1.1
A, B, C	25262.3009, 2254.7611, 2138.8410
A_s, B_s, C_s	25189.0403, 2248.2223, 2132.6384
Charge, Multiplicity	0, 1
Predicted log column density	9.896±3.376
Electronic energy	-211.24599

geom631



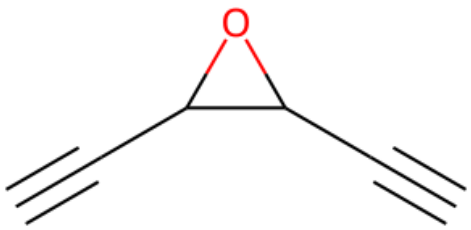
SMILES: C#CCCO

Nearest TMC-1 molecule (distance): CC#C (4.94)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	but-3-yn-1-ol
$\mu_{a,b,c}$	1.1, 0.8, 0.7
A, B, C	10595.4420, 3317.3086, 2726.9529
A_s, B_s, C_s	10564.7152, 3307.6884, 2719.0447
Charge, Multiplicity	0, 1
Predicted log column density	11.892±3.728
Electronic energy	-231.10739

geom632



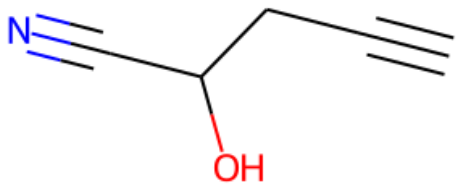
SMILES: C#CC1OC1C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (6.29)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	2,3-diethynyloxirane
$\mu_{a,b,c}$	0.0, 1.9, 0.0
A, B, C	10314.0631, 1403.5484, 1313.4418
A_s, B_s, C_s	10284.1523, 1399.4781, 1309.6329
Charge, Multiplicity	0, 1
Predicted log column density	10.038±6.550
Electronic energy	-305.96815

geom633



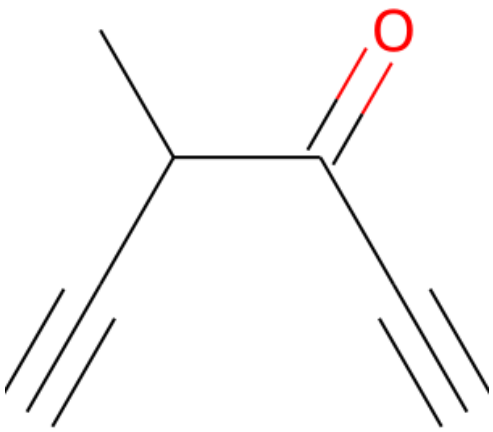
SMILES: C#CCC(O)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.88)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	2-hydroxypent-4-ynenitrile
$\mu_{a,b,c}$	2.8, 1.6, 1.3
A, B, C	3692.6907, 2088.9487, 1700.8531
A_s, B_s, C_s	3681.9819, 2082.8908, 1695.9206
Charge, Multiplicity	0, 1
Predicted log column density	11.534±4.504
Electronic energy	-323.31024

geom634



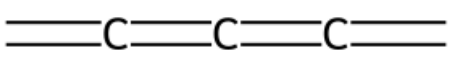
SMILES: C#CC(=O)C(C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#C (6.34)

Is DFT optimized?: True

Property	Value
Formula	C7H6O
Molecular weight	106.124
IUPAC name	
$\mu_{a,b,c}$	0.2, 2.3, 1.6
A, B, C	2569.6294, 1869.3684, 1193.3852
A_s, B_s, C_s	2562.1774, 1863.9473, 1189.9244
Charge, Multiplicity	0, 1
Predicted log column density	10.002±4.977
Electronic energy	-345.31136

geom635



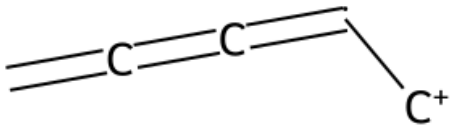
SMILES: C=C=C=C=C

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (2.58)

Is DFT optimized?: True

Property	Value
Formula	C5H4
Molecular weight	64.087
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	144904.1615, 2085.8125, 2085.8116
A_s, B_s, C_s	144483.9395, 2079.7637, 2079.7628
Charge, Multiplicity	0, 1
Predicted log column density	11.216±1.686
Electronic energy	-192.72732

geom636



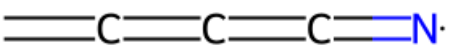
SMILES: C=C=C=[C][CH2+]

Nearest TMC-1 molecule (distance): C=C=C=[C] (3.31)

Is DFT optimized?: True

Property	Value
Formula	C5H4+
Molecular weight	64.087
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	142760.8921, 2092.9736, 2072.3350
A_s, B_s, C_s	142346.8855, 2086.9040, 2066.3253
Charge, Multiplicity	1, 2
Predicted log column density	11.286±1.473
Electronic energy	-192.41538

geom637



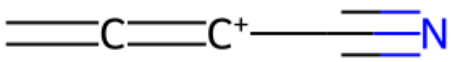
SMILES: C=C=C=C=[N]

Nearest TMC-1 molecule (distance): C=C=CC#N (3.71)

Is DFT optimized?: True

Property	Value
Formula	C4H2N
Molecular weight	64.067
IUPAC name	
$\mu_{a,b,c}$	4.7, 0.0, 0.0
A, B, C	287415.7191, 2189.5378, 2172.9840
A_s, B_s, C_s	286582.2135, 2183.1882, 2166.6823
Charge, Multiplicity	0, 2
Predicted log column density	11.674±1.542
Electronic energy	-208.17217

geom638



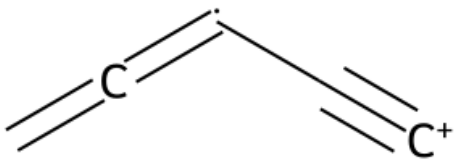
SMILES: C=C=[C+]C#N

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (3.73)

Is DFT optimized?: True

Property	Value
Formula	C4H2N+
Molecular weight	64.067
IUPAC name	but-2-ynenitrile
$\mu_{a,b,c}$	7.5, 0.0, 0.0
A, B, C	283755.4696, 2206.6658, 2189.6385
A_s, B_s, C_s	282932.5788, 2200.2664, 2183.2886
Charge, Multiplicity	1, 1
Predicted log column density	12.260±1.683
Electronic energy	-207.83140

geom639



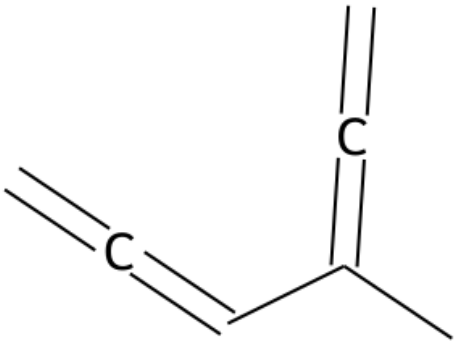
SMILES: [C+]#C[C]=C=C

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (3.63)

Is DFT optimized?: True

Property	Value
Formula	C5H2+
Molecular weight	62.071
IUPAC name	penta-1,2-dien-4-yne
$\mu_{a,b,c}$	2.5, 0.0, 0.0
A, B, C	284983.5078, 2319.8448, 2301.1164
A_s, B_s, C_s	284157.0557, 2313.1173, 2294.4431
Charge, Multiplicity	1, 2
Predicted log column density	11.432±1.644
Electronic energy	-191.05615

geom640



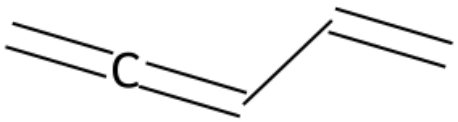
SMILES: C=C=CC(C)=C=C

Nearest TMC-1 molecule (distance): C=C=C=[C] (4.67)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.3, 0.0
A, B, C	6999.7036, 1361.9968, 1166.7516
A_s, B_s, C_s	6979.4045, 1358.0470, 1163.3680
Charge, Multiplicity	0, 1
Predicted log column density	10.539±3.171
Electronic energy	-271.35075

geom641



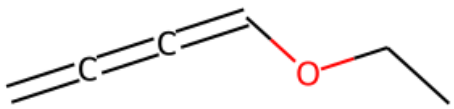
SMILES: C=C=CC=C

Nearest TMC-1 molecule (distance): C=C=C=[C] (4.93)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.1, 0.0
A, B, C	34347.0206, 2316.3477, 2202.9748
A_s, B_s, C_s	34247.4143, 2309.6303, 2196.5862
Charge, Multiplicity	0, 1
Predicted log column density	12.322±2.583
Electronic energy	-193.99076

geom642



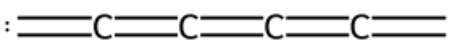
SMILES: C=C=C=COCC

Nearest TMC-1 molecule (distance): C=C=C=[C] (5.06)

Is DFT optimized?: True

Property	Value
Formula	C6H8O
Molecular weight	96.129
IUPAC name	
$\mu_{a,b,c}$	2.1, 1.3, 0.1
A, B, C	16213.8898, 881.4142, 844.9884
A_s, B_s, C_s	16166.8695, 878.8581, 842.5380
Charge, Multiplicity	0, 1
Predicted log column density	13.249±4.819
Electronic energy	-308.46610

geom643



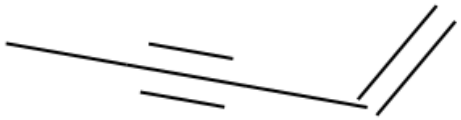
SMILES: [C]=C=C=C=C

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (2.66)

Is DFT optimized?: True

Property	Value
Formula	C6H2
Molecular weight	74.082
IUPAC name	
$\mu_{a,b,c}$	1.3, 0.0, 0.0
A, B, C	290297.8392, 1338.1697, 1332.0295
A_s, B_s, C_s	289455.9754, 1334.2890, 1328.1666
Charge, Multiplicity	0, 3
Predicted log column density	10.457±1.066
Electronic energy	-229.42321

geom644



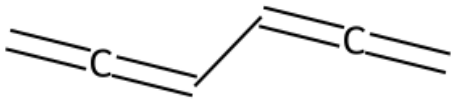
SMILES: C=CC#CC

Nearest TMC-1 molecule (distance): C=CC#C (4.33)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	pent-1-en-3-yne
$\mu_{a,b,c}$	0.6, 0.1, 0.0
A, B, C	34768.8783, 2116.2179, 2020.0226
A_s, B_s, C_s	34668.0485, 2110.0809, 2014.1646
Charge, Multiplicity	0, 1
Predicted log column density	11.935±1.764
Electronic energy	-193.99155

geom645



SMILES: C=C=CC=C=C

Nearest TMC-1 molecule (distance): C=C=C=[C] (5.22)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	32031.0620, 1361.9575, 1330.3798
A_s, B_s, C_s	31938.1719, 1358.0078, 1326.5217
Charge, Multiplicity	0, 1
Predicted log column density	12.448±2.759
Electronic energy	-232.04267

geom646

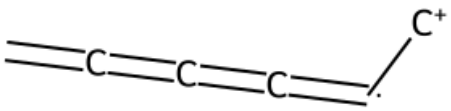
SMILES: C=CSC#CC

Nearest TMC-1 molecule (distance): C=C=C=[C] (5.30)

Is DFT optimized?: True

Property	Value
Formula	C5H6S
Molecular weight	98.170
IUPAC name	1-ethenylsulfanylprop-1-yne
$\mu_{a,b,c}$	0.9, 1.3, 0.0
A, B, C	10955.5825, 1174.8972, 1068.2445
A_s, B_s, C_s	10923.8113, 1171.4900, 1065.1466
Charge, Multiplicity	0, 1
Predicted log column density	11.920±4.016
Electronic energy	-592.15124

geom647



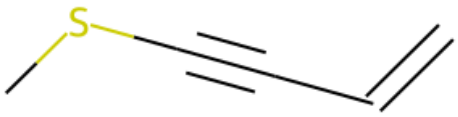
SMILES: C=C=C=C=[C][CH2+]

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (2.67)

Is DFT optimized?: True

Property	Value
Formula	C6H4+
Molecular weight	76.098
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	143155.2005, 1238.4823, 1230.3926
A_s, B_s, C_s	142740.0504, 1234.8907, 1226.8245
Charge, Multiplicity	1, 2
Predicted log column density	10.368±1.286
Electronic energy	-230.48455

geom648



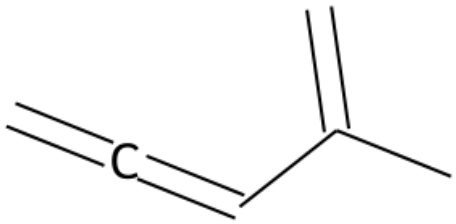
SMILES: C=CC#CSC

Nearest TMC-1 molecule (distance): C=CC#N (4.95)

Is DFT optimized?: True

Property	Value
Formula	C5H6S
Molecular weight	98.170
IUPAC name	4-methylsulfanylbut-1-en-3-yne
$\mu_{a,b,c}$	0.5, 1.6, 0.0
A, B, C	12334.0542, 1078.0836, 997.8610
A_s, B_s, C_s	12298.2854, 1074.9571, 994.9672
Charge, Multiplicity	0, 1
Predicted log column density	10.756±4.399
Electronic energy	-592.15523

geom649



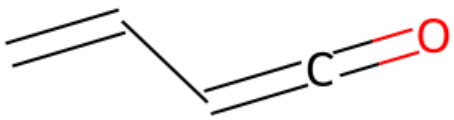
SMILES: C=C=CC(=C)C

Nearest TMC-1 molecule (distance): C=C=C=[C] (5.33)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	
$\mu_{a,b,c}$	0.3, 0.4, 0.0
A, B, C	8218.0565, 2181.0239, 1763.3546
A_s, B_s, C_s	8194.2241, 2174.6989, 1758.2408
Charge, Multiplicity	0, 1
Predicted log column density	10.499±4.007
Electronic energy	-233.29968

geom650



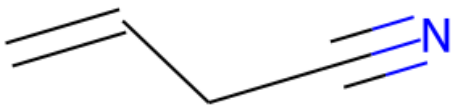
SMILES: C=CC=C=O

Nearest TMC-1 molecule (distance): C=CC#N (4.94)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	
$\mu_{a,b,c}$	1.0, 0.5, 0.0
A, B, C	40082.2397, 2375.4330, 2242.5316
A_s, B_s, C_s	39966.0012, 2368.5442, 2236.0283
Charge, Multiplicity	0, 1
Predicted log column density	11.063±2.907
Electronic energy	-229.92252

geom651



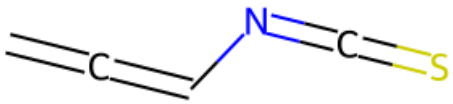
SMILES: C=CCC#N

Nearest TMC-1 molecule (distance): C=CC#N (3.16)

Is DFT optimized?: True

Property	Value
Formula	C4H5N
Molecular weight	67.091
IUPAC name	but-3-enenitrile
$\mu_{a,b,c}$	3.7, 1.8, 0.2
A, B, C	19188.9742, 2625.0939, 2504.5922
A_s, B_s, C_s	19133.3262, 2617.4811, 2497.3289
Charge, Multiplicity	0, 1
Predicted log column density	10.103±2.373
Electronic energy	-210.07357

geom652



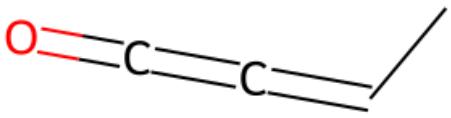
SMILES: C=C=CN=C=S

Nearest TMC-1 molecule (distance): C=C=C=O (4.77)

Is DFT optimized?: True

Property	Value
Formula	C4H3NS
Molecular weight	97.142
IUPAC name	
$\mu_{a,b,c}$	3.3, 0.8, 0.0
A, B, C	32534.8229, 954.0003, 932.7974
A_s, B_s, C_s	32440.4719, 951.2337, 930.0923
Charge, Multiplicity	0, 1
Predicted log column density	12.815±2.599
Electronic energy	-606.99631

geom653



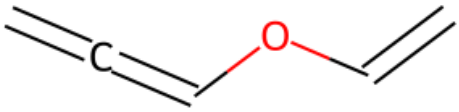
SMILES: CC=C=C=O

Nearest TMC-1 molecule (distance): C=C=C=O (3.43)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	
$\mu_{a,b,c}$	3.2, 1.0, 0.0
A, B, C	52375.0720, 2140.8326, 2083.2350
A_s, B_s, C_s	52223.1843, 2134.6242, 2077.1936
Charge, Multiplicity	0, 1
Predicted log column density	11.518±2.164
Electronic energy	-229.89989

geom654



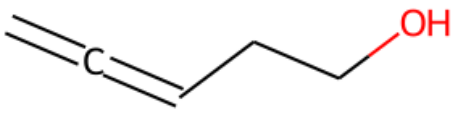
SMILES: C=C=COC=C

Nearest TMC-1 molecule (distance): C=C=C=[C] (5.77)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	
$\mu_{a,b,c}$	0.4, 1.3, 0.1
A, B, C	26738.0611, 1461.5163, 1400.3076
A_s, B_s, C_s	26660.5207, 1457.2779, 1396.2468
Charge, Multiplicity	0, 1
Predicted log column density	12.299±3.482
Electronic energy	-269.16697

geom655



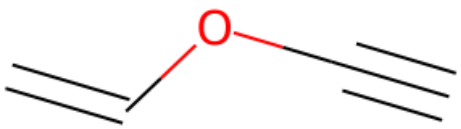
SMILES: C=C=CCCO

Nearest TMC-1 molecule (distance): C=C=[C] (5.34)

Is DFT optimized?: True

Property	Value
Formula	C5H8O
Molecular weight	84.118
IUPAC name	
$\mu_{a,b,c}$	1.6, 0.2, 0.5
A, B, C	8712.3281, 1667.6160, 1606.1829
A_s, B_s, C_s	8687.0624, 1662.7799, 1601.5250
Charge, Multiplicity	0, 1
Predicted log column density	10.006±3.646
Electronic energy	-270.41516

geom656



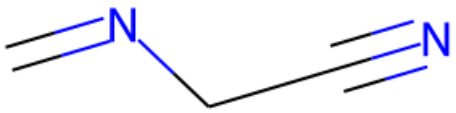
SMILES: C#COC=C

Nearest TMC-1 molecule (distance): C=CC#C (2.78)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	ethynoxyethene
$\mu_{a,b,c}$	0.8, 1.2, 0.0
A, B, C	43206.3411, 2676.1365, 2520.0492
A_s, B_s, C_s	43081.0427, 2668.3757, 2512.7410
Charge, Multiplicity	0, 1
Predicted log column density	12.285±2.831
Electronic energy	-229.84698

geom657



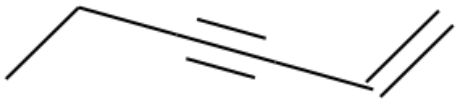
SMILES: C=NCC#N

Nearest TMC-1 molecule (distance): [C]#NC#N (3.77)

Is DFT optimized?: True

Property	Value
Formula	C3H4N2
Molecular weight	68.079
IUPAC name	2-(methylideneamino)acetonitrile
$\mu_{a,b,c}$	4.1, 2.2, 1.7
A, B, C	21125.2960, 2798.2616, 2666.6507
A_s, B_s, C_s	21064.0326, 2790.1466, 2658.9174
Charge, Multiplicity	0, 1
Predicted log column density	9.094±2.657
Electronic energy	-226.09998

geom658



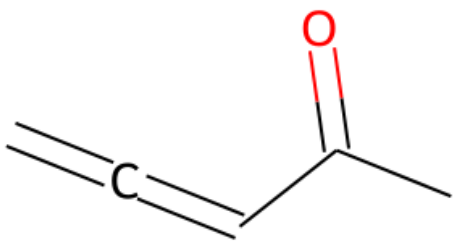
SMILES: C=CC#CCC

Nearest TMC-1 molecule (distance): C=CC#C (4.92)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	hex-1-en-3-yne
$\mu_{a,b,c}$	0.6, 0.1, 0.0
A, B, C	12329.6904, 1413.5233, 1289.6722
A_s, B_s, C_s	12293.9342, 1409.4241, 1285.9321
Charge, Multiplicity	0, 1
Predicted log column density	10.152±3.109
Electronic energy	-233.29460

geom659



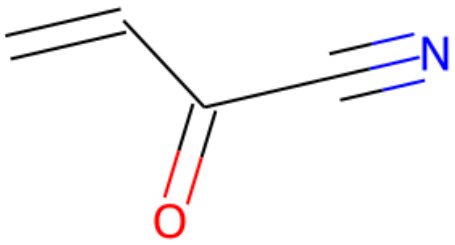
SMILES: C=C=CC(C)=O

Nearest TMC-1 molecule (distance): C=C=[C] (5.38)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	
$\mu_{a,b,c}$	3.4, 1.7, 0.0
A, B, C	8431.3242, 2187.2204, 1777.4798
A_s, B_s, C_s	8406.8734, 2180.8774, 1772.3251
Charge, Multiplicity	0, 1
Predicted log column density	11.169±3.714
Electronic energy	-269.22045

geom660



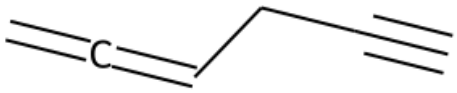
SMILES: C=CC(=O)C#N

Nearest TMC-1 molecule (distance): C=CC#N (3.47)

Is DFT optimized?: True

Property	Value
Formula	C4H3NO
Molecular weight	81.074
IUPAC name	prop-2-enoyl cyanide
$\mu_{a,b,c}$	4.0, 1.9, 0.0
A, B, C	8995.1724, 2449.6462, 1925.3251
A_s, B_s, C_s	8969.0864, 2442.5423, 1919.7417
Charge, Multiplicity	0, 1
Predicted log column density	10.594±2.917
Electronic energy	-284.05121

geom661



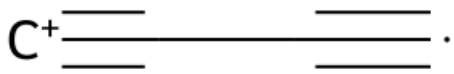
SMILES: C#CCC=C=C

Nearest TMC-1 molecule (distance): C=CC#C (5.23)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.4, 0.1
A, B, C	14156.8676, 1545.7756, 1492.8693
A_s, B_s, C_s	14115.8126, 1541.2929, 1488.5399
Charge, Multiplicity	0, 1
Predicted log column density	11.752±2.364
Electronic energy	-232.03037

geom662



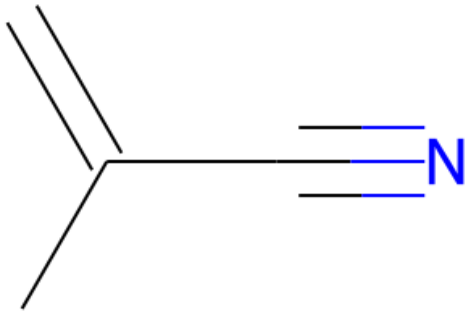
SMILES: [C]#CC#[C+]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.56)

Is DFT optimized?: True

Property	Value
Formula	C4+
Molecular weight	48.044
IUPAC name	buta-1,3-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 5164.8823, 5164.8823
A_s, B_s, C_s	∞, 5149.9041, 5149.9041
Charge, Multiplicity	1, 2
Predicted log column density	12.592±1.706
Electronic energy	-151.42949

geom663



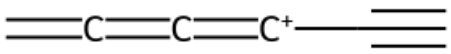
SMILES: C=C(C)C#N

Nearest TMC-1 molecule (distance): C=CC#N (4.73)

Is DFT optimized?: True

Property	Value
Formula	C4H5N
Molecular weight	67.091
IUPAC name	2-methylprop-2-enenitrile
$\mu_{a,b,c}$	4.1, 0.2, 0.0
A, B, C	9266.4688, 4165.1464, 2925.8440
A_s, B_s, C_s	9239.5960, 4153.0675, 2917.3591
Charge, Multiplicity	0, 1
Predicted log column density	10.308±4.186
Electronic energy	-210.08005

geom664



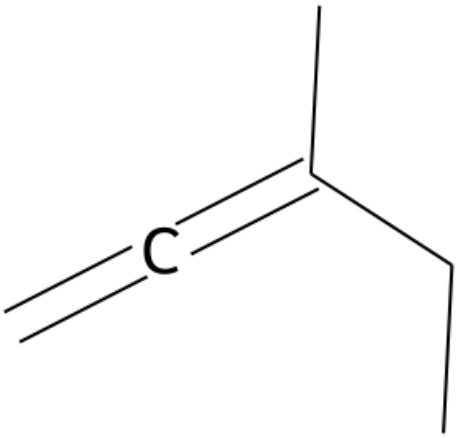
SMILES: C#C[C+]=C=C

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (3.73)

Is DFT optimized?: True

Property	Value
Formula	C6H3+
Molecular weight	75.090
IUPAC name	hex-1-en-3,5-diyne
$\mu_{a,b,c}$	1.1, 0.0, 0.0
A, B, C	285043.3834, 1288.8620, 1283.0607
A_s, B_s, C_s	284216.7576, 1285.1243, 1279.3398
Charge, Multiplicity	1, 1
Predicted log column density	12.364±1.855
Electronic energy	-229.85763

geom665



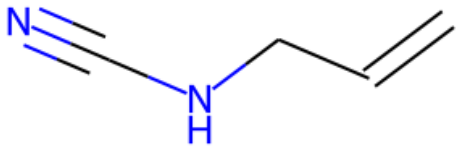
SMILES: C=C=C(C)CC

Nearest TMC-1 molecule (distance): C=C=[C] (5.42)

Is DFT optimized?: True

Property	Value
Formula	C6H10
Molecular weight	82.146
IUPAC name	
$\mu_{a,b,c}$	0.6, 0.2, 0.1
A, B, C	5526.0613, 2252.9412, 1780.3498
A_s, B_s, C_s	5510.0357, 2246.4077, 1775.1867
Charge, Multiplicity	0, 1
Predicted log column density	9.929±4.680
Electronic energy	-234.53209

geom666



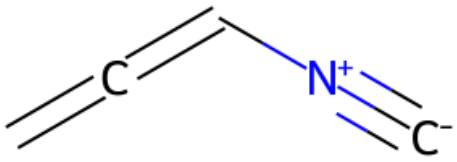
SMILES: C=CCNC#N

Nearest TMC-1 molecule (distance): C=CC#N (4.48)

Is DFT optimized?: True

Property	Value
Formula	C4H6N2
Molecular weight	82.106
IUPAC name	prop-2-enylcyanamide
$\mu_{a,b,c}$	5.0, 0.6, 0.8
A, B, C	22720.5073, 1466.6675, 1449.7251
A_s, B_s, C_s	22654.6178, 1462.4142, 1445.5209
Charge, Multiplicity	0, 1
Predicted log column density	11.389±4.460
Electronic energy	-265.39991

geom667



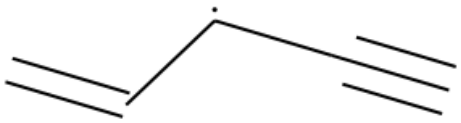
SMILES: [C−]#[N+]C=C=C

Nearest TMC-1 molecule (distance): C#C[N+]#[C−] (5.23)

Is DFT optimized?: True

Property	Value
Formula	C4H3N
Molecular weight	65.075
IUPAC name	
$\mu_{a,b,c}$	3.8, 1.3, 0.0
A, B, C	27738.8288, 2815.0473, 2601.6623
A_s, B_s, C_s	27658.3862, 2806.8837, 2594.1175
Charge, Multiplicity	0, 1
Predicted log column density	11.418±1.891
Electronic energy	-208.78726

geom668



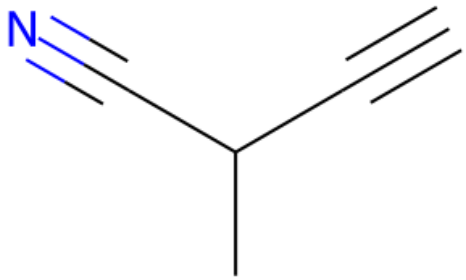
SMILES: C#C[CH]C=C

Nearest TMC-1 molecule (distance): C=CC#C (2.24)

Is DFT optimized?: True

Property	Value
Formula	C5H5
Molecular weight	65.095
IUPAC name	pent-1-en-4-yne
$\mu_{a,b,c}$	0.4, 0.1, 0.0
A, B, C	40829.9579, 2399.5081, 2266.3203
A_s, B_s, C_s	40711.5510, 2392.5495, 2259.7479
Charge, Multiplicity	0, 2
Predicted log column density	11.715±2.353
Electronic energy	-193.34537

geom669



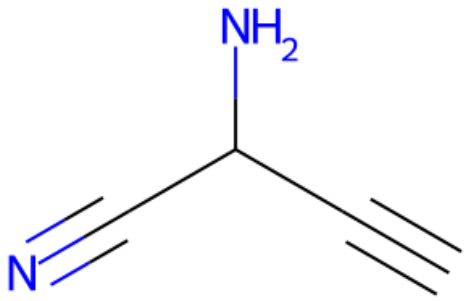
SMILES: C#CC(C)C#N

Nearest TMC-1 molecule (distance): [C]#CC#N (4.54)

Is DFT optimized?: True

Property	Value
Formula	C5H5N
Molecular weight	79.102
IUPAC name	2-methylbut-3-ynenitrile
$\mu_{a,b,c}$	3.0, 2.5, 0.8
A, B, C	5530.8093, 2798.3213, 1980.6854
A_s, B_s, C_s	5514.7699, 2790.2062, 1974.9414
Charge, Multiplicity	0, 1
Predicted log column density	10.575±4.029
Electronic energy	-248.11565

geom670



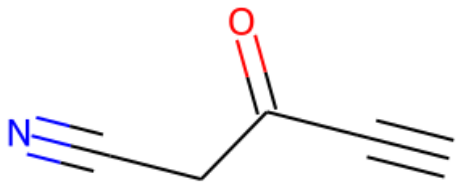
SMILES: C#CC(N)C#N

Nearest TMC-1 molecule (distance): [C]#CC#N (4.86)

Is DFT optimized?: True

Property	Value
Formula	C4H4N2
Molecular weight	80.090
IUPAC name	
$\mu_{a,b,c}$	4.3, 1.7, 0.3
A, B, C	5599.3800, 2851.1290, 2005.0579
A_s, B_s, C_s	5583.1418, 2842.8607, 1999.2433
Charge, Multiplicity	0, 1
Predicted log column density	9.563±4.242
Electronic energy	-264.13773

geom671



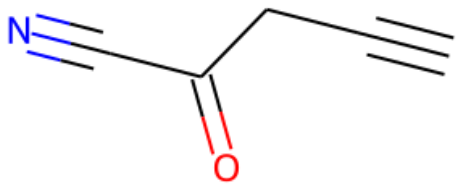
SMILES: C#CC(=O)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (3.74)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	3-oxopent-4-ynenitrile
$\mu_{a,b,c}$	0.9, 0.3, 1.6
A, B, C	3806.5574, 2286.5838, 1477.0323
A_s, B_s, C_s	3795.5184, 2279.9527, 1472.7489
Charge, Multiplicity	0, 1
Predicted log column density	11.356±3.927
Electronic energy	-322.09895

geom672



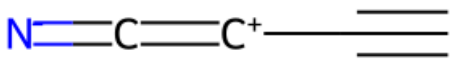
SMILES: C#CCC(=O)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (3.89)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	2.7, 1.9, 0.0
A, B, C	8910.1526, 1446.3289, 1253.8757
A_s, B_s, C_s	8884.3132, 1442.1346, 1250.2395
Charge, Multiplicity	0, 1
Predicted log column density	12.148±3.832
Electronic energy	-322.09118

geom673



SMILES: C#C[C+]=C=[N-]

Nearest TMC-1 molecule (distance): C#CC#[C-] (3.56)

Is DFT optimized?: True

Property	Value
Formula	C4HN
Molecular weight	63.059
IUPAC name	but-1-en-3-ynylideneazanide
$\mu_{a,b,c}$	4.6, 0.0, 0.0
A, B, C	12304989249.8903, 2298.5123, 2298.5119
A_s, B_s, C_s	12269304781.0656, 2291.8466, 2291.8462
Charge, Multiplicity	0, 1
Predicted log column density	13.580±3.189
Electronic energy	-207.47627

geom674

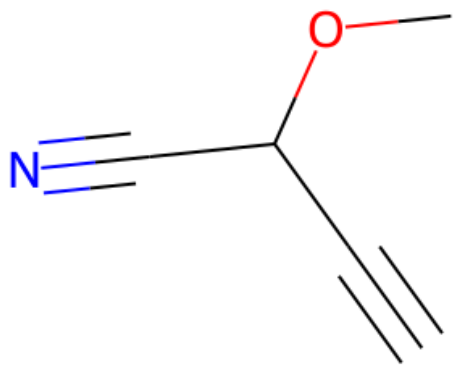
SMILES: C#CCCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (2.67)

Is DFT optimized?: True

Property	Value
Formula	C5H5N
Molecular weight	79.102
IUPAC name	pent-4-ynenitrile
$\mu_{a,b,c}$	3.5, 0.9, 0.0
A, B, C	25351.2581, 1468.2513, 1412.1482
A_s, B_s, C_s	25277.7395, 1463.9934, 1408.0530
Charge, Multiplicity	0, 1
Predicted log column density	11.215±2.713
Electronic energy	-248.12202

geom675



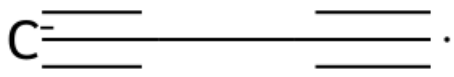
SMILES: C#CC(C#N)OC

Nearest TMC-1 molecule (distance): C#CCC#N (5.50)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	2-methoxybut-3-ynenitrile
$\mu_{a,b,c}$	0.4, 2.7, 1.6
A, B, C	3477.6898, 2305.7155, 1451.1654
A_s, B_s, C_s	3467.6045, 2299.0289, 1446.9571
Charge, Multiplicity	0, 1
Predicted log column density	11.304±4.810
Electronic energy	-323.28620

geom676



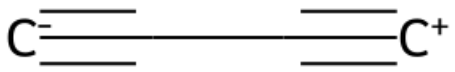
SMILES: [C]#CC#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (1.26)

Is DFT optimized?: True

Property	Value
Formula	C4-
Molecular weight	48.044
IUPAC name	buta-1,3-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 4994.0852, 4994.0852
A_s, B_s, C_s	∞, 4979.6024, 4979.6024
Charge, Multiplicity	-1, 2
Predicted log column density	12.501±1.447
Electronic energy	-152.10100

geom677



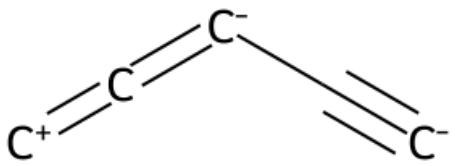
SMILES: [C+]#CC#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (1.63)

Is DFT optimized?: True

Property	Value
Formula	C4
Molecular weight	48.044
IUPAC name	buta-1,3-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 5080.4231, 5080.4231
A_s, B_s, C_s	∞, 5065.6898, 5065.6898
Charge, Multiplicity	0, 1
Predicted log column density	11.963±1.623
Electronic energy	-151.85129

geom678



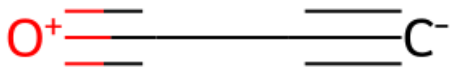
SMILES: [C−]#C[C−]=C=[CH+]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (1.88)

Is DFT optimized?: True

Property	Value
Formula	C5H-
Molecular weight	61.063
IUPAC name	penta-1,2-dien-4-yne
$\mu_{a,b,c}$	3.0, 1.6, 0.0
A, B, C	559378.7145, 2387.9176, 2377.7684
A_s, B_s, C_s	557756.5162, 2380.9926, 2370.8728
Charge, Multiplicity	-1, 1
Predicted log column density	11.948±1.889
Electronic energy	-190.84436

geom679



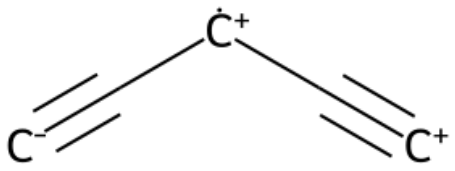
SMILES: [C−]#CC#[O+]

Nearest TMC-1 molecule (distance): [C−]#CC#[S+] (2.42)

Is DFT optimized?: True

Property	Value
Formula	C3O
Molecular weight	52.032
IUPAC name	prop-2-ynylidyneoxidanium
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	∞, 4774.2741, 4774.2741
A_s, B_s, C_s	∞, 4760.4287, 4760.4287
Charge, Multiplicity	0, 1
Predicted log column density	10.238±1.756
Electronic energy	-189.32347

geom680



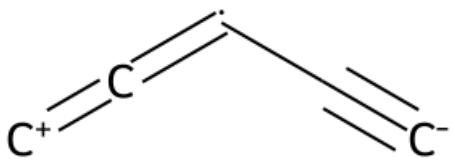
SMILES: [C+]#C[C+]C#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.46)

Is DFT optimized?: True

Property	Value
Formula	C5+
Molecular weight	60.055
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	2796556119555.9014, 2576.1914, 2576.1914
A_s, B_s, C_s	2788446106809.1895, 2568.7205, 2568.7205
Charge, Multiplicity	1, 2
Predicted log column density	11.855±1.794
Electronic energy	-189.66770

geom681



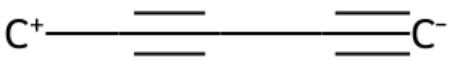
SMILES: [C−]#C[C]=C=[CH+]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (1.70)

Is DFT optimized?: True

Property	Value
Formula	C5H
Molecular weight	61.063
IUPAC name	
$\mu_{a,b,c}$	5.2, 0.0, 0.0
A, B, C	844430780.9450, 2383.9980, 2383.9913
A_s, B_s, C_s	841981931.6803, 2377.0844, 2377.0777
Charge, Multiplicity	0, 2
Predicted log column density	11.643±1.564
Electronic energy	-190.76550

geom682



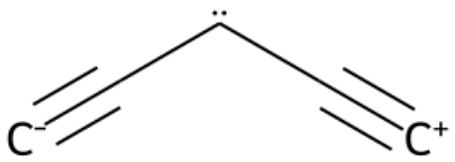
SMILES: [C−]#CC#C[CH2+]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.01)

Is DFT optimized?: True

Property	Value
Formula	C5H2
Molecular weight	62.071
IUPAC name	penta-1,3-diyne
$\mu_{a,b,c}$	6.3, 0.0, 0.0
A, B, C	289928.5205, 2301.2922, 2283.1699
A_s, B_s, C_s	289087.7278, 2294.6185, 2276.5487
Charge, Multiplicity	0, 1
Predicted log column density	11.502±1.512
Electronic energy	-191.41054

geom683



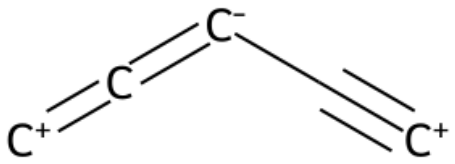
SMILES: [C+]#C[C]C#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.12)

Is DFT optimized?: True

Property	Value
Formula	C5
Molecular weight	60.055
IUPAC name	penta-1,4-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	638125080149.3307, 2551.1505, 2551.1505
A_s, B_s, C_s	636274517416.8976, 2543.7522, 2543.7521
Charge, Multiplicity	0, 3
Predicted log column density	11.401±1.674
Electronic energy	-190.01132

geom684



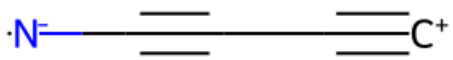
SMILES: [C+]#C[C−]=C=[CH+]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.80)

Is DFT optimized?: True

Property	Value
Formula	C5H+
Molecular weight	61.063
IUPAC name	
$\mu_{a,b,c}$	3.8, 0.0, 0.0
A, B, C	2941710881.8629, 2401.0860, 2401.0841
A_s, B_s, C_s	2933179920.3055, 2394.1229, 2394.1209
Charge, Multiplicity	1, 1
Predicted log column density	12.350±2.060
Electronic energy	-190.44858

geom685



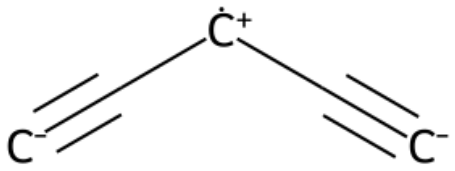
SMILES: [C+]#CC#C[N−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (2.82)

Is DFT optimized?: True

Property	Value
Formula	C4N
Molecular weight	62.051
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	∞, 2413.0984, 2413.0984
A_s, B_s, C_s	∞, 2406.1004, 2406.1004
Charge, Multiplicity	0, 2
Predicted log column density	12.675±2.279
Electronic energy	-206.84028

geom686



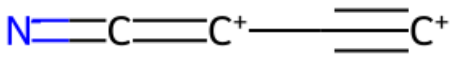
SMILES: [C−]#C[C+]C#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (3.68)

Is DFT optimized?: True

Property	Value
Formula	C5-
Molecular weight	60.055
IUPAC name	penta-1,4-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	11332475431930.6035, 2505.0974, 2505.0974
A_s, B_s, C_s	11299611253178.0039, 2497.8326, 2497.8326
Charge, Multiplicity	-1, 2
Predicted log column density	11.263±1.858
Electronic energy	-190.22684

geom687



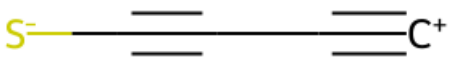
SMILES: [C+]#C[C+]=C=[N−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (3.57)

Is DFT optimized?: True

Property	Value
Formula	C4N+
Molecular weight	62.051
IUPAC name	
$\mu_{a,b,c}$	2.7, 0.0, 0.0
A, B, C	15038011552.5184, 2418.0536, 2418.0532
A_s, B_s, C_s	14994401319.0161, 2411.0412, 2411.0408
Charge, Multiplicity	1, 1
Predicted log column density	12.959±3.233
Electronic energy	-206.47923

geom688



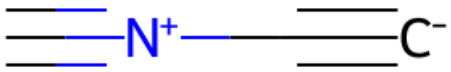
SMILES: [C+]#CC#C[S−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (3.20)

Is DFT optimized?: True

Property	Value
Formula	C4S
Molecular weight	80.111
IUPAC name	buta-1,3-diyne-1-thiolate
$\mu_{a,b,c}$	3.8, 0.0, 0.0
A, B, C	949205189.4885, 1511.2377, 1511.2357
A_s, B_s, C_s	946452494.4390, 1506.8551, 1506.8531
Charge, Multiplicity	0, 1
Predicted log column density	13.686±1.705
Electronic energy	-550.27942

geom689



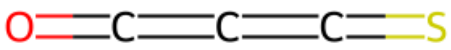
SMILES: [C−]#C[N+]#C

Nearest TMC-1 molecule (distance): C#C[N+]#[C−] (2.43)

Is DFT optimized?: False

Property	Value
Formula	C3HN
Molecular weight	51.048
IUPAC name	
$\mu_{a,b,c}$	9.4, 0.0, 0.0
A, B, C	∞, 4720.1363, 4720.1363
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.046±1.878
Electronic energy	-169.35206

geom690



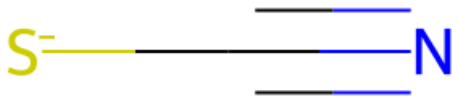
SMILES: O=C=C=C=S

Nearest TMC-1 molecule (distance): C=C=C=O (3.95)

Is DFT optimized?: True

Property	Value
Formula	C3OS
Molecular weight	84.099
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.6, 0.0
A, B, C	354101670.9368, 1405.9482, 1405.9426
A_s, B_s, C_s	353074776.0911, 1401.8710, 1401.8654
Charge, Multiplicity	0, 1
Predicted log column density	12.315±1.810
Electronic energy	-587.58196

geom691



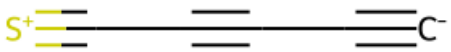
SMILES: N#C[S−]

Nearest TMC-1 molecule (distance): [C+]#C[S−] (3.57)

Is DFT optimized?: True

Property	Value
Formula	CNS-
Molecular weight	58.085
IUPAC name	thiocyanate
$\mu_{a,b,c}$	1.5, 0.0, 0.0
A, B, C	∞, 5938.4187, 5938.4187
A_s, B_s, C_s	∞, 5921.1973, 5921.1973
Charge, Multiplicity	-1, 1
Predicted log column density	13.282±2.291
Electronic energy	-491.05862

geom692



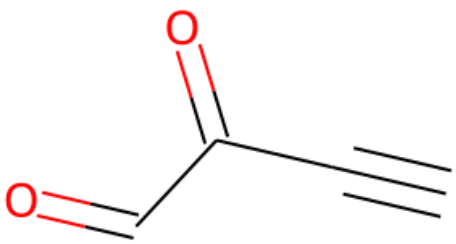
SMILES: [C−]#CC#CC#[S+]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (4.32)

Is DFT optimized?: True

Property	Value
Formula	C5S
Molecular weight	92.122
IUPAC name	penta-2,4-diynylidynesulfanium
$\mu_{a,b,c}$	5.0, 0.0, 0.0
A, B, C	∞, 919.8705, 919.8705
A_s, B_s, C_s	∞, 917.2028, 917.2028
Charge, Multiplicity	0, 1
Predicted log column density	11.382±1.546
Electronic energy	-588.38736

geom693



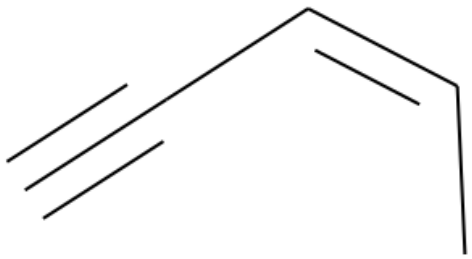
SMILES: C#CC(=O)C=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (3.53)

Is DFT optimized?: True

Property	Value
Formula	C4H2O2
Molecular weight	82.058
IUPAC name	2-oxobut-3-ynal
$\mu_{a,b,c}$	1.1, 0.8, 0.0
A, B, C	5108.6942, 3519.4170, 2083.8427
A_s, B_s, C_s	5093.8789, 3509.2107, 2077.7995
Charge, Multiplicity	0, 1
Predicted log column density	10.212±2.934
Electronic energy	-303.86643

geom694



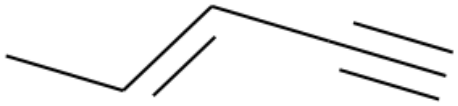
SMILES: C#C/C=C\C

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.20)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	(Z)-pent-3-en-1-yne
$\mu_{a,b,c}$	0.9, 0.2, 0.0
A, B, C	11905.1477, 3341.4485, 2652.0012
A_s, B_s, C_s	11870.6228, 3331.7583, 2644.3104
Charge, Multiplicity	0, 1
Predicted log column density	13.155±2.111
Electronic energy	-193.98772

geom695



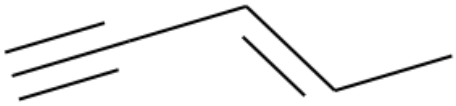
SMILES: C#CC=CC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.20)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	pent-3-en-1-yne
$\mu_{a,b,c}$	1.1, 0.2, 0.0
A, B, C	38483.6349, 2242.5502, 2147.2472
A_s, B_s, C_s	38372.0323, 2236.0468, 2141.0202
Charge, Multiplicity	0, 1
Predicted log column density	13.155±2.111
Electronic energy	-193.98717

geom696



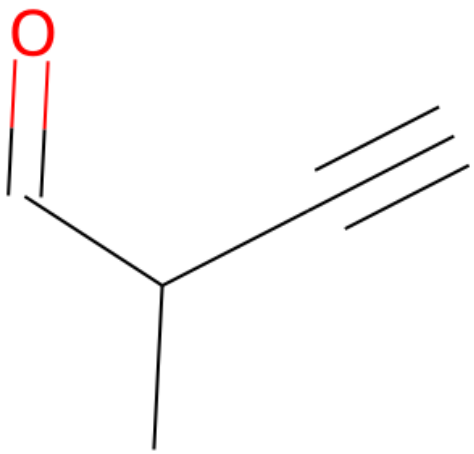
SMILES: C#C/C=C/C

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.20)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	(E)-pent-3-en-1-yne
$\mu_{a,b,c}$	1.1, 0.2, 0.0
A, B, C	38447.7914, 2242.9744, 2147.5244
A_s, B_s, C_s	38336.2928, 2236.4697, 2141.2966
Charge, Multiplicity	0, 1
Predicted log column density	13.155±2.111
Electronic energy	-193.98717

geom697



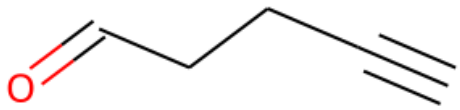
SMILES: C#CC(C)C=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.66)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	2-methylbut-3-ynal
$\mu_{a,b,c}$	2.0, 0.3, 1.2
A, B, C	6480.8957, 2514.2515, 1960.1091
A_s, B_s, C_s	6462.1011, 2506.9601, 1954.4248
Charge, Multiplicity	0, 1
Predicted log column density	9.089±4.027
Electronic energy	-269.19823

geom698



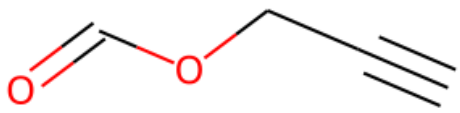
SMILES: C#CCCC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.68)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	pent-4-ynal
$\mu_{a,b,c}$	0.4, 2.9, 0.9
A, B, C	4477.4823, 3332.9666, 2070.7982
A_s, B_s, C_s	4464.4976, 3323.3009, 2064.7929
Charge, Multiplicity	0, 1
Predicted log column density	8.556±3.009
Electronic energy	-269.19533

geom699



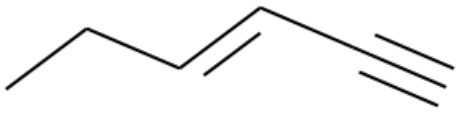
SMILES: C#CCOC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.73)

Is DFT optimized?: True

Property	Value
Formula	C4H4O2
Molecular weight	84.074
IUPAC name	prop-2-ynyl formate
$\mu_{a,b,c}$	0.8, 1.6, 0.3
A, B, C	7791.0413, 2425.6285, 2093.0384
A_s, B_s, C_s	7768.4473, 2418.5942, 2086.9686
Charge, Multiplicity	0, 1
Predicted log column density	12.209±3.792
Electronic energy	-305.10516

geom700



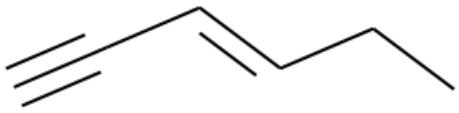
SMILES: C#CC=CCC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.78)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	hex-3-en-1-yne
$\mu_{a,b,c}$	1.2, 0.0, 0.1
A, B, C	16232.9227, 1385.0293, 1346.1118
A_s, B_s, C_s	16185.8472, 1381.0127, 1342.2080
Charge, Multiplicity	0, 1
Predicted log column density	10.423±3.261
Electronic energy	-233.29043

geom701



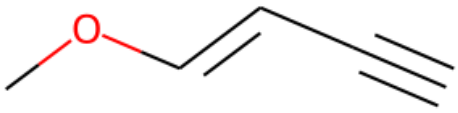
SMILES: C#C/C=C/CC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.78)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	(E)-hex-3-en-1-yne
$\mu_{a,b,c}$	1.2, 0.0, 0.1
A, B, C	16214.9319, 1385.2844, 1346.8121
A_s, B_s, C_s	16167.9086, 1381.2671, 1342.9063
Charge, Multiplicity	0, 1
Predicted log column density	10.423±3.261
Electronic energy	-233.29043

geom702



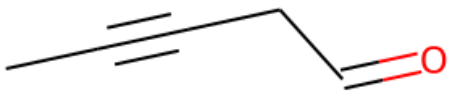
SMILES: C#CC=COC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.79)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	1-methoxybut-1-en-3-yne
$\mu_{a,b,c}$	2.1, 1.5, 0.0
A, B, C	22962.6491, 1437.8200, 1364.9556
A_s, B_s, C_s	22896.0574, 1433.6503, 1360.9972
Charge, Multiplicity	0, 1
Predicted log column density	13.908±3.975
Electronic energy	-269.17095

geom703



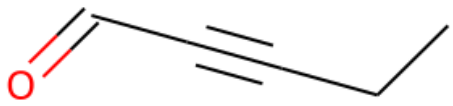
SMILES: CC#CCC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.85)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	pent-3-ynal
$\mu_{a,b,c}$	3.2, 0.2, 0.7
A, B, C	18659.7241, 1302.9783, 1244.6449
A_s, B_s, C_s	18605.6109, 1299.1997, 1241.0355
Charge, Multiplicity	0, 1
Predicted log column density	8.632±3.049
Electronic energy	-269.20680

geom704



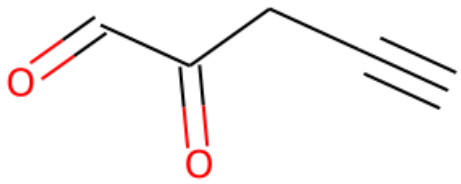
SMILES: CCC#CC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.92)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	pent-2-ynal
$\mu_{a,b,c}$	3.6, 1.8, 0.8
A, B, C	14072.6980, 1366.4424, 1287.6173
A_s, B_s, C_s	14031.8871, 1362.4797, 1283.8832
Charge, Multiplicity	0, 1
Predicted log column density	9.347±3.287
Electronic energy	-269.20330

geom705



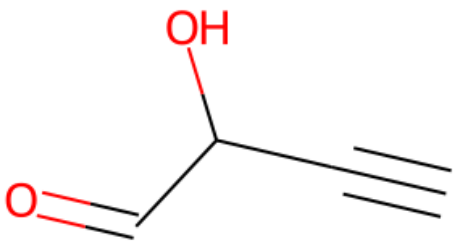
SMILES: C#CCC(=O)C=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (4.97)

Is DFT optimized?: True

Property	Value
Formula	C5H4O2
Molecular weight	96.085
IUPAC name	2-oxopent-4-ynal
$\mu_{a,b,c}$	0.1, 0.6, 0.0
A, B, C	6734.8217, 1561.7761, 1277.5617
A_s, B_s, C_s	6715.2907, 1557.2470, 1273.8568
Charge, Multiplicity	0, 1
Predicted log column density	11.190±3.587
Electronic energy	-343.17683

geom706



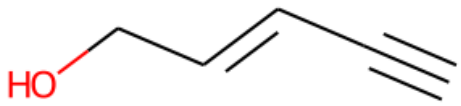
SMILES: C#CC(O)C=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.10)

Is DFT optimized?: True

Property	Value
Formula	C4H4O2
Molecular weight	84.074
IUPAC name	2-hydroxybut-3-ynal
$\mu_{a,b,c}$	1.3, 1.8, 1.3
A, B, C	6858.1943, 2626.6573, 2090.1002
A_s, B_s, C_s	6838.3056, 2619.0400, 2084.0389
Charge, Multiplicity	0, 1
Predicted log column density	9.193±4.589
Electronic energy	-305.08252

geom707



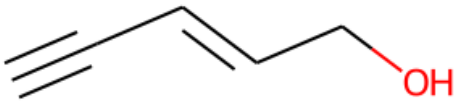
SMILES: C#CC=CCO

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.10)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	pent-2-en-4-yn-1-ol
$\mu_{a,b,c}$	1.0, 0.5, 0.8
A, B, C	18809.7055, 1373.6231, 1337.3777
A_s, B_s, C_s	18755.1573, 1369.6396, 1333.4993
Charge, Multiplicity	0, 1
Predicted log column density	9.834±3.097
Electronic energy	-269.17573

geom708



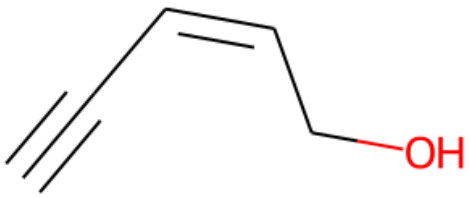
SMILES: C#C/C=C/CO

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.10)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	(E)-pent-2-en-4-yn-1-ol
$\mu_{a,b,c}$	1.0, 0.5, 0.8
A, B, C	18804.4594, 1373.7001, 1337.4844
A_s, B_s, C_s	18749.9265, 1369.7164, 1333.6057
Charge, Multiplicity	0, 1
Predicted log column density	9.834±3.097
Electronic energy	-269.17573

geom709



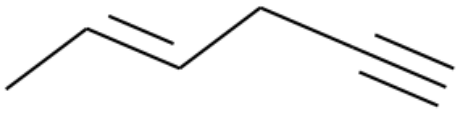
SMILES: C#C/C=C\CO

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.10)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	(Z)-pent-2-en-4-yn-1-ol
$\mu_{a,b,c}$	1.3, 0.2, 0.5
A, B, C	8167.5284, 1925.0137, 1653.9113
A_s, B_s, C_s	8143.8426, 1919.4312, 1649.1149
Charge, Multiplicity	0, 1
Predicted log column density	9.834±3.097
Electronic energy	-269.17591

geom710



SMILES: C#CCC=CC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.18)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	hex-4-en-1-yne
$\mu_{a,b,c}$	0.9, 0.3, 0.0
A, B, C	12501.1506, 1463.1064, 1380.5886
A_s, B_s, C_s	12464.8973, 1458.8634, 1376.5849
Charge, Multiplicity	0, 1
Predicted log column density	12.834±2.857
Electronic energy	-233.28567

geom711

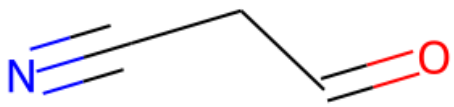
SMILES: C#CC=C(C)C

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.18)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	4-methylpent-3-en-1-yne
$\mu_{a,b,c}$	1.3, 0.4, 0.0
A, B, C	8348.2736, 2120.2991, 1727.0276
A_s, B_s, C_s	8324.0636, 2114.1502, 1722.0192
Charge, Multiplicity	0, 1
Predicted log column density	10.209±4.973
Electronic energy	-233.29725

geom712



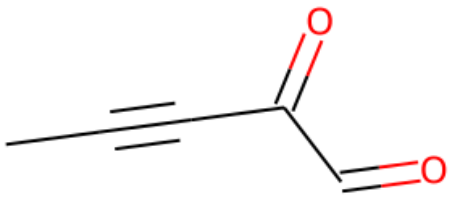
SMILES: N#CCC=O

Nearest TMC-1 molecule (distance): CCC#N (4.32)

Is DFT optimized?: True

Property	Value
Formula	C3H3NO
Molecular weight	69.063
IUPAC name	3-oxopropanenitrile
$\mu_{a,b,c}$	1.0, 1.2, 0.2
A, B, C	30180.4989, 2514.6651, 2356.8257
A_s, B_s, C_s	30092.9755, 2507.3726, 2349.9909
Charge, Multiplicity	0, 1
Predicted log column density	8.454±2.846
Electronic energy	-245.98573

geom713



SMILES: CC#CC(=O)C=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.38)

Is DFT optimized?: True

Property	Value
Formula	C5H4O2
Molecular weight	96.085
IUPAC name	
$\mu_{a,b,c}$	2.7, 0.6, 0.0
A, B, C	4570.2684, 1597.4092, 1192.5158
A_s, B_s, C_s	4557.0147, 1592.7767, 1189.0575
Charge, Multiplicity	0, 1
Predicted log column density	9.530±3.017
Electronic energy	-343.18457

geom714

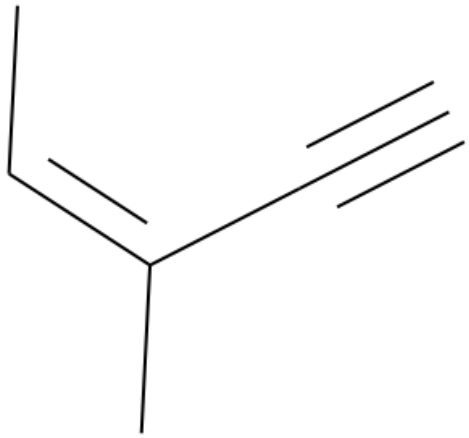
SMILES: O=CC#CCO

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.41)

Is DFT optimized?: True

Property	Value
Formula	C4H4O2
Molecular weight	84.074
IUPAC name	4-hydroxybut-2-ynal
$\mu_{a,b,c}$	2.2, 1.0, 1.2
A, B, C	23190.7977, 1274.7633, 1221.1632
A_s, B_s, C_s	23123.5444, 1271.0664, 1217.6218
Charge, Multiplicity	0, 1
Predicted log column density	9.291±3.589
Electronic energy	-305.08384

geom715



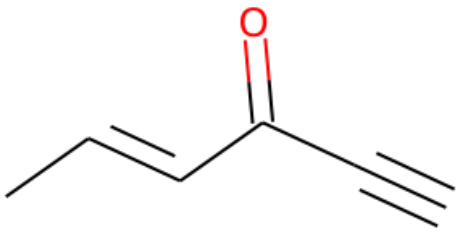
SMILES: C#CC(C)=CC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.45)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	3-methylpent-3-en-1-yne
$\mu_{a,b,c}$	1.1, 0.2, 0.0
A, B, C	7234.8407, 2231.2697, 1742.2929
A_s, B_s, C_s	7213.8596, 2224.7990, 1737.2403
Charge, Multiplicity	0, 1
Predicted log column density	12.872±4.843
Electronic energy	-233.29193

geom716



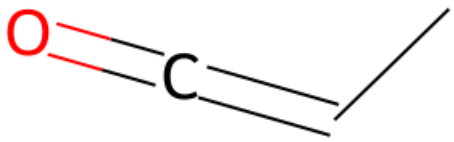
SMILES: C#CC(=O)C=CC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.45)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	hex-4-en-1-yn-3-one
$\mu_{a,b,c}$	1.5, 3.0, 0.0
A, B, C	6766.3958, 1359.5233, 1140.0329
A_s, B_s, C_s	6746.7733, 1355.5807, 1136.7268
Charge, Multiplicity	0, 1
Predicted log column density	13.039±3.991
Electronic energy	-307.27523

geom717



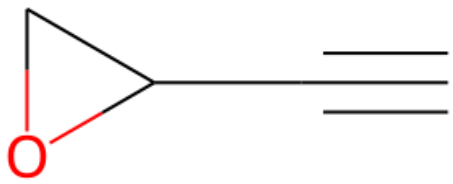
SMILES: CC=C=O

Nearest TMC-1 molecule (distance): C=C=O (3.69)

Is DFT optimized?: True

Property	Value
Formula	C3H4O
Molecular weight	56.064
IUPAC name	
$\mu_{a,b,c}$	2.0, 0.4, 0.0
A, B, C	39143.5744, 4445.2145, 4094.6107
A_s, B_s, C_s	39030.0581, 4432.3234, 4082.7363
Charge, Multiplicity	0, 1
Predicted log column density	11.882±2.134
Electronic energy	-191.85083

geom718



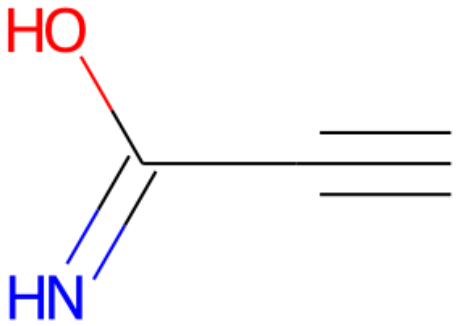
SMILES: C#CC1CO1

Nearest TMC-1 molecule (distance): CC#C (5.10)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	2-ethynyloxirane
$\mu_{a,b,c}$	0.4, 1.9, 0.7
A, B, C	18774.2983, 3395.6406, 3252.5605
A_s, B_s, C_s	18719.8528, 3385.7933, 3243.1281
Charge, Multiplicity	0, 1
Predicted log column density	10.800±4.341
Electronic energy	-229.85613

geom719



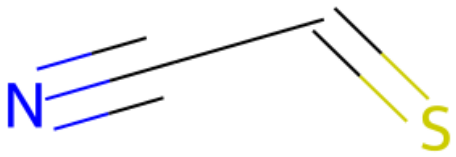
SMILES: C#CC(=N)O

Nearest TMC-1 molecule (distance): C#[C]=O (5.44)

Is DFT optimized?: True

Property	Value
Formula	C3H3NO
Molecular weight	69.063
IUPAC name	prop-2-ynamide
$\mu_{a,b,c}$	4.3, 1.0, 0.0
A, B, C	11147.3174, 4172.0359, 3035.8347
A_s, B_s, C_s	11114.9902, 4159.9370, 3027.0308
Charge, Multiplicity	0, 1
Predicted log column density	12.354±3.936
Electronic energy	-245.92400

geom720



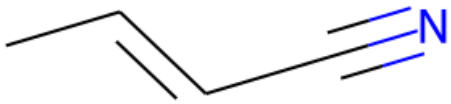
SMILES: N#CC=S

Nearest TMC-1 molecule (distance): N#C[CH+] (4.18)

Is DFT optimized?: True

Property	Value
Formula	C2HNS
Molecular weight	71.104
IUPAC name	methanethioyl cyanide
$\mu_{a,b,c}$	1.8, 1.9, 0.0
A, B, C	43053.2663, 3184.5386, 2965.2097
A_s, B_s, C_s	42928.4119, 3175.3034, 2956.6106
Charge, Multiplicity	0, 1
Predicted log column density	13.974±2.372
Electronic energy	-529.63006

geom721



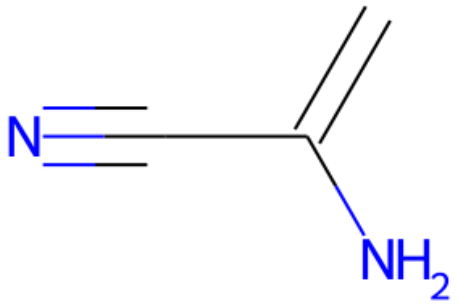
SMILES: CC=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (4.73)

Is DFT optimized?: True

Property	Value
Formula	C4H5N
Molecular weight	67.091
IUPAC name	but-2-enenitrile
$\mu_{a,b,c}$	4.9, 0.7, 0.0
A, B, C	38296.2370, 2288.0655, 2188.4867
A_s, B_s, C_s	38185.1779, 2281.4301, 2182.1401
Charge, Multiplicity	0, 1
Predicted log column density	13.159±2.077
Electronic energy	-210.07902

geom722



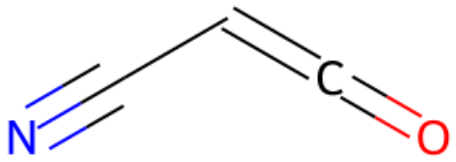
SMILES: C=C(N)C#N

Nearest TMC-1 molecule (distance): [CH2]C#N (4.11)

Is DFT optimized?: True

Property	Value
Formula	C3H4N2
Molecular weight	68.079
IUPAC name	2-aminoprop-2-enenitrile
$\mu_{a,b,c}$	4.1, 0.6, 1.1
A, B, C	9972.4006, 4278.0898, 3001.9547
A_s, B_s, C_s	9943.4806, 4265.6833, 2993.2490
Charge, Multiplicity	0, 1
Predicted log column density	10.905±3.259
Electronic energy	-226.11109

geom723



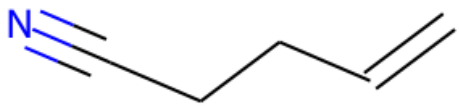
SMILES: N#CC=C=O

Nearest TMC-1 molecule (distance): C=C=CC#N (3.93)

Is DFT optimized?: True

Property	Value
Formula	C3HNO
Molecular weight	67.047
IUPAC name	
$\mu_{a,b,c}$	2.9, 2.3, 0.0
A, B, C	29295.0288, 2801.6445, 2557.0954
A_s, B_s, C_s	29210.0732, 2793.5198, 2549.6799
Charge, Multiplicity	0, 1
Predicted log column density	10.415±1.876
Electronic energy	-244.75462

geom724



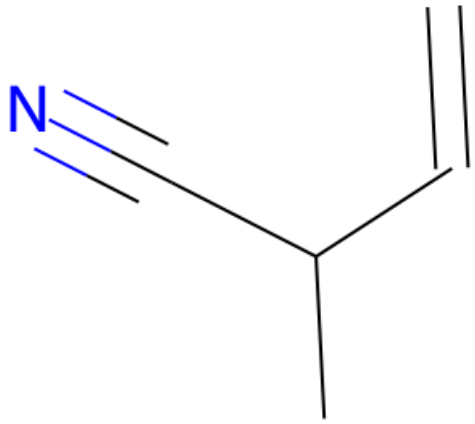
SMILES: C=CCCC#N

Nearest TMC-1 molecule (distance): C=CC#N (4.97)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	pent-4-enenitrile
$\mu_{a,b,c}$	3.9, 1.3, 0.1
A, B, C	17605.1913, 1422.8653, 1397.7677
A_s, B_s, C_s	17554.1362, 1418.7390, 1393.7142
Charge, Multiplicity	0, 1
Predicted log column density	8.901±3.238
Electronic energy	-249.37979

geom725



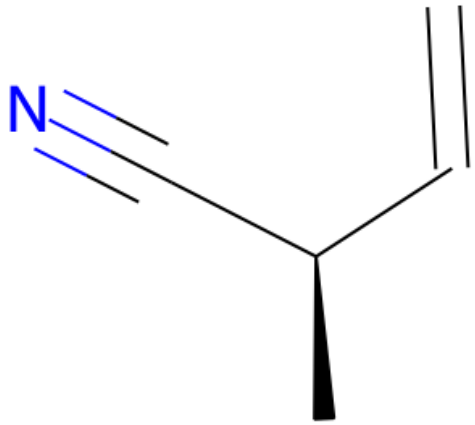
SMILES: C=CC(C)C#N

Nearest TMC-1 molecule (distance): C=CC#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	2-methylbut-3-enenitrile
$\mu_{a,b,c}$	2.9, 2.9, 1.1
A, B, C	5945.6844, 2554.9532, 2009.7904
A_s, B_s, C_s	5928.4419, 2547.5438, 2003.9620
Charge, Multiplicity	0, 1
Predicted log column density	9.535±4.115
Electronic energy	-249.37861

geom726



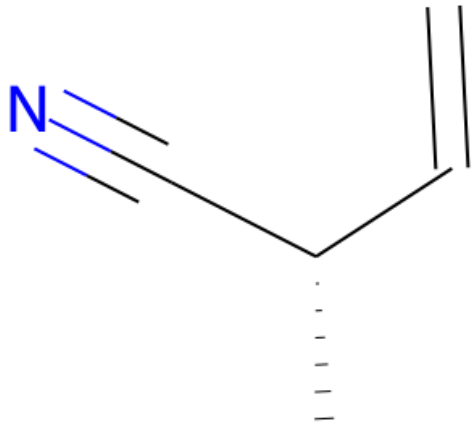
SMILES: C=C[C@@H](C)C#N

Nearest TMC-1 molecule (distance): C=CC#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	(2R)-2-methylbut-3-enenitrile
$\mu_{a,b,c}$	3.5, 2.2, 0.5
A, B, C	5445.5366, 2593.7028, 1911.4722
A_s, B_s, C_s	5429.7445, 2586.1810, 1905.9289
Charge, Multiplicity	0, 1
Predicted log column density	9.535±4.115
Electronic energy	-249.37855

geom727



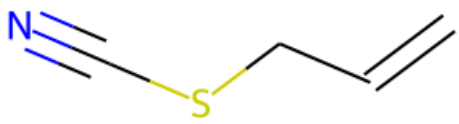
SMILES: C=C[C@H](C)C#N

Nearest TMC-1 molecule (distance): C=CC#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	(2S)-2-methylbut-3-enenitrile
$\mu_{a,b,c}$	3.5, 2.2, 0.5
A, B, C	5444.7924, 2593.5124, 1911.2149
A_s, B_s, C_s	5429.0025, 2585.9912, 1905.6723
Charge, Multiplicity	0, 1
Predicted log column density	9.535±4.115
Electronic energy	-249.37855

geom728



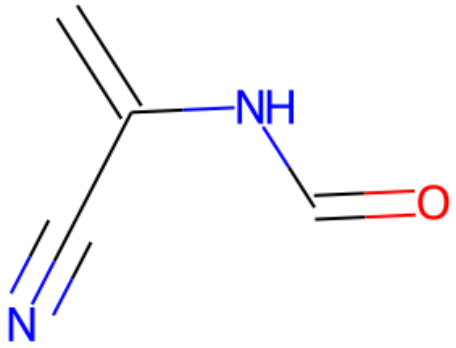
SMILES: C=CCSC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.11)

Is DFT optimized?: True

Property	Value
Formula	C4H5NS
Molecular weight	99.158
IUPAC name	prop-2-enyl thiocyanate
$\mu_{a,b,c}$	4.7, 0.1, 0.1
A, B, C	11492.6922, 1305.6658, 1229.0957
A_s, B_s, C_s	11459.3634, 1301.8794, 1225.5313
Charge, Multiplicity	0, 1
Predicted log column density	10.109±5.285
Electronic energy	-608.23497

geom729



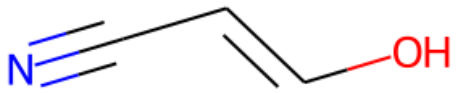
SMILES: C=C(C#N)NC=O

Nearest TMC-1 molecule (distance): C=CC#N (5.18)

Is DFT optimized?: True

Property	Value
Formula	C4H4N2O
Molecular weight	96.089
IUPAC name	N-(1-cyanoethenyl)formamide
$\mu_{a,b,c}$	1.7, 3.8, 0.0
A, B, C	4555.3329, 1888.8048, 1335.1885
A_s, B_s, C_s	4542.1225, 1883.3273, 1331.3165
Charge, Multiplicity	0, 1
Predicted log column density	10.110±3.883
Electronic energy	-339.41381

geom730



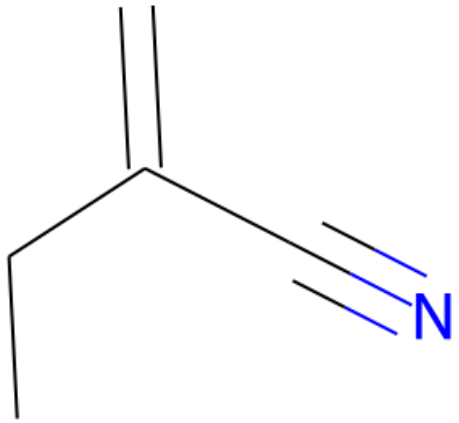
SMILES: N#CC=CO

Nearest TMC-1 molecule (distance): C=CC#N (5.20)

Is DFT optimized?: True

Property	Value
Formula	C3H3NO
Molecular weight	69.063
IUPAC name	3-hydroxyprop-2-enenitrile
$\mu_{a,b,c}$	4.3, 1.9, 0.0
A, B, C	44281.8209, 2385.7844, 2263.8162
A_s, B_s, C_s	44153.4036, 2378.8656, 2257.2511
Charge, Multiplicity	0, 1
Predicted log column density	11.002±2.339
Electronic energy	-245.97512

geom731



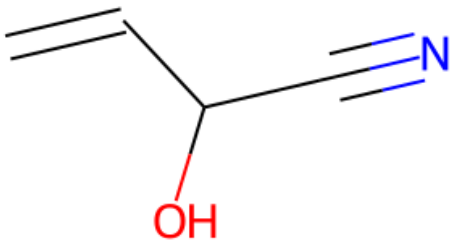
SMILES: C=C(C#N)CC

Nearest TMC-1 molecule (distance): CCC#N (4.90)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	2-methylidenebutanenitrile
$\mu_{a,b,c}$	3.3, 2.5, 0.1
A, B, C	4618.4719, 3100.7945, 2027.0651
A_s, B_s, C_s	4605.0783, 3091.8022, 2021.1866
Charge, Multiplicity	0, 1
Predicted log column density	10.099±4.487
Electronic energy	-249.38398

geom732



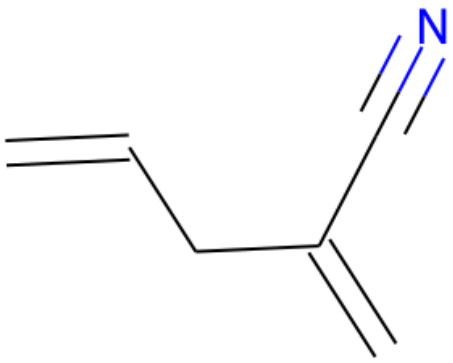
SMILES: C=CC(O)C#N

Nearest TMC-1 molecule (distance): C=CC#N (5.35)

Is DFT optimized?: True

Property	Value
Formula	C4H5NO
Molecular weight	83.090
IUPAC name	2-hydroxybut-3-enenitrile
$\mu_{a,b,c}$	3.4, 0.3, 0.1
A, B, C	6943.5009, 2520.5247, 2000.8455
A_s, B_s, C_s	6923.3647, 2513.2152, 1995.0430
Charge, Multiplicity	0, 1
Predicted log column density	9.641±4.633
Electronic energy	-285.26020

geom733



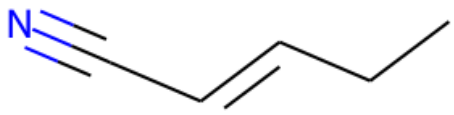
SMILES: C=CCC(=C)C#N

Nearest TMC-1 molecule (distance): C=CC#N (5.44)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	2-methylidenepent-4-enenitrile
$\mu_{a,b,c}$	1.1, 3.9, 0.1
A, B, C	3735.2038, 2048.6160, 1425.6523
A_s, B_s, C_s	3724.3717, 2042.6750, 1421.5179
Charge, Multiplicity	0, 1
Predicted log column density	9.165±3.948
Electronic energy	-287.44654

geom734



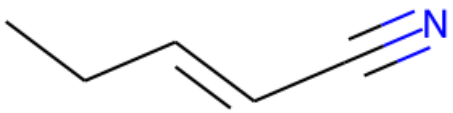
SMILES: CCC=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.49)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	pent-2-enenitrile
$\mu_{a,b,c}$	4.9, 1.1, 0.2
A, B, C	16247.8003, 1401.0577, 1358.7305
A_s, B_s, C_s	16200.6817, 1396.9946, 1354.7901
Charge, Multiplicity	0, 1
Predicted log column density	10.430±3.207
Electronic energy	-249.38515

geom735



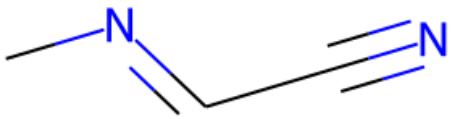
SMILES: CC/C=C/C#N

Nearest TMC-1 molecule (distance): C=CC#N (5.49)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	(E)-pent-2-enenitrile
$\mu_{a,b,c}$	4.9, 1.1, 0.2
A, B, C	16197.9509, 1402.2611, 1360.4343
A_s, B_s, C_s	16150.9768, 1398.1945, 1356.4890
Charge, Multiplicity	0, 1
Predicted log column density	10.430±3.207
Electronic energy	-249.38515

geom736



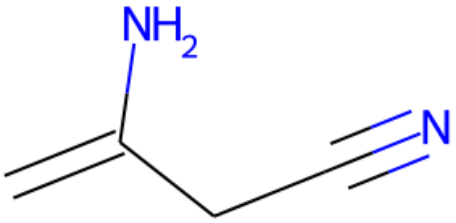
SMILES: CN=CC#N

Nearest TMC-1 molecule (distance): [C]#NC#N (4.76)

Is DFT optimized?: True

Property	Value
Formula	C3H4N2
Molecular weight	68.079
IUPAC name	2-methyliminoacetonitrile
$\mu_{a,b,c}$	4.2, 2.3, 0.0
A, B, C	45475.7107, 2415.2128, 2326.4248
A_s, B_s, C_s	45343.8312, 2408.2087, 2319.6781
Charge, Multiplicity	0, 1
Predicted log column density	10.214±3.299
Electronic energy	-226.10411

geom737



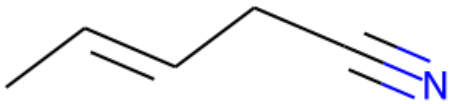
SMILES: C=C(N)CC#N

Nearest TMC-1 molecule (distance): [CH2]C#N (5.17)

Is DFT optimized?: True

Property	Value
Formula	C4H6N2
Molecular weight	82.106
IUPAC name	3-aminobut-3-enenitrile
$\mu_{a,b,c}$	2.8, 0.4, 0.7
A, B, C	7529.9636, 2350.3324, 1983.9360
A_s, B_s, C_s	7508.1267, 2343.5164, 1978.1825
Charge, Multiplicity	0, 1
Predicted log column density	10.816±3.798
Electronic energy	-265.41961

geom738



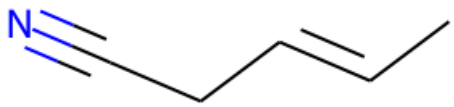
SMILES: C/C=C/CC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	(E)-pent-3-enenitrile
$\mu_{a,b,c}$	3.8, 2.3, 0.1
A, B, C	12743.7954, 1476.8936, 1398.0418
A_s, B_s, C_s	12706.8384, 1472.6106, 1393.9875
Charge, Multiplicity	0, 1
Predicted log column density	11.547±3.074
Electronic energy	-249.38235

geom739



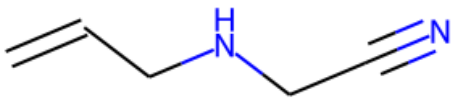
SMILES: CC=CCC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	pent-3-enenitrile
$\mu_{a,b,c}$	3.8, 2.3, 0.1
A, B, C	12837.8238, 1473.1348, 1395.2217
A_s, B_s, C_s	12800.5941, 1468.8627, 1391.1755
Charge, Multiplicity	0, 1
Predicted log column density	11.547±3.074
Electronic energy	-249.38235

geom740



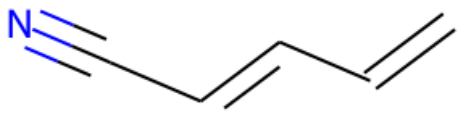
SMILES: C=CCNCC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.64)

Is DFT optimized?: True

Property	Value
Formula	C5H8N2
Molecular weight	96.133
IUPAC name	2-(prop-2-enylamino)acetonitrile
$\mu_{a,b,c}$	3.7, 2.3, 1.1
A, B, C	11874.8523, 952.0598, 919.2717
A_s, B_s, C_s	11840.4153, 949.2989, 916.6058
Charge, Multiplicity	0, 1
Predicted log column density	11.424±4.691
Electronic energy	-304.69916

geom741



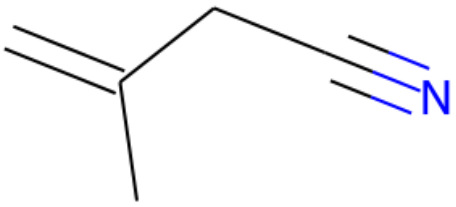
SMILES: C=CC=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.66)

Is DFT optimized?: True

Property	Value
Formula	C5H5N
Molecular weight	79.102
IUPAC name	penta-2,4-dienenitrile
$\mu_{a,b,c}$	4.8, 1.0, 0.0
A, B, C	26098.9338, 1442.4898, 1366.9391
A_s, B_s, C_s	26023.2469, 1438.3066, 1362.9750
Charge, Multiplicity	0, 1
Predicted log column density	11.712±3.264
Electronic energy	-248.15081

geom742



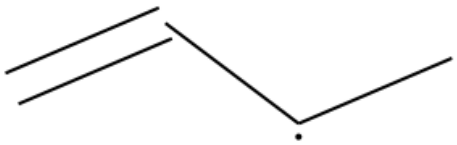
SMILES: C=C(C)CC#N

Nearest TMC-1 molecule (distance): CCC#N (5.27)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	3-methylbut-3-enenitrile
$\mu_{a,b,c}$	3.5, 0.8, 1.7
A, B, C	6778.4995, 2328.7816, 1967.3744
A_s, B_s, C_s	6758.8419, 2322.0281, 1961.6690
Charge, Multiplicity	0, 1
Predicted log column density	11.262±4.583
Electronic energy	-249.38348

geom743



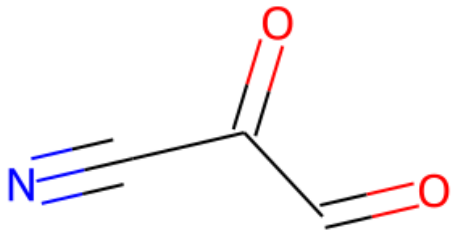
SMILES: C=C[CH]C

Nearest TMC-1 molecule (distance): CC=C (2.12)

Is DFT optimized?: True

Property	Value
Formula	C4H7
Molecular weight	55.100
IUPAC name	but-1-ene
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	37983.3280, 3992.5565, 3695.3545
A_s, B_s, C_s	37873.1763, 3980.9781, 3684.6380
Charge, Multiplicity	0, 2
Predicted log column density	13.248±2.291
Electronic energy	-156.52773

geom744



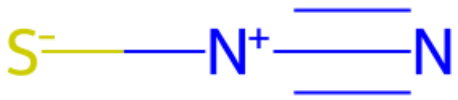
SMILES: N#CC(=O)C=O

Nearest TMC-1 molecule (distance): C=C=CC#N (5.78)

Is DFT optimized?: True

Property	Value
Formula	C3HNO2
Molecular weight	83.046
IUPAC name	2-oxoacetyl cyanide
$\mu_{a,b,c}$	2.4, 1.6, 0.0
A, B, C	5197.3534, 3572.4664, 2117.1910
A_s, B_s, C_s	5182.2811, 3562.1062, 2111.0511
Charge, Multiplicity	0, 1
Predicted log column density	9.703±3.120
Electronic energy	-319.94848

geom745



SMILES: N#[N+][S-]

Nearest TMC-1 molecule (distance): [C-]#[NH+] (3.93)

Is DFT optimized?: False

Property	Value
Formula	N2S
Molecular weight	60.081
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	∞, 6330.4038, 6330.4038
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.977±2.735
Electronic energy	-507.59962

geom746

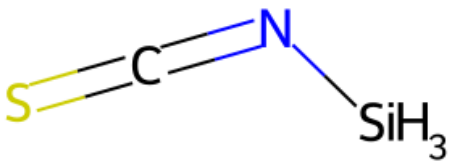
SMILES: S=C=S

Nearest TMC-1 molecule (distance): O=C=S (2.53)

Is DFT optimized?: True

Property	Value
Formula	CS2
Molecular weight	76.145
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 3266.6713, 3266.6713
A_s, B_s, C_s	∞, 3257.1980, 3257.1980
Charge, Multiplicity	0, 1
Predicted log column density	15.698±2.355
Electronic energy	-834.42686

geom747



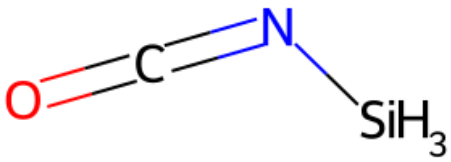
SMILES: [SiH3]N=C=S

Nearest TMC-1 molecule (distance): O=C=S (3.10)

Is DFT optimized?: True

Property	Value
Formula	CH3NSSi
Molecular weight	89.195
IUPAC name	isothiocyanatosilane
$\mu_{a,b,c}$	2.7, 0.0, 0.0
A, B, C	84726.6448, 1499.4019, 1499.4008
A_s, B_s, C_s	84480.9376, 1495.0536, 1495.0526
Charge, Multiplicity	0, 1
Predicted log column density	12.397±2.531
Electronic energy	-782.28819

geom748



SMILES: O=C=N[SiH3]

Nearest TMC-1 molecule (distance): O=C=S (3.23)

Is DFT optimized?: True

Property	Value
Formula	CH3NOSi
Molecular weight	73.127
IUPAC name	isocyanatosilane
$\mu_{a,b,c}$	2.5, 0.0, 0.0
A, B, C	85189.3704, 2441.4314, 2441.4289
A_s, B_s, C_s	84942.3212, 2434.3513, 2434.3488
Charge, Multiplicity	0, 1
Predicted log column density	8.985±2.251
Electronic energy	-459.33393

geom749

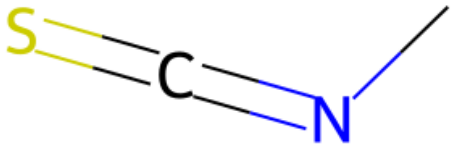
SMILES: CN=C=O

Nearest TMC-1 molecule (distance): O=C=S (3.38)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO
Molecular weight	57.052
IUPAC name	methylimino(oxo)methane
$\mu_{a,b,c}$	3.2, 0.8, 0.0
A, B, C	86115.1476, 4286.2077, 4191.5367
A_s, B_s, C_s	85865.4136, 4273.7777, 4179.3813
Charge, Multiplicity	0, 1
Predicted log column density	9.845±2.859
Electronic energy	-207.92284

geom750



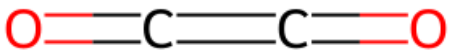
SMILES: CN=C=S

Nearest TMC-1 molecule (distance): O=C=S (3.50)

Is DFT optimized?: False

Property	Value
Formula	C2H3NS
Molecular weight	73.120
IUPAC name	methylimino(sulfanylidene)methane
$\mu_{a,b,c}$	0.5, 0.5, 2.4
A, B, C	36182.7808, 3076.7801, 2887.8576
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.259±3.164
Electronic energy	-530.86674

geom751



SMILES: O=C=C=O

Nearest TMC-1 molecule (distance): C=C=C=O (3.48)

Is DFT optimized?: True

Property	Value
Formula	C2O2
Molecular weight	56.020
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 4291.4591, 4291.4591
A_s, B_s, C_s	∞, 4279.0139, 4279.0139
Charge, Multiplicity	0, 1
Predicted log column density	10.030±1.817
Electronic energy	-226.45614

geom752

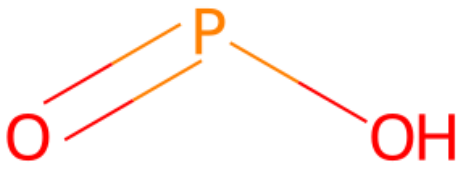
SMILES: O=[N+]=O

Nearest TMC-1 molecule (distance): [C−]#[S+] (2.98)

Is DFT optimized?: True

Property	Value
Formula	NO2+
Molecular weight	46.005
IUPAC name	nitronium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 12554.6051, 12554.6051
A_s, B_s, C_s	∞, 12518.1967, 12518.1967
Charge, Multiplicity	1, 1
Predicted log column density	11.941±2.216
Electronic energy	-204.64821

geom753



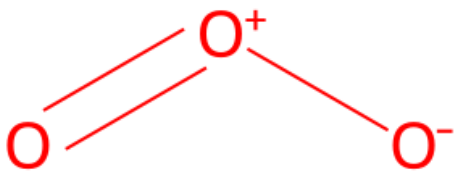
SMILES: O=PO

Nearest TMC-1 molecule (distance): CO (2.50)

Is DFT optimized?: True

Property	Value
Formula	HO2P
Molecular weight	63.980
IUPAC name	phosphenous acid
$\mu_{a,b,c}$	2.3, 1.2, 1.0
A, B, C	29076.1507, 8268.0991, 6917.6356
A_s, B_s, C_s	28991.8299, 8244.1216, 6897.5744
Charge, Multiplicity	0, 1
Predicted log column density	12.926±2.326
Electronic energy	-493.56042

geom754



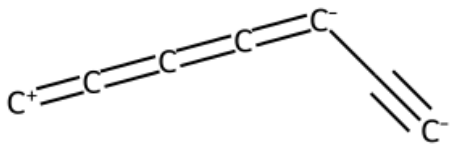
SMILES: O=[O+][O−]

Nearest TMC-1 molecule (distance): N (2.41)

Is DFT optimized?: True

Property	Value
Formula	O3
Molecular weight	47.997
IUPAC name	ozone
$\mu_{a,b,c}$	0.0, 0.0, 0.7
A, B, C	114529.2211, 13823.0914, 12334.3932
A_s, B_s, C_s	114197.0864, 13783.0044, 12298.6235
Charge, Multiplicity	0, 1
Predicted log column density	12.278±2.327
Electronic energy	-225.34034

geom755



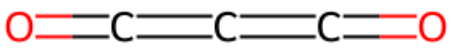
SMILES: [C−]#C[C−]=C=C=C=[CH+]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (5.28)

Is DFT optimized?: True

Property	Value
Formula	C7H-
Molecular weight	85.085
IUPAC name	
$\mu_{a,b,c}$	5.1, 1.8, 0.0
A, B, C	278324.3536, 877.2958, 874.5415
A_s, B_s, C_s	277517.2130, 874.7517, 872.0054
Charge, Multiplicity	-1, 1
Predicted log column density	11.000±2.150
Electronic energy	-266.98094

geom756



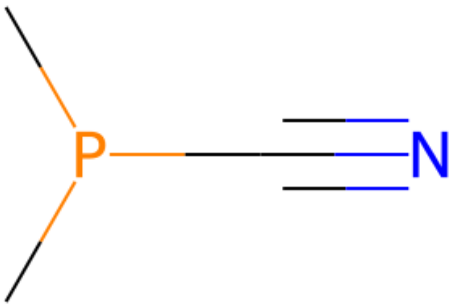
SMILES: O=C=C=C=O

Nearest TMC-1 molecule (distance): C=C=C=O (4.00)

Is DFT optimized?: True

Property	Value
Formula	C3O2
Molecular weight	68.031
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 2201.3698, 2201.3698
A_s, B_s, C_s	∞, 2194.9858, 2194.9858
Charge, Multiplicity	0, 1
Predicted log column density	9.587±1.944
Electronic energy	-264.62915

geom757



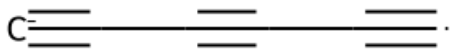
SMILES: CP(C)C#N

Nearest TMC-1 molecule (distance): [C−]#CC#[S+] (5.35)

Is DFT optimized?: True

Property	Value
Formula	C3H6NP
Molecular weight	87.062
IUPAC name	dimethylphosphanylformonitrile
$\mu_{a,b,c}$	4.3, 0.0, 0.6
A, B, C	5691.8769, 3084.0390, 2390.2699
A_s, B_s, C_s	5675.3705, 3075.0953, 2383.3381
Charge, Multiplicity	0, 1
Predicted log column density	10.222±4.682
Electronic energy	-513.94933

geom758



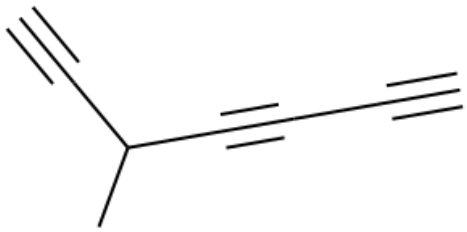
SMILES: [C]#CC#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (4.52)

Is DFT optimized?: True

Property	Value
Formula	C6-
Molecular weight	72.066
IUPAC name	hexa-1,3,5-triyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 1434.8295, 1434.8295
A_s, B_s, C_s	∞, 1430.6685, 1430.6685
Charge, Multiplicity	-1, 2
Predicted log column density	11.656±1.578
Electronic energy	-228.22553

geom759



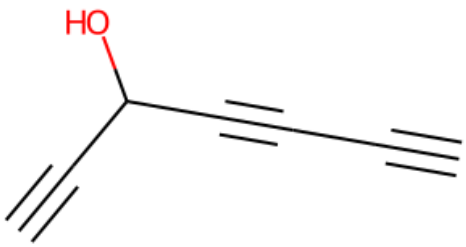
SMILES: C#CC#CC(C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (4.58)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	
$\mu_{a,b,c}$	0.6, 0.7, 0.1
A, B, C	4580.3340, 922.6951, 794.4124
A_s, B_s, C_s	4567.0511, 920.0193, 792.1086
Charge, Multiplicity	0, 1
Predicted log column density	10.001±4.166
Electronic energy	-308.14459

geom760



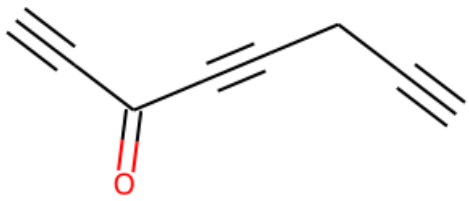
SMILES: C#CC#CC(O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (4.58)

Is DFT optimized?: True

Property	Value
Formula	C7H4O
Molecular weight	104.108
IUPAC name	
$\mu_{a,b,c}$	0.4, 1.4, 0.7
A, B, C	4711.1166, 926.2723, 797.8159
A_s, B_s, C_s	4697.4544, 923.5861, 795.5022
Charge, Multiplicity	0, 1
Predicted log column density	10.105±4.254
Electronic energy	-344.02592

geom761



SMILES: C#CCC#CC(=O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.35)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	1.2, 3.9, 0.1
A, B, C	4439.5041, 649.1458, 575.7041
A_s, B_s, C_s	4426.6296, 647.2632, 574.0346
Charge, Multiplicity	0, 1
Predicted log column density	9.461±4.302
Electronic energy	-382.11529

geom762

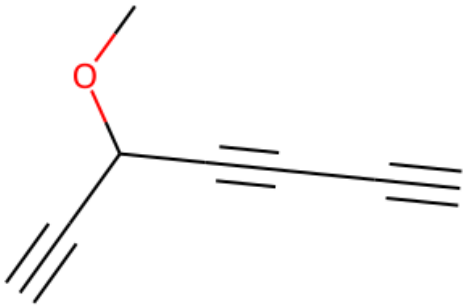
SMILES: C#CCC#CCC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.40)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	octa-1,4,7-triyne
$\mu_{a,b,c}$	0.0, 0.0, 0.5
A, B, C	6639.3915, 701.5323, 700.7147
A_s, B_s, C_s	6620.1373, 699.4978, 698.6827
Charge, Multiplicity	0, 1
Predicted log column density	10.546±3.326
Electronic energy	-308.13456

geom763



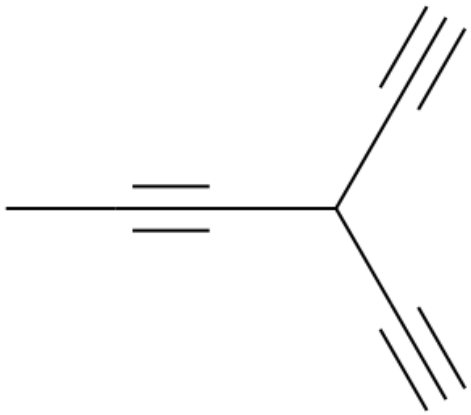
SMILES: C#CC#CC(C#C)OC

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.41)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	1.3, 0.6, 0.9
A, B, C	3293.8679, 753.9583, 628.4846
A_s, B_s, C_s	3284.3157, 751.7718, 626.6620
Charge, Multiplicity	0, 1
Predicted log column density	10.760±4.641
Electronic energy	-383.31681

geom764



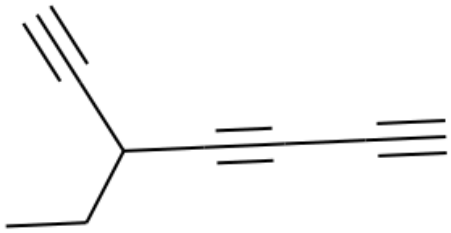
SMILES: C#CC(C#C)C#CC

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.52)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	3-ethynylhexa-1,4-diyne
$\mu_{a,b,c}$	1.0, 0.0, 0.1
A, B, C	2671.9276, 1293.9143, 916.7578
A_s, B_s, C_s	2664.1790, 1290.1619, 914.0992
Charge, Multiplicity	0, 1
Predicted log column density	9.595±4.488
Electronic energy	-308.13010

geom765



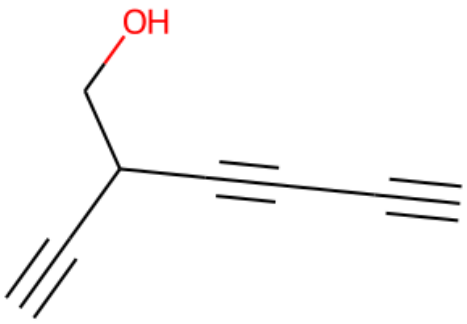
SMILES: C#CC#CC(C#C)CC

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.58)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.6, 0.0
A, B, C	3172.5744, 731.2411, 612.2714
A_s, B_s, C_s	3163.3739, 729.1205, 610.4958
Charge, Multiplicity	0, 1
Predicted log column density	8.538±5.121
Electronic energy	-347.44894

geom766



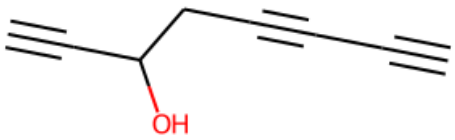
SMILES: C#CC#CC(C#C)CO

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.59)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	1.3, 1.1, 0.8
A, B, C	2801.5554, 814.4942, 699.5728
A_s, B_s, C_s	2793.4309, 812.1322, 697.5440
Charge, Multiplicity	0, 1
Predicted log column density	8.098±4.727
Electronic energy	-383.33462

geom767



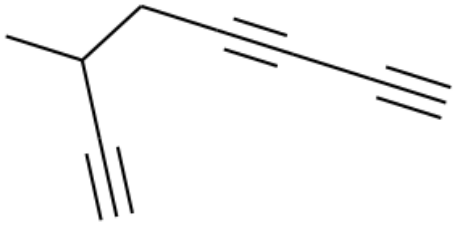
SMILES: C#CC#CCC(O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.61)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	0.4, 0.7, 1.1
A, B, C	2797.9907, 820.5004, 737.6197
A_s, B_s, C_s	2789.8765, 818.1209, 735.4806
Charge, Multiplicity	0, 1
Predicted log column density	10.011±4.837
Electronic energy	-383.34064

geom768



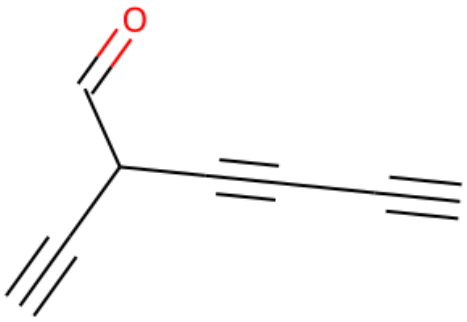
SMILES: C#CC#CCC(C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.62)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.2, 0.0
A, B, C	6359.5861, 585.8444, 551.1303
A_s, B_s, C_s	6341.1433, 584.1454, 549.5320
Charge, Multiplicity	0, 1
Predicted log column density	10.965±4.572
Electronic energy	-347.45538

geom769



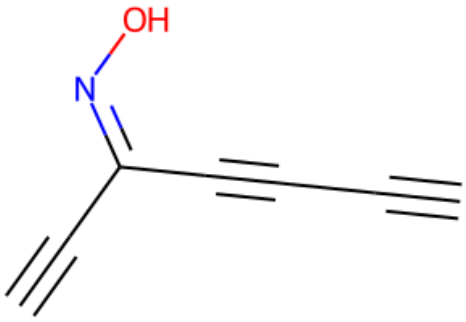
SMILES: C#CC#CC(C#C)C=O

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.63)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	1.2, 2.0, 0.7
A, B, C	2672.8773, 819.8353, 647.3435
A_s, B_s, C_s	2665.1260, 817.4578, 645.4662
Charge, Multiplicity	0, 1
Predicted log column density	7.751±4.228
Electronic energy	-382.11822

geom770



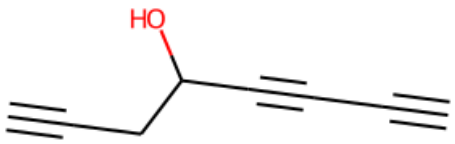
SMILES: C#CC#CC(C#C)=NO

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	0.4, 0.3, 0.0
A, B, C	3793.4655, 742.1743, 620.7310
A_s, B_s, C_s	3782.4644, 740.0219, 618.9309
Charge, Multiplicity	0, 1
Predicted log column density	7.339±5.361
Electronic energy	-398.10863

geom771



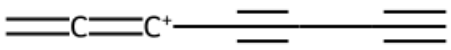
SMILES: C#CC#CC(O)CC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.64)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	0.0, 1.3, 0.8
A, B, C	2679.2870, 850.6303, 721.8824
A_s, B_s, C_s	2671.5170, 848.1635, 719.7889
Charge, Multiplicity	0, 1
Predicted log column density	11.011±4.535
Electronic energy	-383.34057

geom772



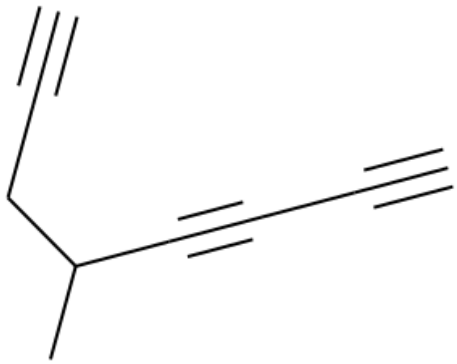
SMILES: C#CC#C[C+]=C=C

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (4.02)

Is DFT optimized?: True

Property	Value
Formula	C7H3+
Molecular weight	87.101
IUPAC name	hepta-1,2-dien-4,6-diyne
$\mu_{a,b,c}$	2.3, 0.0, 0.0
A, B, C	286396.1895, 819.3206, 816.9835
A_s, B_s, C_s	285565.6406, 816.9446, 814.6143
Charge, Multiplicity	1, 1
Predicted log column density	11.939±1.724
Electronic energy	-267.92477

geom773



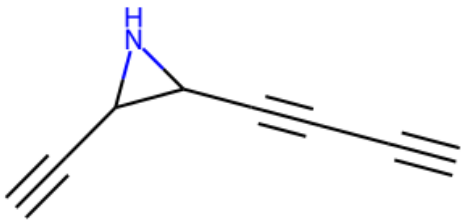
SMILES: C#CC#CC(C)CC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.75)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	5-methylocta-1,3,7-triyne
$\mu_{a,b,c}$	0.5, 0.3, 0.0
A, B, C	5762.1920, 595.8521, 552.4112
A_s, B_s, C_s	5745.4816, 594.1242, 550.8092
Charge, Multiplicity	0, 1
Predicted log column density	11.962±4.425
Electronic energy	-347.45536

geom774



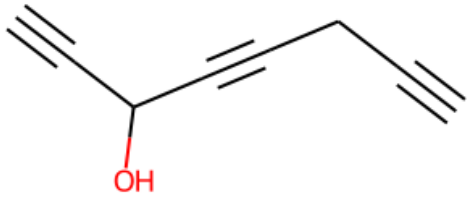
SMILES: C#CC#CC1NC1C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.89)

Is DFT optimized?: True

Property	Value
Formula	C8H5N
Molecular weight	115.135
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.8, 0.8
A, B, C	7247.9413, 592.9746, 568.2988
A_s, B_s, C_s	7226.9223, 591.2550, 566.6507
Charge, Multiplicity	0, 1
Predicted log column density	9.410±5.885
Electronic energy	-362.23229

geom775



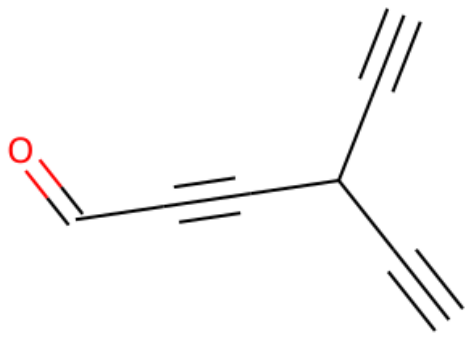
SMILES: C#CCC#CC(O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.90)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	octa-1,4,7-triyn-3-ol
$\mu_{a,b,c}$	1.2, 1.3, 0.4
A, B, C	3035.6051, 681.5207, 649.5204
A_s, B_s, C_s	3026.8019, 679.5443, 647.6368
Charge, Multiplicity	0, 1
Predicted log column density	9.287±4.883
Electronic energy	-383.32168

geom776



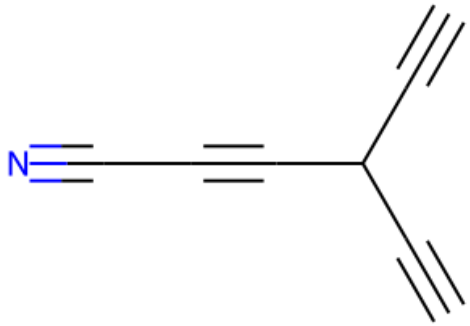
SMILES: C#CC(C#C)C#CC=O

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (5.92)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	3.0, 1.5, 0.1
A, B, C	2627.6832, 822.1177, 646.2161
A_s, B_s, C_s	2620.0629, 819.7335, 644.3421
Charge, Multiplicity	0, 1
Predicted log column density	7.644±4.648
Electronic energy	-382.10145

geom777



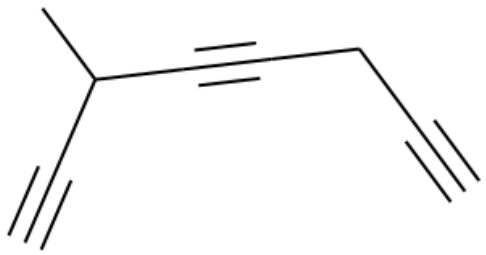
SMILES: C#CC(C#C)C#CC#N

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.00)

Is DFT optimized?: True

Property	Value
Formula	C8H3N
Molecular weight	113.119
IUPAC name	
$\mu_{a,b,c}$	4.6, 0.0, 0.8
A, B, C	2662.3943, 849.7630, 668.5944
A_s, B_s, C_s	2654.6733, 847.2987, 666.6555
Charge, Multiplicity	0, 1
Predicted log column density	9.082±4.407
Electronic energy	-361.02516

geom778



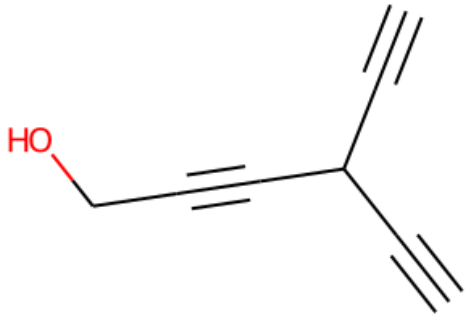
SMILES: C#CCC#CC(C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.00)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.7, 0.2
A, B, C	3407.0446, 649.8711, 592.9166
A_s, B_s, C_s	3397.1642, 647.9865, 591.1972
Charge, Multiplicity	0, 1
Predicted log column density	9.174±4.886
Electronic energy	-347.43929

geom779



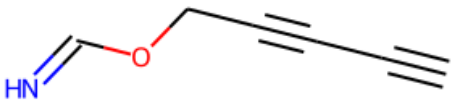
SMILES: C#CC(C#C)C#CCO

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.07)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	1.0, 1.2, 0.2
A, B, C	2571.9180, 769.7395, 624.1369
A_s, B_s, C_s	2564.4594, 767.5073, 622.3269
Charge, Multiplicity	0, 1
Predicted log column density	7.801±5.482
Electronic energy	-383.31499

geom780



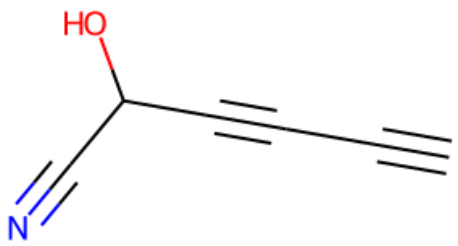
SMILES: C#CC#CCOC=N

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (5.96)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	2.5, 1.8, 0.0
A, B, C	12729.9369, 638.1491, 610.0299
A_s, B_s, C_s	12693.0201, 636.2985, 608.2609
Charge, Multiplicity	0, 1
Predicted log column density	13.497±4.739
Electronic energy	-361.33513

geom781



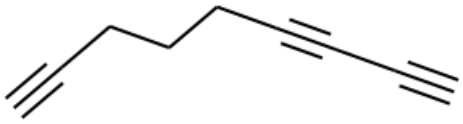
SMILES: C#CC#CC(O)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.44)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO
Molecular weight	105.096
IUPAC name	
$\mu_{a,b,c}$	3.2, 1.6, 0.0
A, B, C	4830.0092, 925.4466, 799.8613
A_s, B_s, C_s	4816.0022, 922.7628, 797.5417
Charge, Multiplicity	0, 1
Predicted log column density	10.120±4.146
Electronic energy	-360.11659

geom782



SMILES: C#CC#CCCCC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.21)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	nona-1,3,8-triyne
$\mu_{a,b,c}$	0.6, 0.7, 0.0
A, B, C	6602.8021, 460.6475, 434.0705
A_s, B_s, C_s	6583.6540, 459.3116, 432.8117
Charge, Multiplicity	0, 1
Predicted log column density	9.881±3.438
Electronic energy	-347.45402

geom783

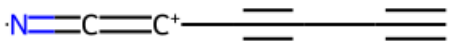
SMILES: C#CCC#CCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.46)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	2.2, 3.2, 1.2
A, B, C	4892.7413, 794.1802, 722.3157
A_s, B_s, C_s	4878.5523, 791.8771, 720.2209
Charge, Multiplicity	0, 1
Predicted log column density	9.324±3.067
Electronic energy	-324.22884

geom784



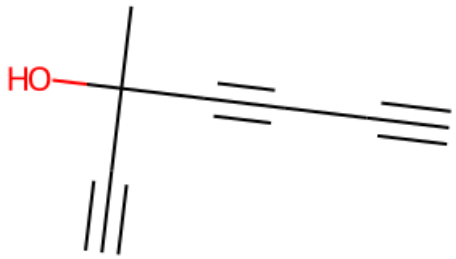
SMILES: C#CC#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (3.70)

Is DFT optimized?: True

Property	Value
Formula	C6HN+
Molecular weight	87.081
IUPAC name	
$\mu_{a,b,c}$	7.5, 0.0, 0.0
A, B, C	286946851.1697, 842.5864, 842.5840
A_s, B_s, C_s	286114705.3013, 840.1429, 840.1405
Charge, Multiplicity	1, 2
Predicted log column density	12.161±1.766
Electronic energy	-283.31961

geom785



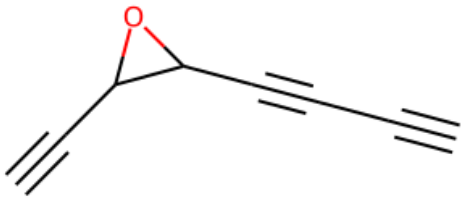
SMILES: C#CC#CC(C)(O)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.24)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.8, 1.4
A, B, C	3076.6766, 815.0004, 739.9002
A_s, B_s, C_s	3067.7542, 812.6369, 737.7544
Charge, Multiplicity	0, 1
Predicted log column density	14.903±5.721
Electronic energy	-383.33236

geom786



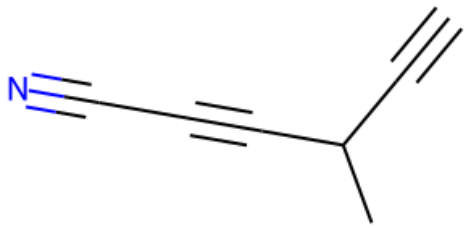
SMILES: C#CC#CC1OC1C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.25)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	0.1, 1.9, 0.3
A, B, C	8323.9730, 583.0648, 562.8984
A_s, B_s, C_s	8299.8334, 581.3739, 561.2660
Charge, Multiplicity	0, 1
Predicted log column density	9.611±6.711
Electronic energy	-382.09100

geom787



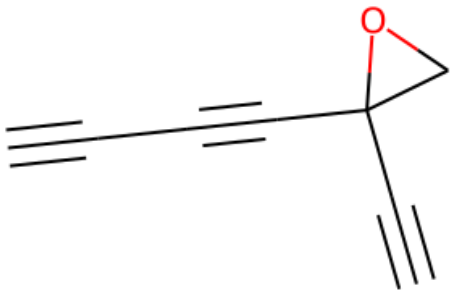
SMILES: C#CC(C)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.58)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	4.9, 1.3, 0.5
A, B, C	4548.5634, 926.8339, 796.5416
A_s, B_s, C_s	4535.3726, 924.1461, 794.2316
Charge, Multiplicity	0, 1
Predicted log column density	10.000±4.132
Electronic energy	-324.23251

geom788



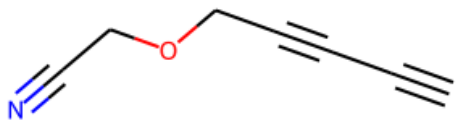
SMILES: C#CC#CC1(C#C)CO1

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.33)

Is DFT optimized?: True

Property	Value
Formula	C8H4O
Molecular weight	116.119
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.5, 1.9
A, B, C	3410.0786, 838.0967, 703.7490
A_s, B_s, C_s	3400.1894, 835.6662, 701.7081
Charge, Multiplicity	0, 1
Predicted log column density	9.177±6.153
Electronic energy	-382.08652

geom789



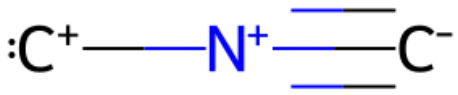
SMILES: C#CC#CCOCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (6.24)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	2.2, 4.3, 0.0
A, B, C	6491.4110, 495.9198, 463.4222
A_s, B_s, C_s	6472.5859, 494.4817, 462.0783
Charge, Multiplicity	0, 1
Predicted log column density	11.312±4.403
Electronic energy	-399.41139

geom790



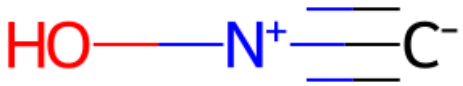
SMILES: [C+][N+]#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (3.85)

Is DFT optimized?: True

Property	Value
Formula	C2N+
Molecular weight	38.029
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 13659.8317, 13659.8317
A_s, B_s, C_s	∞, 13620.2182, 13620.2182
Charge, Multiplicity	1, 3
Predicted log column density	12.088±1.687
Electronic energy	-130.23759

geom791



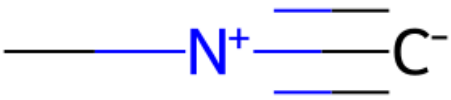
SMILES: [C−]#[N+]O

Nearest TMC-1 molecule (distance): [C−]#[NH+] (4.16)

Is DFT optimized?: True

Property	Value
Formula	CHNO
Molecular weight	43.025
IUPAC name	hydroxyazaniumylidynemethane
$\mu_{a,b,c}$	3.0, 1.7, 0.0
A, B, C	623510.5930, 11110.9974, 10916.4653
A_s, B_s, C_s	621702.4123, 11078.7755, 10884.8076
Charge, Multiplicity	0, 1
Predicted log column density	11.520±1.747
Electronic energy	-168.48996

geom792



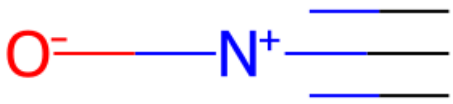
SMILES: [C−]#[N+]C

Nearest TMC-1 molecule (distance): [C−]#[S+] (3.99)

Is DFT optimized?: True

Property	Value
Formula	C2H3N
Molecular weight	41.053
IUPAC name	isocyanomethane
$\mu_{a,b,c}$	3.9, 0.0, 0.0
A, B, C	157749.0689, 10067.2357, 10066.9327
A_s, B_s, C_s	157291.5966, 10038.0408, 10037.7386
Charge, Multiplicity	0, 1
Predicted log column density	12.174±1.772
Electronic energy	-132.67480

geom793



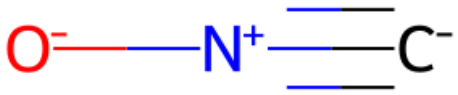
SMILES: C#[N+][O-]

Nearest TMC-1 molecule (distance): [C+]#C[O-] (3.79)

Is DFT optimized?: True

Property	Value
Formula	CHNO
Molecular weight	43.025
IUPAC name	formonitrile oxide
$\mu_{a,b,c}$	0.0, 0.0, 3.6
A, B, C	3877986092.4943, 11462.7759, 11462.7420
A_s, B_s, C_s	3866739932.8261, 11429.5338, 11429.5000
Charge, Multiplicity	0, 1
Predicted log column density	12.258±2.726
Electronic energy	-168.51634

geom794



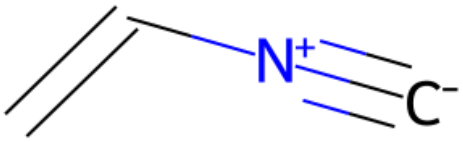
SMILES: [C−]#[N+][O−]

Nearest TMC-1 molecule (distance): [C−]#[NH+] (4.81)

Is DFT optimized?: False

Property	Value
Formula	CNO-
Molecular weight	42.017
IUPAC name	oxidoazaniumylidynemethane
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	∞, 11088.5850, 11088.5850
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-1, 1
Predicted log column density	11.153±2.475
Electronic energy	-167.95855

geom795



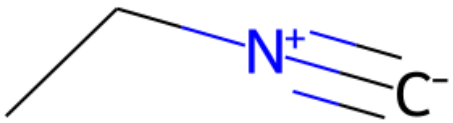
SMILES: [C−]#[N+]C=C

Nearest TMC-1 molecule (distance): C#C[N+]#[C−] (5.22)

Is DFT optimized?: True

Property	Value
Formula	C3H3N
Molecular weight	53.064
IUPAC name	isocyanoethene
$\mu_{a,b,c}$	3.4, 0.8, 0.0
A, B, C	51761.2746, 5374.5206, 4868.9637
A_s, B_s, C_s	51611.1669, 5358.9345, 4854.8438
Charge, Multiplicity	0, 1
Predicted log column density	11.162±1.942
Electronic energy	-170.74016

geom796



SMILES: [C−]#[N+]CC

Nearest TMC-1 molecule (distance): C#C[N+]#[C−] (5.30)

Is DFT optimized?: True

Property	Value
Formula	C3H5N
Molecular weight	55.080
IUPAC name	isocyanoethane
$\mu_{a,b,c}$	3.8, 1.3, 0.0
A, B, C	28138.8903, 5077.2004, 4545.9750
A_s, B_s, C_s	28057.2876, 5062.4765, 4532.7917
Charge, Multiplicity	0, 1
Predicted log column density	11.061±2.934
Electronic energy	-171.98091

geom797

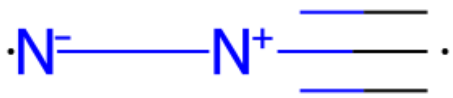
SMILES: CC#[N+][O-]

Nearest TMC-1 molecule (distance): [CH+]=C=[C-] (4.03)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO
Molecular weight	57.052
IUPAC name	acetonitrile oxide
$\mu_{a,b,c}$	4.8, 0.0, 0.0
A, B, C	158957.3964, 3898.8294, 3898.7886
A_s, B_s, C_s	158496.4200, 3887.5228, 3887.4821
Charge, Multiplicity	0, 1
Predicted log column density	11.847±3.208
Electronic energy	-207.83145

geom798



SMILES: [C]#[N+][N−]

Nearest TMC-1 molecule (distance): [C−]#[NH+] (3.37)

Is DFT optimized?: True

Property	Value
Formula	CN2
Molecular weight	40.025
IUPAC name	methylidyneazaniumylazanide
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	∞, 13088.3071, 13088.3071
A_s, B_s, C_s	∞, 13050.3510, 13050.3510
Charge, Multiplicity	0, 3
Predicted log column density	13.622±2.757
Electronic energy	-147.39267

geom799

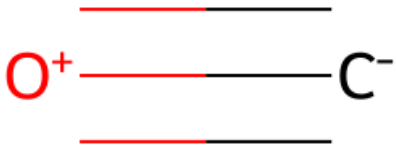
SMILES: C=[N+]=[N−]

Nearest TMC-1 molecule (distance): [C−]#[NH+] (5.54)

Is DFT optimized?: True

Property	Value
Formula	CH2N2
Molecular weight	42.041
IUPAC name	diazomethane
$\mu_{a,b,c}$	0.0, 1.8, 0.0
A, B, C	274584.0626, 11362.0558, 10910.5850
A_s, B_s, C_s	273787.7688, 11329.1058, 10878.9443
Charge, Multiplicity	0, 1
Predicted log column density	14.101±4.128
Electronic energy	-148.68648

geom800



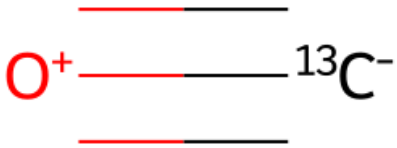
SMILES: [C−]#[O+]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (4.42)

Is DFT optimized?: False

Property	Value
Formula	CO
Molecular weight	28.010
IUPAC name	carbon monoxide
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	∞, 65975.5774, 65975.5774
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.173±2.418
Electronic energy	-113.26045

geom801



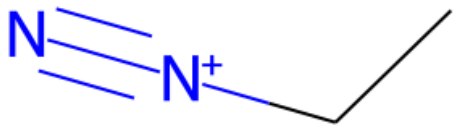
SMILES: [13C−]#[O+]

Nearest TMC-1 molecule (distance): [CH+]=C=[C−] (4.42)

Is DFT optimized?: False

Property	Value
Formula	CO
Molecular weight	29.002
IUPAC name	(113C)methylidyneoxidanium
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	∞, 65975.5774, 65975.5774
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.173±2.418
Electronic energy	-113.26045

geom802



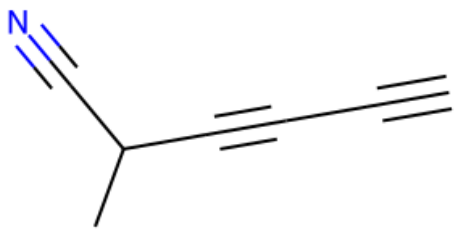
SMILES: CC[N+]#N

Nearest TMC-1 molecule (distance): N=C=O (4.96)

Is DFT optimized?: True

Property	Value
Formula	C2H5N2+
Molecular weight	57.076
IUPAC name	ethanediazonium
$\mu_{a,b,c}$	0.8, 1.3, 0.0
A, B, C	27217.3119, 4859.9015, 4354.0552
A_s, B_s, C_s	27138.3817, 4845.8078, 4341.4284
Charge, Multiplicity	1, 1
Predicted log column density	12.122±3.611
Electronic energy	-188.34686

geom803



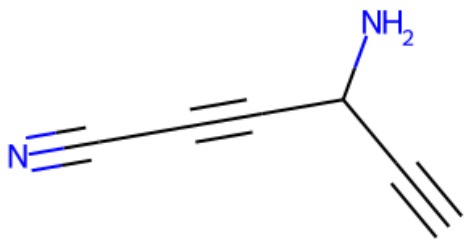
SMILES: C#CC#CC(C)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.54)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	1.8, 3.4, 0.8
A, B, C	4714.2314, 919.6606, 795.4513
A_s, B_s, C_s	4700.5601, 916.9936, 793.1445
Charge, Multiplicity	0, 1
Predicted log column density	10.066±3.966
Electronic energy	-324.23810

geom804



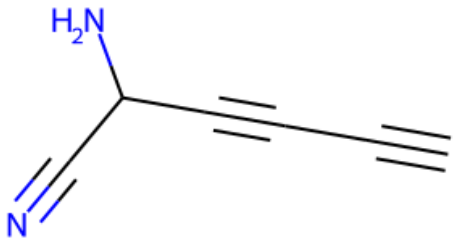
SMILES: C#CC(N)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.65)

Is DFT optimized?: True

Property	Value
Formula	C6H4N2
Molecular weight	104.112
IUPAC name	
$\mu_{a,b,c}$	5.7, 0.0, 0.0
A, B, C	4567.6703, 934.1930, 800.0032
A_s, B_s, C_s	4554.4240, 931.4838, 797.6832
Charge, Multiplicity	0, 1
Predicted log column density	8.997±4.092
Electronic energy	-340.25514

geom805



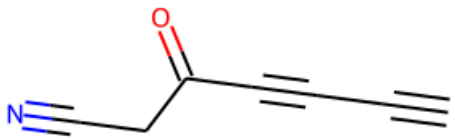
SMILES: C#CC#CC(N)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (4.65)

Is DFT optimized?: True

Property	Value
Formula	C6H4N2
Molecular weight	104.112
IUPAC name	
$\mu_{a,b,c}$	3.4, 3.2, 0.5
A, B, C	4783.1527, 921.7668, 796.9964
A_s, B_s, C_s	4769.2815, 919.0937, 794.6851
Charge, Multiplicity	0, 1
Predicted log column density	9.053±4.069
Electronic energy	-340.26019

geom806



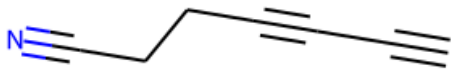
SMILES: C#CC#CC(=O)CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.08)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	1.3, 0.5, 1.6
A, B, C	2374.6899, 973.5389, 701.7891
A_s, B_s, C_s	2367.8033, 970.7156, 699.7539
Charge, Multiplicity	0, 1
Predicted log column density	10.243±3.861
Electronic energy	-398.22168

geom807



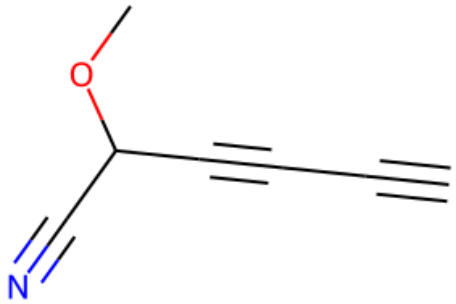
SMILES: C#CC#CCCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.14)

Is DFT optimized?: True

Property	Value
Formula	C7H5N
Molecular weight	103.124
IUPAC name	
$\mu_{a,b,c}$	3.4, 0.6, 0.0
A, B, C	19328.9892, 612.1503, 597.7535
A_s, B_s, C_s	19272.9352, 610.3751, 596.0200
Charge, Multiplicity	0, 1
Predicted log column density	9.701±3.016
Electronic energy	-324.24489

geom808



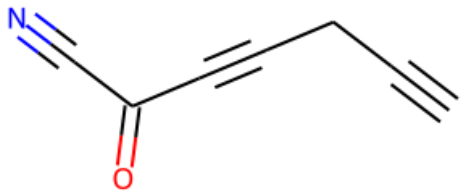
SMILES: C#CC#CC(C#N)OC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.34)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	0.6, 2.6, 1.7
A, B, C	3419.1823, 749.1869, 629.3540
A_s, B_s, C_s	3409.2667, 747.0142, 627.5289
Charge, Multiplicity	0, 1
Predicted log column density	10.795±4.621
Electronic energy	-399.40829

geom809



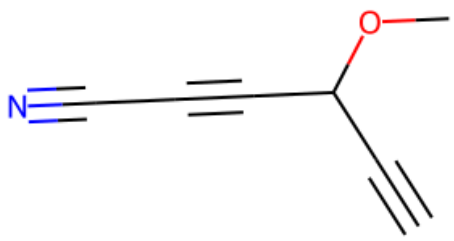
SMILES: C#CCC#CC(=O)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.38)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	4.8, 0.9, 1.1
A, B, C	3961.0530, 651.3179, 604.9649
A_s, B_s, C_s	3949.5660, 649.4291, 603.2105
Charge, Multiplicity	0, 1
Predicted log column density	9.047±3.941
Electronic energy	-398.20069

geom810



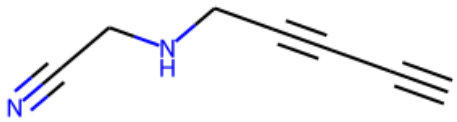
SMILES: C#CC(C#CC#N)OC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.41)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	3.7, 0.8, 1.5
A, B, C	2396.9502, 890.3931, 666.3228
A_s, B_s, C_s	2389.9991, 887.8110, 664.3904
Charge, Multiplicity	0, 1
Predicted log column density	10.729±4.626
Electronic energy	-399.40349

geom811



SMILES: C#CC#CCNCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.47)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	2.4, 3.3, 1.2
A, B, C	6671.3233, 478.4936, 449.4275
A_s, B_s, C_s	6651.9765, 477.1060, 448.1241
Charge, Multiplicity	0, 1
Predicted log column density	11.205±4.644
Electronic energy	-379.56045

geom812

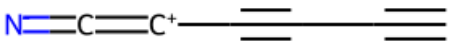
SMILES: C#CC(=O)C#CCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.47)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	2.0, 6.0, 0.5
A, B, C	4595.7319, 644.6715, 570.2844
A_s, B_s, C_s	4582.4043, 642.8019, 568.6306
Charge, Multiplicity	0, 1
Predicted log column density	8.251±4.258
Electronic energy	-398.20713

geom813



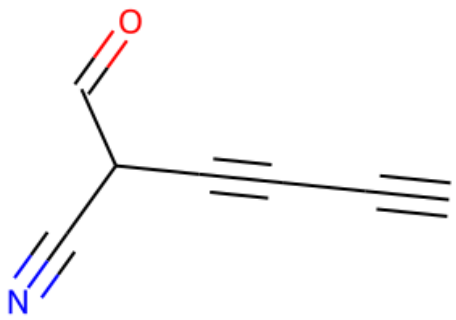
SMILES: C#CC#C[C+]=C=[N-]

Nearest TMC-1 molecule (distance): C#CC#CC#[C-] (3.79)

Is DFT optimized?: True

Property	Value
Formula	C6HN
Molecular weight	87.081
IUPAC name	hex-1-en-3,5-diynylideneazanide
$\mu_{a,b,c}$	5.6, 0.0, 0.0
A, B, C	1571886728.5457, 839.7794, 839.7790
A_s, B_s, C_s	1567328257.0329, 837.3441, 837.3436
Charge, Multiplicity	0, 1
Predicted log column density	12.627±3.093
Electronic energy	-283.61613

geom814



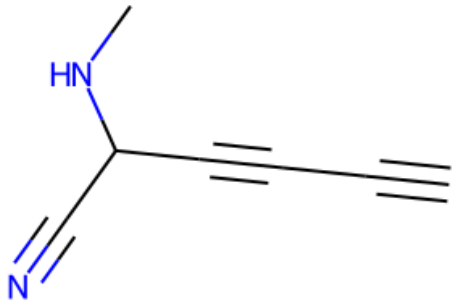
SMILES: C#CC#CC(C#N)C=O

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.51)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	3.2, 1.2, 0.0
A, B, C	2676.3624, 824.3808, 649.8643
A_s, B_s, C_s	2668.6009, 821.9901, 647.9797
Charge, Multiplicity	0, 1
Predicted log column density	7.744±4.049
Electronic energy	-398.20793

geom815



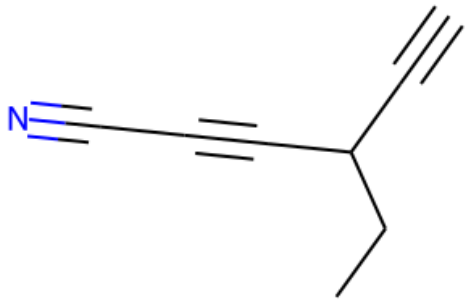
SMILES: C#CC#CC(C#N)NC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	1.4, 4.0, 1.7
A, B, C	3314.0687, 742.8276, 621.7188
A_s, B_s, C_s	3304.4579, 740.6734, 619.9158
Charge, Multiplicity	0, 1
Predicted log column density	9.691±5.364
Electronic energy	-379.55436

geom816



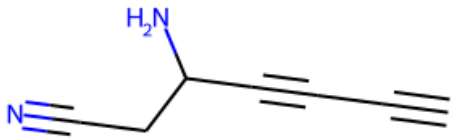
SMILES: C#CC(C#CC#N)CC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.58)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	5.1, 0.9, 0.4
A, B, C	2195.8879, 896.7579, 657.3375
A_s, B_s, C_s	2189.5198, 894.1573, 655.4312
Charge, Multiplicity	0, 1
Predicted log column density	8.495±5.065
Electronic energy	-363.53708

geom817



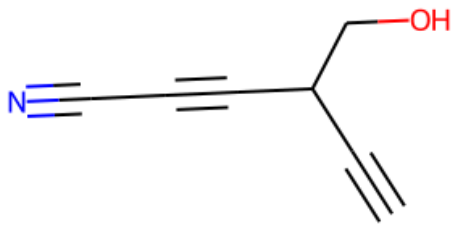
SMILES: C#CC#CC(N)CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.59)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	1.3, 3.9, 1.0
A, B, C	2205.5455, 913.3893, 666.9520
A_s, B_s, C_s	2199.1495, 910.7405, 665.0178
Charge, Multiplicity	0, 1
Predicted log column density	8.215±4.365
Electronic energy	-379.57580

geom818



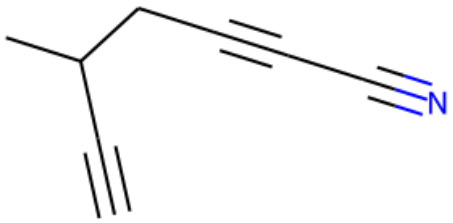
SMILES: C#CC(C#CC#N)CO

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.59)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	4.2, 1.1, 0.2
A, B, C	3286.3079, 726.8919, 612.3479
A_s, B_s, C_s	3276.7776, 724.7839, 610.5721
Charge, Multiplicity	0, 1
Predicted log column density	8.038±4.675
Electronic energy	-399.42348

geom819



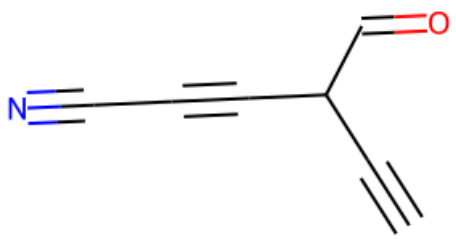
SMILES: C#CC(C)CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.62)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	4.8, 0.5, 0.5
A, B, C	6379.7914, 584.4338, 549.6246
A_s, B_s, C_s	6361.2900, 582.7389, 548.0307
Charge, Multiplicity	0, 1
Predicted log column density	10.936±4.551
Electronic energy	-363.54366

geom820



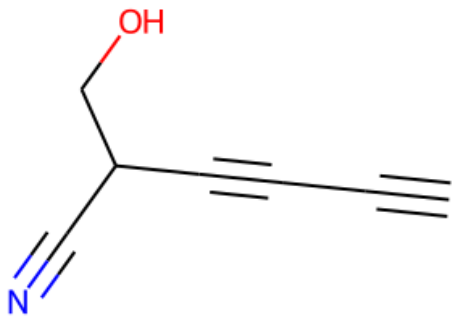
SMILES: C#CC(C#CC#N)C=O

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H3NO
Molecular weight	117.107
IUPAC name	
$\mu_{a,b,c}$	5.8, 1.7, 1.5
A, B, C	2582.4860, 886.8913, 685.6996
A_s, B_s, C_s	2574.9968, 884.3193, 683.7111
Charge, Multiplicity	0, 1
Predicted log column density	7.683±4.204
Electronic energy	-398.20308

geom821



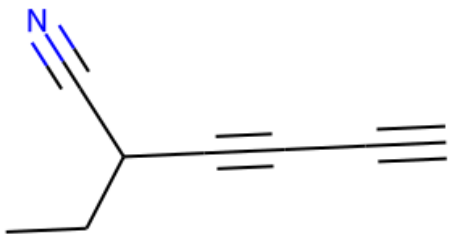
SMILES: C#CC#CC(C#N)CO

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	2.7, 2.2, 0.0
A, B, C	2318.8212, 887.5077, 660.9514
A_s, B_s, C_s	2312.0966, 884.9339, 659.0347
Charge, Multiplicity	0, 1
Predicted log column density	8.085±4.664
Electronic energy	-399.42856

geom822



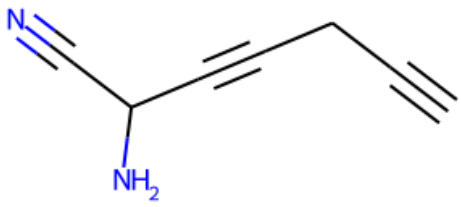
SMILES: C#CC#CC(C#N)CC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.64)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	1.0, 3.7, 0.8
A, B, C	3315.2978, 726.1070, 613.5445
A_s, B_s, C_s	3305.6835, 724.0013, 611.7652
Charge, Multiplicity	0, 1
Predicted log column density	8.548±5.046
Electronic energy	-363.54288

geom823



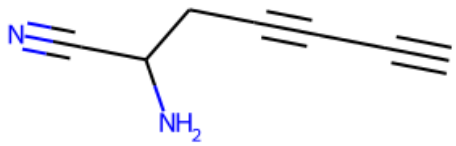
SMILES: C#CCC#CC(N)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.66)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	3.0, 4.2, 0.0
A, B, C	2874.7431, 723.5991, 641.4169
A_s, B_s, C_s	2866.4064, 721.5007, 639.5568
Charge, Multiplicity	0, 1
Predicted log column density	8.229±4.619
Electronic energy	-379.55623

geom824



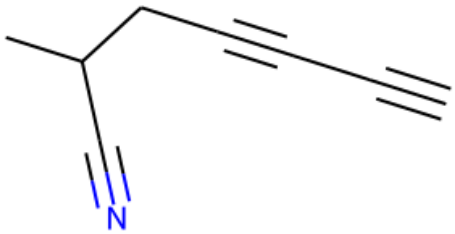
SMILES: C#CC#CCC(N)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.70)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	4.2, 0.2, 0.5
A, B, C	6659.8027, 592.3633, 556.6335
A_s, B_s, C_s	6640.4892, 590.6454, 555.0192
Charge, Multiplicity	0, 1
Predicted log column density	8.421±4.714
Electronic energy	-379.57441

geom825



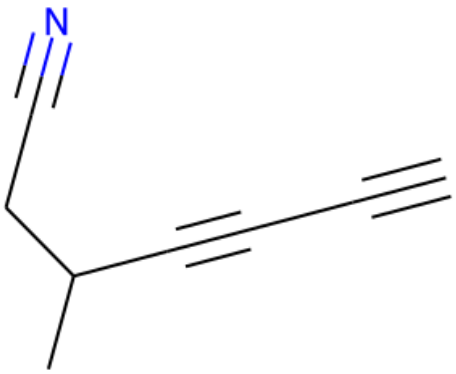
SMILES: C#CC#CCC(C)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.70)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	3.3, 1.2, 0.1
A, B, C	6335.4505, 587.1153, 552.2855
A_s, B_s, C_s	6317.0777, 585.4127, 550.6839
Charge, Multiplicity	0, 1
Predicted log column density	10.983±4.406
Electronic energy	-363.55039

geom826



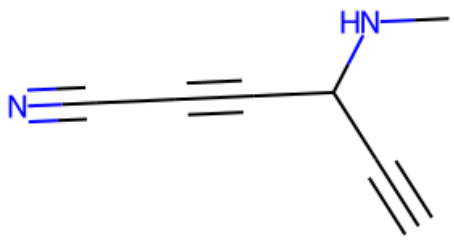
SMILES: C#CC#CC(C)CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.73)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	3.3, 1.2, 0.1
A, B, C	6344.3468, 587.0996, 552.2359
A_s, B_s, C_s	6325.9482, 585.3970, 550.6344
Charge, Multiplicity	0, 1
Predicted log column density	10.764±4.373
Electronic energy	-363.55039

geom827



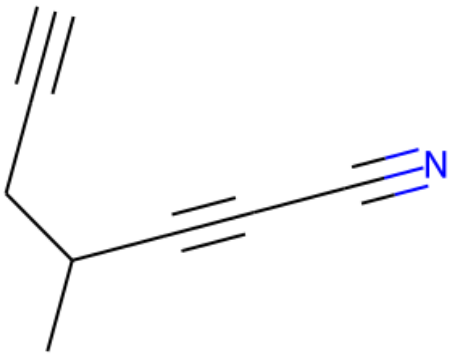
SMILES: C#CC(C#CC#N)NC

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.73)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	5.6, 0.6, 0.0
A, B, C	3211.8459, 744.5921, 621.8131
A_s, B_s, C_s	3202.5316, 742.4328, 620.0099
Charge, Multiplicity	0, 1
Predicted log column density	9.625±5.646
Electronic energy	-379.55163

geom828



SMILES: C#CCC(C)C#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.75)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	
$\mu_{a,b,c}$	4.9, 1.0, 0.3
A, B, C	5776.0162, 594.4281, 551.2845
A_s, B_s, C_s	5759.2657, 592.7043, 549.6858
Charge, Multiplicity	0, 1
Predicted log column density	11.936±4.401
Electronic energy	-363.54372

geom829

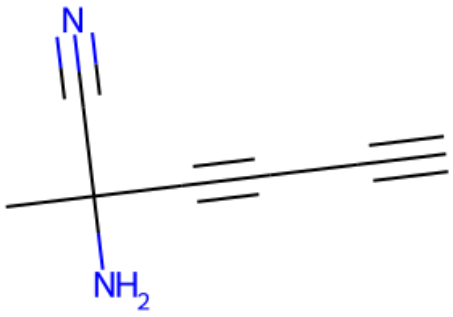
SMILES: C#CC(O)C#CCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.75)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	1.1, 2.0, 0.8
A, B, C	2976.8040, 738.1457, 606.7690
A_s, B_s, C_s	2968.1713, 736.0051, 605.0094
Charge, Multiplicity	0, 1
Predicted log column density	8.063±4.810
Electronic energy	-399.41521

geom830



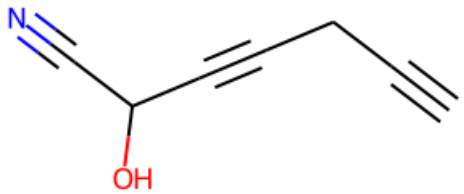
SMILES: C#CC#CC(C)(N)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.77)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	1.5, 4.4, 1.2
A, B, C	3109.4857, 811.0348, 743.8599
A_s, B_s, C_s	3100.4682, 808.6828, 741.7027
Charge, Multiplicity	0, 1
Predicted log column density	14.174±5.582
Electronic energy	-379.56528

geom831



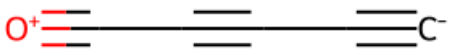
SMILES: C#CCC#CC(O)C#N

Nearest TMC-1 molecule (distance): C#CC#CC#N (5.77)

Is DFT optimized?: True

Property	Value
Formula	C7H5NO
Molecular weight	119.123
IUPAC name	
$\mu_{a,b,c}$	3.1, 2.5, 0.1
A, B, C	2900.1723, 724.5780, 642.5131
A_s, B_s, C_s	2891.7618, 722.4767, 640.6498
Charge, Multiplicity	0, 1
Predicted log column density	9.275±4.706
Electronic energy	-399.41365

geom832



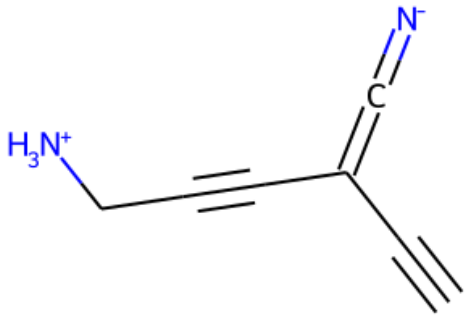
SMILES: [C−]#CC#CC#[O+]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (4.86)

Is DFT optimized?: True

Property	Value
Formula	C5O
Molecular weight	76.054
IUPAC name	
$\mu_{a,b,c}$	3.6, 0.0, 0.0
A, B, C	∞, 1359.1035, 1359.1035
A_s, B_s, C_s	∞, 1355.1621, 1355.1621
Charge, Multiplicity	0, 1
Predicted log column density	9.876±1.813
Electronic energy	-265.43087

geom833



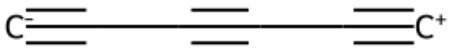
SMILES: C#CC(=C=[N-])C#CC[NH3+]

Nearest TMC-1 molecule (distance): C#CC#CC#[C-] (6.54)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2
Molecular weight	118.139
IUPAC name	
$\mu_{a,b,c}$	4.8, 3.3, 0.6
A, B, C	2125.1631, 622.6110, 541.0343
A_s, B_s, C_s	2119.0001, 620.8055, 539.4653
Charge, Multiplicity	0, 1
Predicted log column density	5.323±5.635
Electronic energy	-379.52832

geom834



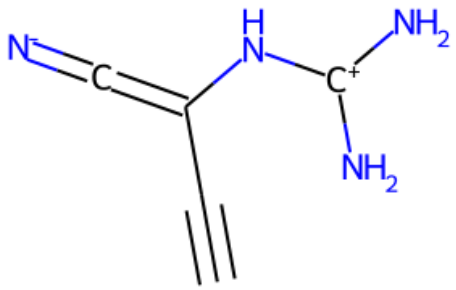
SMILES: [C+]#CC#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (4.83)

Is DFT optimized?: True

Property	Value
Formula	C6
Molecular weight	72.066
IUPAC name	hexa-1,3,5-triyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 1445.6523, 1445.6523
A_s, B_s, C_s	∞, 1441.4599, 1441.4599
Charge, Multiplicity	0, 1
Predicted log column density	11.381±1.706
Electronic energy	-228.13216

geom835



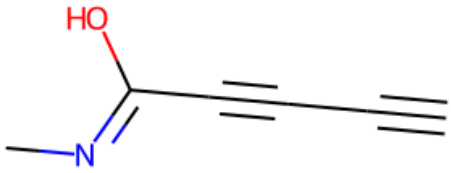
SMILES: C#CC(=C=[N-])N[C+](N)N

Nearest TMC-1 molecule (distance): C#CC#[NH+] (6.97)

Is DFT optimized?: True

Property	Value
Formula	C5H6N4
Molecular weight	122.131
IUPAC name	
$\mu_{a,b,c}$	11.1, 3.5, 0.6
A, B, C	2138.4726, 1195.1007, 900.7836
A_s, B_s, C_s	2132.2710, 1191.6349, 898.1713
Charge, Multiplicity	0, 1
Predicted log column density	11.607±4.665
Electronic energy	-412.88949

geom836



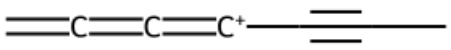
SMILES: C#CC#CC(O)=NC

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (5.77)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	1.5, 2.1, 0.0
A, B, C	8863.1745, 791.6427, 730.0444
A_s, B_s, C_s	8837.4713, 789.3469, 727.9273
Charge, Multiplicity	0, 1
Predicted log column density	8.914±4.276
Electronic energy	-361.34687

geom837



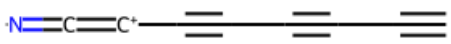
SMILES: C=C=C=[C+]C#CC

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (4.33)

Is DFT optimized?: True

Property	Value
Formula	C7H5+
Molecular weight	89.117
IUPAC name	
$\mu_{a,b,c}$	1.1, 0.1, 0.1
A, B, C	101538.4720, 762.7556, 760.7825
A_s, B_s, C_s	101244.0104, 760.5436, 758.5762
Charge, Multiplicity	1, 1
Predicted log column density	11.831±1.889
Electronic energy	-269.19038

geom838



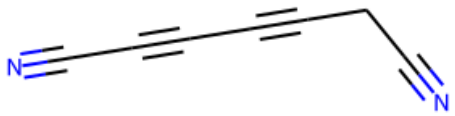
SMILES: C#CC#CC#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (3.70)

Is DFT optimized?: False

Property	Value
Formula	C8HN+
Molecular weight	111.103
IUPAC name	
$\mu_{a,b,c}$	-, -, -
A, B, C	38585.8620, 371.0490, 367.5149
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 2
Predicted log column density	11.859±1.756
Electronic energy	-

geom839



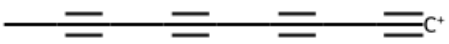
SMILES: N#CC#CC#CCC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (5.21)

Is DFT optimized?: True

Property	Value
Formula	C7H2N2
Molecular weight	114.107
IUPAC name	hepta-2,4-diynedinitrile
$\mu_{a,b,c}$	2.9, 4.0, 0.0
A, B, C	9854.9052, 447.9846, 429.6488
A_s, B_s, C_s	9826.3259, 446.6854, 428.4028
Charge, Multiplicity	0, 1
Predicted log column density	9.752±2.233
Electronic energy	-377.14088

geom840



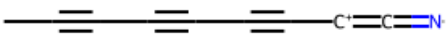
SMILES: [C+]#CC#CC#CC#CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (4.75)

Is DFT optimized?: False

Property	Value
Formula	C9H3+
Molecular weight	111.123
IUPAC name	
$\mu_{a,b,c}$	-, -, -
A, B, C	158199.7073, 342.1593, 342.1593
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 1
Predicted log column density	12.026±1.763
Electronic energy	-

geom841



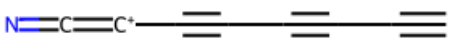
SMILES: CC#CC#CC#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (5.22)

Is DFT optimized?: False

Property	Value
Formula	C9H3N+
Molecular weight	125.130
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.1, 0.2
A, B, C	24897.7212, 255.2372, 253.0514
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	12.036±1.868
Electronic energy	-398.63369

geom842



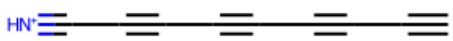
SMILES: C#CC#CC#C[C+]=C=[N−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (3.79)

Is DFT optimized?: True

Property	Value
Formula	C8HN
Molecular weight	111.103
IUPAC name	
$\mu_{a,b,c}$	6.4, 0.0, 0.0
A, B, C	793966102.9575, 397.7451, 397.7449
A_s, B_s, C_s	791663601.2589, 396.5917, 396.5915
Charge, Multiplicity	0, 1
Predicted log column density	12.389±3.080
Electronic energy	-359.74943

geom843



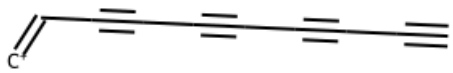
SMILES: C#CC#CC#CC#CC#[NH+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (3.27)

Is DFT optimized?: True

Property	Value
Formula	C9H2N+
Molecular weight	124.122
IUPAC name	
$\mu_{a,b,c}$	7.6, 0.0, 0.0
A, B, C	∞, 285.2517, 285.2517
A_s, B_s, C_s	∞, 284.4245, 284.4245
Charge, Multiplicity	1, 1
Predicted log column density	10.854±1.679
Electronic energy	-398.19521

geom844



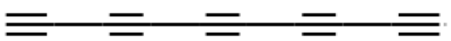
SMILES: C#CC#CC#CC#C[C]=[CH+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (3.16)

Is DFT optimized?: True

Property	Value
Formula	C10H2+
Molecular weight	122.126
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	9817123534.0983, 293.9851, 293.9850
A_s, B_s, C_s	9788653875.8494, 293.1325, 293.1325
Charge, Multiplicity	1, 2
Predicted log column density	11.889±1.621
Electronic energy	-381.48456

geom845



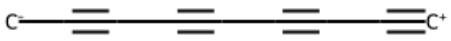
SMILES: [C]#CC#CC#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (3.10)

Is DFT optimized?: True

Property	Value
Formula	C10H
Molecular weight	121.118
IUPAC name	deca-1,3,5,7,9-pentayne
$\mu_{a,b,c}$	1.3, 0.0, 0.0
A, B, C	∞, 299.3321, 299.3321
A_s, B_s, C_s	∞, 298.4640, 298.4640
Charge, Multiplicity	0, 2
Predicted log column density	11.876±1.612
Electronic energy	-381.07003

geom846



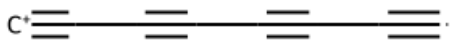
SMILES: [C+]#CC#CC#CC#C[CH2−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (5.15)

Is DFT optimized?: True

Property	Value
Formula	C9H2
Molecular weight	110.115
IUPAC name	
$\mu_{a,b,c}$	9.8, 0.0, 0.0
A, B, C	289496.4634, 404.0338, 403.4707
A_s, B_s, C_s	288656.9236, 402.8621, 402.3007
Charge, Multiplicity	0, 1
Predicted log column density	11.672±2.295
Electronic energy	-343.64942

geom847



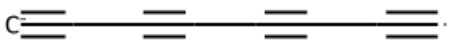
SMILES: [C]#CC#CC#CC#[C+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (5.40)

Is DFT optimized?: True

Property	Value
Formula	C8+
Molecular weight	96.088
IUPAC name	octa-1,3,5,7-tetrayne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 610.0774, 610.0774
A_s, B_s, C_s	∞, 608.3082, 608.3082
Charge, Multiplicity	1, 2
Predicted log column density	11.953±1.815
Electronic energy	-303.87490

geom848



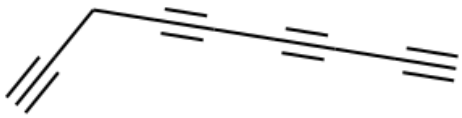
SMILES: [C]#CC#CC#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (4.52)

Is DFT optimized?: True

Property	Value
Formula	C8-
Molecular weight	96.088
IUPAC name	octa-1,3,5,7-tetrayne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 602.5155, 602.5155
A_s, B_s, C_s	∞, 600.7682, 600.7682
Charge, Multiplicity	-1, 2
Predicted log column density	11.374±1.659
Electronic energy	-304.43356

geom849



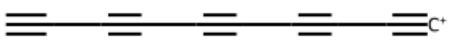
SMILES: C#CC#CC#CCC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#CC#C (2.70)

Is DFT optimized?: True

Property	Value
Formula	C9H4
Molecular weight	112.131
IUPAC name	nona-1,3,5,8-tetrayne
$\mu_{a,b,c}$	0.7, 0.5, 0.0
A, B, C	9374.3046, 452.2320, 432.5703
A_s, B_s, C_s	9347.1191, 450.9206, 431.3158
Charge, Multiplicity	0, 1
Predicted log column density	11.152±2.114
Electronic energy	-344.96403

geom850



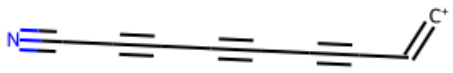
SMILES: [C+]#CC#CC#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (3.61)

Is DFT optimized?: False

Property	Value
Formula	C10H+
Molecular weight	121.118
IUPAC name	deca-1,3,5,7,9-pentayne
$\mu_{a,b,c}$	-, -, -
A, B, C	∞, 267.5942, 267.5942
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 1
Predicted log column density	11.617±1.708
Electronic energy	-

geom851



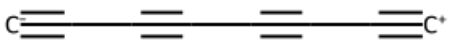
SMILES: [CH+]=[C]C#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (4.57)

Is DFT optimized?: True

Property	Value
Formula	C9HN+
Molecular weight	123.114
IUPAC name	
$\mu_{a,b,c}$	9.2, 0.0, 0.0
A, B, C	202816317.3511, 291.5617, 291.5612
A_s, B_s, C_s	202228150.0308, 290.7161, 290.7157
Charge, Multiplicity	1, 2
Predicted log column density	11.751±1.659
Electronic energy	-397.54266

geom852



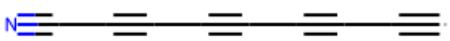
SMILES: [C+]#CC#CC#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (4.83)

Is DFT optimized?: True

Property	Value
Formula	C8
Molecular weight	96.088
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 607.1544, 607.1544
A_s, B_s, C_s	∞, 605.3937, 605.3937
Charge, Multiplicity	0, 1
Predicted log column density	11.115±1.784
Electronic energy	-304.25926

geom853



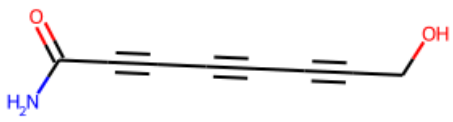
SMILES: [C]#CC#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (4.52)

Is DFT optimized?: True

Property	Value
Formula	C9N
Molecular weight	122.106
IUPAC name	nona-2,4,6,8-tetraynenitrile
$\mu_{a,b,c}$	4.6, 0.0, 0.0
A, B, C	∞, 297.4608, 297.4608
A_s, B_s, C_s	∞, 296.5981, 296.5981
Charge, Multiplicity	0, 2
Predicted log column density	11.737±1.654
Electronic energy	-397.15355

geom854



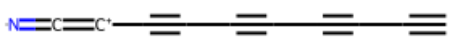
SMILES: NC(=O)C#CC#CC#CCO

Nearest TMC-1 molecule (distance): CC#CC#CC#N (6.34)

Is DFT optimized?: True

Property	Value
Formula	C8H5NO2
Molecular weight	147.133
IUPAC name	8-hydroxyocta-2,4,6-triynamide
$\mu_{a,b,c}$	1.2, 5.0, 1.4
A, B, C	7467.3180, 223.7527, 221.1127
A_s, B_s, C_s	7445.6628, 223.1038, 220.4714
Charge, Multiplicity	0, 1
Predicted log column density	8.500±4.798
Electronic energy	-512.70197

geom855



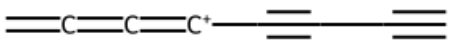
SMILES: C#CC#CC#CC#C[C+]=C=[N]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (3.98)

Is DFT optimized?: False

Property	Value
Formula	C10HN+
Molecular weight	135.125
IUPAC name	
$\mu_{a,b,c}$	-, -, -
A, B, C	21201.1305, 203.8440, 201.9028
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 2
Predicted log column density	11.622±1.809
Electronic energy	-

geom856



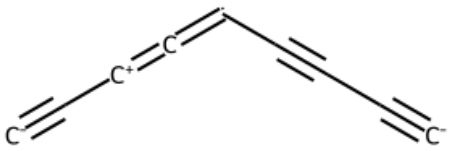
SMILES: C#CC#C[C+]=C=C=C

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (4.21)

Is DFT optimized?: True

Property	Value
Formula	C8H3+
Molecular weight	99.112
IUPAC name	
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	285680.5986, 554.8588, 553.7833
A_s, B_s, C_s	284852.1249, 553.2497, 552.1773
Charge, Multiplicity	1, 1
Predicted log column density	11.395±1.816
Electronic energy	-305.99255

geom857



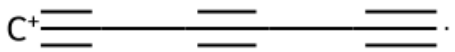
SMILES: [C−]#CC#C[C]=C=[C+]C#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (7.51)

Is DFT optimized?: True

Property	Value
Formula	C9-
Molecular weight	108.099
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	3251829740.0335, 423.1800, 423.1799
A_s, B_s, C_s	3242399433.7874, 421.9527, 421.9527
Charge, Multiplicity	-1, 2
Predicted log column density	10.223±2.087
Electronic energy	-342.49161

geom858



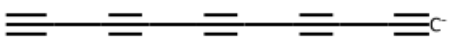
SMILES: [C]#CC#CC#[C+]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (5.40)

Is DFT optimized?: True

Property	Value
Formula	C6+
Molecular weight	72.066
IUPAC name	hexa-1,3,5-triyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 1467.3900, 1467.3900
A_s, B_s, C_s	∞, 1463.1345, 1463.1345
Charge, Multiplicity	1, 2
Predicted log column density	12.226±1.744
Electronic energy	-227.72726

geom859



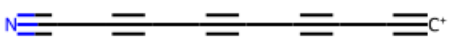
SMILES: [C−]#CC#CC#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (4.07)

Is DFT optimized?: True

Property	Value
Formula	C10H-
Molecular weight	121.118
IUPAC name	deca-1,3,5,7,9-pentayne
$\mu_{a,b,c}$	14.9, 0.0, 0.0
A, B, C	∞, 298.1343, 298.1343
A_s, B_s, C_s	∞, 297.2697, 297.2697
Charge, Multiplicity	-1, 1
Predicted log column density	11.037±1.629
Electronic energy	-381.23392

geom860



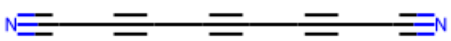
SMILES: [C+]#CC#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (4.83)

Is DFT optimized?: False

Property	Value
Formula	C9N+
Molecular weight	122.106
IUPAC name	nona-2,4,6,8-tetraynenitrile
$\mu_{a,b,c}$	-, -, -
A, B, C	∞, 265.7597, 265.7597
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 1
Predicted log column density	11.481±1.749
Electronic energy	-

geom861



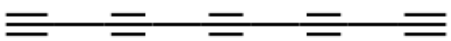
SMILES: N#CC#CC#CC#CC#N

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C8N2
Molecular weight	124.102
IUPAC name	octa-2,4,6-triynedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 287.3341, 287.3341
A_s, B_s, C_s	∞, 286.5009, 286.5009
Charge, Multiplicity	0, 1
Predicted log column density	11.476±1.707
Electronic energy	-413.95953

geom862



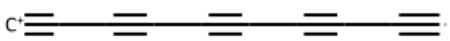
SMILES: C#CC#CC#CC#CC#C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C10H2
Molecular weight	122.126
IUPAC name	deca-1,3,5,7,9-pentayne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 291.0493, 291.0493
A_s, B_s, C_s	∞, 290.2052, 290.2052
Charge, Multiplicity	0, 1
Predicted log column density	11.730±1.641
Electronic energy	-381.79413

geom863



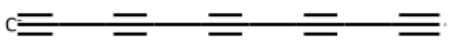
SMILES: [C]#CC#CC#CC#CC#[C+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (6.37)

Is DFT optimized?: True

Property	Value
Formula	C10+
Molecular weight	120.110
IUPAC name	deca-1,3,5,7,9-pentayne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 310.3844, 310.3844
A_s, B_s, C_s	∞, 309.4843, 309.4843
Charge, Multiplicity	1, 2
Predicted log column density	11.732±1.914
Electronic energy	-380.01527

geom864



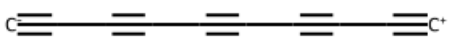
SMILES: [C]#CC#CC#CC#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (6.44)

Is DFT optimized?: True

Property	Value
Formula	C10-
Molecular weight	120.110
IUPAC name	deca-1,3,5,7,9-pentayne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 307.8394, 307.8394
A_s, B_s, C_s	∞, 306.9467, 306.9467
Charge, Multiplicity	-1, 2
Predicted log column density	11.155±1.770
Electronic energy	-380.56105

geom865



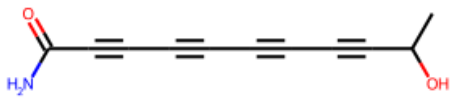
SMILES: [C+]#CC#CC#CC#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (6.94)

Is DFT optimized?: True

Property	Value
Formula	C10
Molecular weight	120.110
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 310.2174, 310.2174
A_s, B_s, C_s	∞, 309.3177, 309.3177
Charge, Multiplicity	0, 1
Predicted log column density	10.898±1.891
Electronic energy	-380.38310

geom866



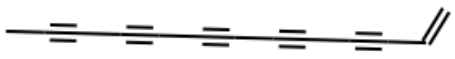
SMILES: CC(O)C#CC#CC#CC(N)=O

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (8.20)

Is DFT optimized?: True

Property	Value
Formula	C11H7NO2
Molecular weight	185.182
IUPAC name	10-hydroxyundeca-2,4,6,8-tetraynamide
$\mu_{a,b,c}$	1.8, 5.2, 0.7
A, B, C	4701.4434, 113.2703, 111.1986
A_s, B_s, C_s	4687.8092, 112.9418, 110.8762
Charge, Multiplicity	0, 1
Predicted log column density	8.837±5.519
Electronic energy	-628.13575

geom867



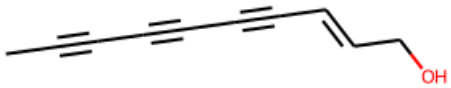
SMILES: C=CC#CC#CC#CC#CC#CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#CC#N (6.82)

Is DFT optimized?: True

Property	Value
Formula	C13H6
Molecular weight	162.191
IUPAC name	tridec-1-en-3,5,7,9,11-pentayne
$\mu_{a,b,c}$	0.8, 0.3, 0.1
A, B, C	24823.8100, 127.3635, 126.8263
A_s, B_s, C_s	24751.8210, 126.9941, 126.4585
Charge, Multiplicity	0, 1
Predicted log column density	11.007±2.062
Electronic energy	-498.49275

geom868



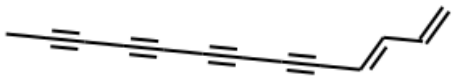
SMILES: CC#CC#CC#CC=CCO

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (9.18)

Is DFT optimized?: True

Property	Value
Formula	C10H8O
Molecular weight	144.173
IUPAC name	dec-2-en-4,6,8-triyn-1-ol
$\mu_{a,b,c}$	2.0, 0.7, 0.6
A, B, C	9877.1724, 207.1979, 204.6893
A_s, B_s, C_s	9848.5286, 206.5970, 204.0957
Charge, Multiplicity	0, 1
Predicted log column density	9.260±3.321
Electronic energy	-460.74044

geom869



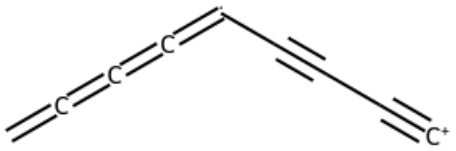
SMILES: C=CC=CC#CC#CC#CC#CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (10.65)

Is DFT optimized?: True

Property	Value
Formula	C13H8
Molecular weight	164.207
IUPAC name	trideca-1,3-dien-5,7,9,11-tetrayne
$\mu_{a,b,c}$	0.1, 0.4, 0.0
A, B, C	10940.0006, 130.2650, 128.8363
A_s, B_s, C_s	10908.2746, 129.8872, 128.4627
Charge, Multiplicity	0, 1
Predicted log column density	10.925±3.378
Electronic energy	-499.74774

geom870



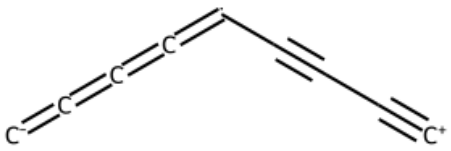
SMILES: [C+]#CC#C[C]=C=C=C

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (7.79)

Is DFT optimized?: True

Property	Value
Formula	C9H2+
Molecular weight	110.115
IUPAC name	
$\mu_{a,b,c}$	4.7, 0.0, 0.0
A, B, C	286701.6929, 404.2072, 403.6381
A_s, B_s, C_s	285870.2580, 403.0350, 402.4676
Charge, Multiplicity	1, 2
Predicted log column density	10.363±1.892
Electronic energy	-343.32980

geom871



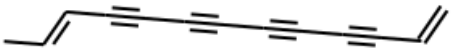
SMILES: [C+]#CC#C[C]=C=C=C=[CH−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (7.35)

Is DFT optimized?: False

Property	Value
Formula	C9H
Molecular weight	109.107
IUPAC name	
$\mu_{a,b,c}$	4.1, 4.5, 14.3
A, B, C	13670.6081, 449.2212, 434.9368
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	9.876±2.284
Electronic energy	-342.85886

geom872



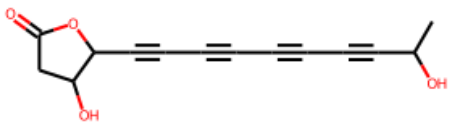
SMILES: C=CC#CC#CC#CC#CC=CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (11.40)

Is DFT optimized?: True

Property	Value
Formula	C13H8
Molecular weight	164.207
IUPAC name	trideca-1,11-dien-3,5,7,9-tetrayne
$\mu_{a,b,c}$	1.2, 0.3, 0.2
A, B, C	14397.4874, 128.8699, 128.0648
A_s, B_s, C_s	14355.7347, 128.4962, 127.6934
Charge, Multiplicity	0, 1
Predicted log column density	11.187±2.747
Electronic energy	-499.74348

geom873



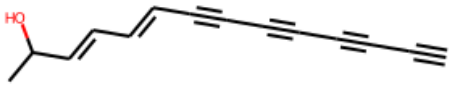
SMILES: CC(O)C#CC#CC#CC#CC1OC(=O)CC1O

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (12.59)

Is DFT optimized?: True

Property	Value
Formula	C14H10O4
Molecular weight	242.230
IUPAC name	4-hydroxy-5-(9-hydroxydeca-1,3,5,7-tetraynyl)oxolan-2-one
$\mu_{a,b,c}$	0.6, 5.0, 0.8
A, B, C	1557.5412, 71.3471, 69.6741
A_s, B_s, C_s	1553.0244, 71.1402, 69.4721
Charge, Multiplicity	0, 1
Predicted log column density	7.808±8.992
Electronic energy	-839.88862

geom874



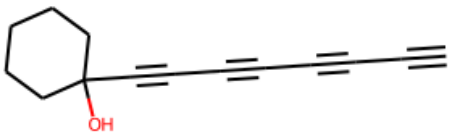
SMILES: C#CC#CC#CC#CC=CC=CC(C)O

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (13.45)

Is DFT optimized?: True

Property	Value
Formula	C14H10O
Molecular weight	194.233
IUPAC name	tetradeca-3,5-dien-7,9,11,13-tetrayn-2-ol
$\mu_{a,b,c}$	1.7, 1.2, 1.4
A, B, C	3614.7389, 94.1402, 93.4657
A_s, B_s, C_s	3604.2561, 93.8672, 93.1946
Charge, Multiplicity	0, 1
Predicted log column density	9.544±6.719
Electronic energy	-614.23639

geom875



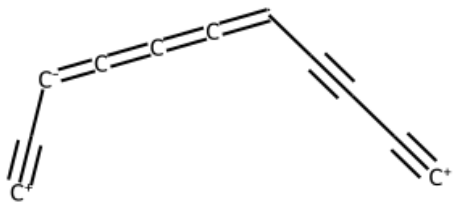
SMILES: C#CC#CC#CC#CC1(O)CCCCC1

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (11.50)

Is DFT optimized?: True

Property	Value
Formula	C14H12O
Molecular weight	196.249
IUPAC name	1-octa-1,3,5,7-tetraynylcyclohexan-1-ol
$\mu_{a,b,c}$	0.5, 1.2, 1.1
A, B, C	1558.8380, 166.2504, 159.9737
A_s, B_s, C_s	1554.3174, 165.7682, 159.5098
Charge, Multiplicity	0, 1
Predicted log column density	6.059±8.573
Electronic energy	-615.49994

geom876



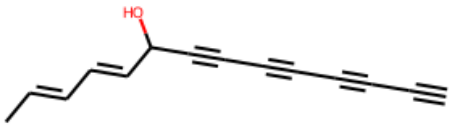
SMILES: [C+]#CC#C[C]=C=C=C=[C−]C#[C+]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (10.41)

Is DFT optimized?: False

Property	Value
Formula	C11+
Molecular weight	132.121
IUPAC name	
$\mu_{a,b,c}$	2.9, 1.2, 4.1
A, B, C	14226.4557, 241.9283, 237.9948
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 2
Predicted log column density	10.219±2.813
Electronic energy	-417.95856

geom877



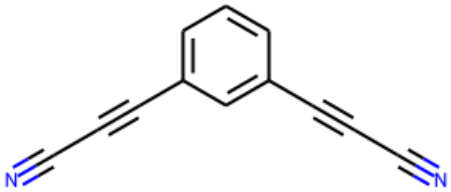
SMILES: C#CC#CC#CC#CC(O)C=CC=CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (13.69)

Is DFT optimized?: True

Property	Value
Formula	C14H10O
Molecular weight	194.233
IUPAC name	tetradeca-2,4-dien-7,9,11,13-tetrayn-6-ol
$\mu_{a,b,c}$	1.1, 1.8, 0.2
A, B, C	1443.7722, 120.3628, 112.5611
A_s, B_s, C_s	1439.5852, 120.0138, 112.2347
Charge, Multiplicity	0, 1
Predicted log column density	10.465±6.643
Electronic energy	-614.22592

geom878



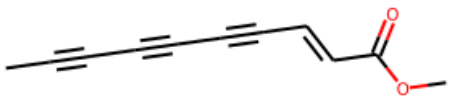
SMILES: N#CC#Cc1cccc(C#CC#N)c1

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (10.71)

Is DFT optimized?: True

Property	Value
Formula	C12H4N2
Molecular weight	176.178
IUPAC name	3-[3-(2-cyanoethynyl)phenyl]prop-2-ynenitrile
$\mu_{a,b,c}$	0.0, 5.5, 0.0
A, B, C	1272.1671, 260.4390, 216.1821
A_s, B_s, C_s	1268.4778, 259.6838, 215.5551
Charge, Multiplicity	0, 1
Predicted log column density	8.655±5.117
Electronic energy	-568.82578

geom879



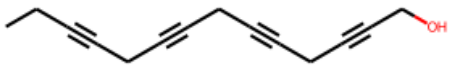
SMILES: CC#CC#CC#CC=CC(=O)OC

Nearest TMC-1 molecule (distance): CC#CC#CC#N (9.92)

Is DFT optimized?: True

Property	Value
Formula	C11H8O2
Molecular weight	172.183
IUPAC name	methyl dec-2-en-4,6,8-triynoate
$\mu_{a,b,c}$	2.0, 1.9, 0.0
A, B, C	6233.9311, 148.9737, 145.7646
A_s, B_s, C_s	6215.8527, 148.5417, 145.3418
Charge, Multiplicity	0, 1
Predicted log column density	11.682±4.988
Electronic energy	-574.06007

geom880



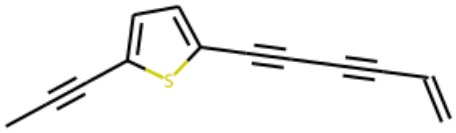
SMILES: CCC#CCC#CCC#CCC#CCO

Nearest TMC-1 molecule (distance): C#CC#CC#CC#CC#N (13.69)

Is DFT optimized?: True

Property	Value
Formula	C14H14O
Molecular weight	198.265
IUPAC name	tetradeca-2,5,8,11-tetrayn-1-ol
$\mu_{a,b,c}$	2.2, 0.9, 0.5
A, B, C	1419.2651, 118.8260, 113.1667
A_s, B_s, C_s	1415.1493, 118.4814, 112.8385
Charge, Multiplicity	0, 1
Predicted log column density	2.448±9.908
Electronic energy	-616.66777

geom881



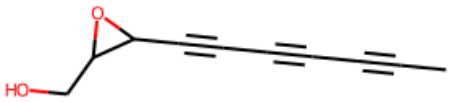
SMILES: C=CC#CC#Cc1ccc(C#CC)s1

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (10.94)

Is DFT optimized?: True

Property	Value
Formula	C13H8S
Molecular weight	196.274
IUPAC name	2-hex-5-en-1,3-diynyl-5-prop-1-ynylthiophene
$\mu_{a,b,c}$	1.1, 0.3, 0.1
A, B, C	3404.6043, 157.5468, 150.8120
A_s, B_s, C_s	3394.7309, 157.0899, 150.3747
Charge, Multiplicity	0, 1
Predicted log column density	8.619±7.054
Electronic energy	-897.98809

geom882



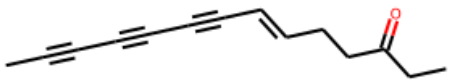
SMILES: CC#CC#CC#CC1OC1CO

Nearest TMC-1 molecule (distance): CC#CC#CC#N (8.97)

Is DFT optimized?: True

Property	Value
Formula	C10H8O2
Molecular weight	160.172
IUPAC name	(3-hepta-1,3,5-triynyloxiran-2-yl)methanol
$\mu_{a,b,c}$	2.6, 0.1, 1.4
A, B, C	6457.4597, 190.1361, 188.6359
A_s, B_s, C_s	6438.7331, 189.5847, 188.0888
Charge, Multiplicity	0, 1
Predicted log column density	8.877±8.123
Electronic energy	-535.92078

geom883



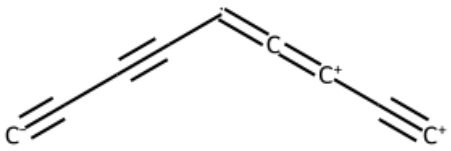
SMILES: CC#CC#CC#CC=CCCC(=O)CC

Nearest TMC-1 molecule (distance): C#CC#CC#CC#N (12.20)

Is DFT optimized?: True

Property	Value
Formula	C14H14O
Molecular weight	198.265
IUPAC name	tetradec-6-en-8,10,12-triyn-3-one
$\mu_{a,b,c}$	0.8, 2.8, 0.0
A, B, C	3531.0433, 96.9308, 95.1538
A_s, B_s, C_s	3520.8033, 96.6497, 94.8779
Charge, Multiplicity	0, 1
Predicted log column density	5.486±6.016
Electronic energy	-616.75936

geom884



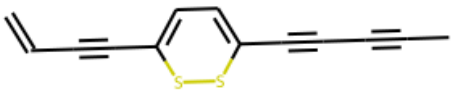
SMILES: [C+]#C[C+]=C=[C]C#CC#[C−]

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C−] (7.31)

Is DFT optimized?: False

Property	Value
Formula	C9+
Molecular weight	108.099
IUPAC name	
$\mu_{a,b,c}$	-, -, -
A, B, C	64342.0637, 403.3720, 400.8595
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 2
Predicted log column density	10.684±2.070
Electronic energy	-

geom885



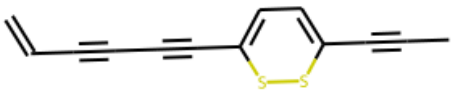
SMILES: C=CC#CC1=CC=C(C#CC#CC)SS1

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C-] (12.43)

Is DFT optimized?: True

Property	Value
Formula	C13H8S2
Molecular weight	228.341
IUPAC name	3-but-3-en-1-ynyl-6-penta-1,3-diynyldithiine
$\mu_{a,b,c}$	0.7, 1.6, 0.2
A, B, C	2416.7913, 139.0652, 133.4535
A_s, B_s, C_s	2409.7826, 138.6620, 133.0665
Charge, Multiplicity	0, 1
Predicted log column density	9.649±8.065
Electronic energy	-1296.13195

geom886



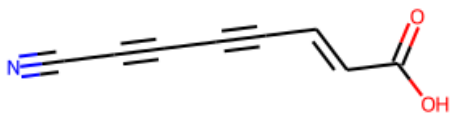
SMILES: C=CC#CC#CC1=CC=C(C#CC)SS1

Nearest TMC-1 molecule (distance): C#CC#CC#CC#[C-] (12.43)

Is DFT optimized?: True

Property	Value
Formula	C13H8S2
Molecular weight	228.341
IUPAC name	3-hex-5-en-1,3-diynyl-6-prop-1-ynyldithiine
$\mu_{a,b,c}$	0.8, 1.8, 0.3
A, B, C	2292.4791, 132.9118, 128.4371
A_s, B_s, C_s	2285.8309, 132.5264, 128.0646
Charge, Multiplicity	0, 1
Predicted log column density	9.649±8.065
Electronic energy	-1296.13138

geom887



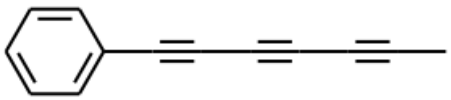
SMILES: N#CC#CC#CC=CC(=O)O

Nearest TMC-1 molecule (distance): CC#CC#CC#N (8.45)

Is DFT optimized?: True

Property	Value
Formula	C8H3NO2
Molecular weight	145.117
IUPAC name	7-cyanohept-2-en-4,6-diynoic acid
$\mu_{a,b,c}$	1.7, 2.6, 0.0
A, B, C	8791.8152, 248.2963, 241.4766
A_s, B_s, C_s	8766.3189, 247.5763, 240.7763
Charge, Multiplicity	0, 1
Predicted log column density	10.204±3.677
Electronic energy	-511.52473

geom888



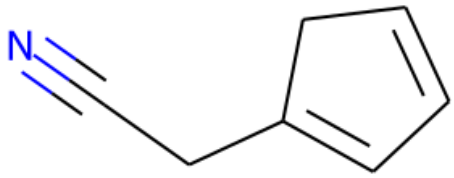
SMILES: CC#CC#CC#Cc1ccccc1

Nearest TMC-1 molecule (distance): CC#CC#CC#N (9.54)

Is DFT optimized?: True

Property	Value
Formula	C13H8
Molecular weight	164.207
IUPAC name	hepta-1,3,5-triynylbenzene
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	5492.1372, 191.6107, 185.3667
A_s, B_s, C_s	5476.2100, 191.0550, 184.8291
Charge, Multiplicity	0, 1
Predicted log column density	10.507±3.670
Electronic energy	-499.85347

geom889



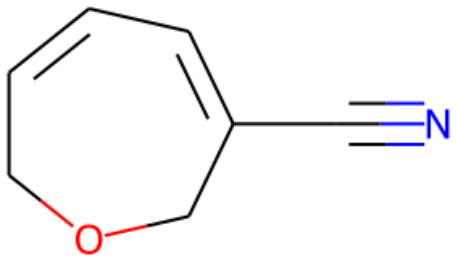
SMILES: N#CCC1=CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (3.24)

Is DFT optimized?: True

Property	Value
Formula	C7H7N
Molecular weight	105.140
IUPAC name	2-cyclopenta-1,3-dien-1-ylacetonitrile
$\mu_{a,b,c}$	2.9, 1.6, 1.9
A, B, C	5338.0757, 1272.0768, 1127.7292
A_s, B_s, C_s	5322.5953, 1268.3877, 1124.4588
Charge, Multiplicity	0, 1
Predicted log column density	10.492±2.923
Electronic energy	-325.55530

geom890



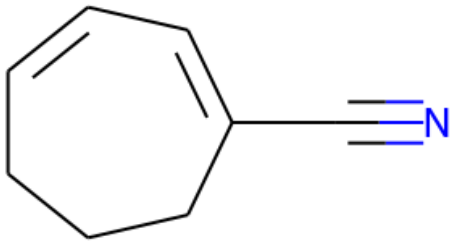
SMILES: N#CC1=CC=CCOC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (3.70)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	5.2, 1.2, 1.4
A, B, C	3578.0568, 1193.3764, 927.8264
A_s, B_s, C_s	3567.6804, 1189.9156, 925.1357
Charge, Multiplicity	0, 1
Predicted log column density	13.603±3.983
Electronic energy	-400.73919

geom891



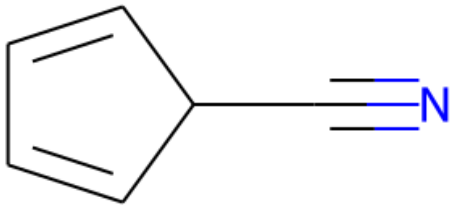
SMILES: N#CC1=CC=CCCC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (3.73)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	cyclohepta-1,3-diene-1-carbonitrile
$\mu_{a,b,c}$	5.3, 0.3, 0.3
A, B, C	3416.3470, 1151.9216, 895.7362
A_s, B_s, C_s	3406.4396, 1148.5811, 893.1386
Charge, Multiplicity	0, 1
Predicted log column density	10.561±3.225
Electronic energy	-364.86384

geom892



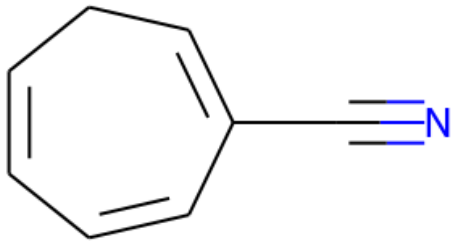
SMILES: N#CC1C=CC=C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (3.87)

Is DFT optimized?: True

Property	Value
Formula	C6H5N
Molecular weight	91.113
IUPAC name	cyclopenta-2,4-diene-1-carbonitrile
$\mu_{a,b,c}$	4.0, 0.0, 1.5
A, B, C	6746.3004, 2107.3492, 1770.2056
A_s, B_s, C_s	6726.7361, 2101.2379, 1765.0720
Charge, Multiplicity	0, 1
Predicted log column density	10.717±3.634
Electronic energy	-286.24377

geom893



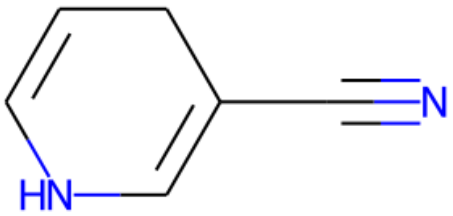
SMILES: N#CC1=CCC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (3.21)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	cyclohepta-1,4,6-triene-1-carbonitrile
$\mu_{a,b,c}$	4.8, 0.6, 0.6
A, B, C	3461.0523, 1242.0997, 991.4886
A_s, B_s, C_s	3451.0152, 1238.4976, 988.6133
Charge, Multiplicity	0, 1
Predicted log column density	11.386±1.971
Electronic energy	-363.63501

geom894



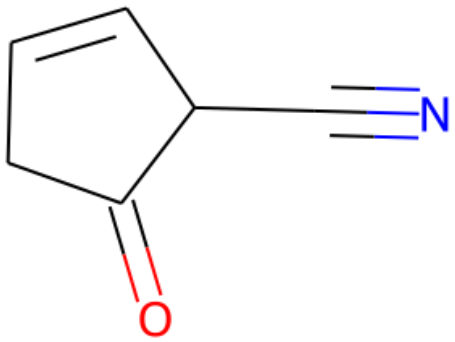
SMILES: N#CC1=CNC=CC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (4.22)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	1,4-dihydropyridine-3-carbonitrile
$\mu_{a,b,c}$	6.1, 1.6, 0.0
A, B, C	5157.8407, 1513.5090, 1178.6248
A_s, B_s, C_s	5142.8830, 1509.1198, 1175.2068
Charge, Multiplicity	0, 1
Predicted log column density	12.281±4.582
Electronic energy	-341.60011

geom895



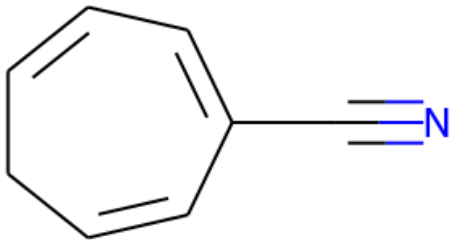
SMILES: N#CC1C=CCC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (3.80)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	5-oxocyclopent-2-ene-1-carbonitrile
$\mu_{a,b,c}$	4.7, 2.8, 1.3
A, B, C	3256.7039, 1986.0131, 1362.1863
A_s, B_s, C_s	3247.2594, 1980.2537, 1358.2359
Charge, Multiplicity	0, 1
Predicted log column density	9.810±3.804
Electronic energy	-361.46441

geom896



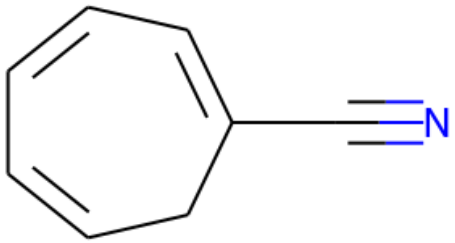
SMILES: N#CC1=CC=CCC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (3.54)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	cyclohepta-1,3,6-triene-1-carbonitrile
$\mu_{a,b,c}$	5.2, 0.1, 0.5
A, B, C	3587.4525, 1231.9402, 972.3945
A_s, B_s, C_s	3577.0489, 1228.3676, 969.5746
Charge, Multiplicity	0, 1
Predicted log column density	11.279±2.340
Electronic energy	-363.63525

geom897



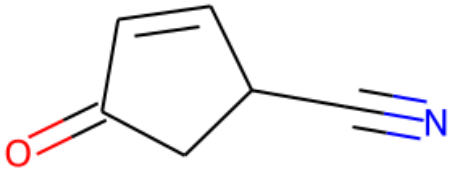
SMILES: N#CC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (2.82)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	cyclohepta-1,3,5-triene-1-carbonitrile
$\mu_{a,b,c}$	4.6, 0.2, 0.7
A, B, C	3464.2471, 1260.7848, 998.4561
A_s, B_s, C_s	3454.2008, 1257.1285, 995.5606
Charge, Multiplicity	0, 1
Predicted log column density	11.872±1.986
Electronic energy	-363.63733

geom898



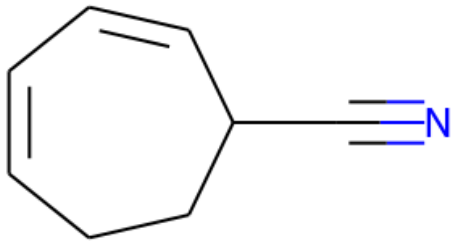
SMILES: N#CC1C=CC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (3.90)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.4, 2.1, 2.3
A, B, C	5296.4799, 1370.0586, 1180.6030
A_s, B_s, C_s	5281.1201, 1366.0854, 1177.1792
Charge, Multiplicity	0, 1
Predicted log column density	10.130±3.510
Electronic energy	-361.47373

geom899



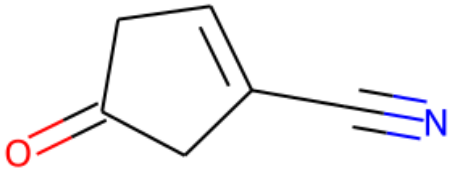
SMILES: N#CC1C=CC=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.35)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	cyclohepta-2,4-diene-1-carbonitrile
$\mu_{a,b,c}$	2.9, 0.0, 2.7
A, B, C	2446.4503, 1463.2255, 1194.0369
A_s, B_s, C_s	2439.3556, 1458.9821, 1190.5742
Charge, Multiplicity	0, 1
Predicted log column density	10.086±3.589
Electronic energy	-364.85677

geom900



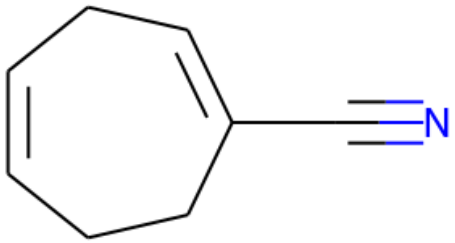
SMILES: N#CC1=CCC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (4.46)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	4-oxocyclopentene-1-carbonitrile
$\mu_{a,b,c}$	1.7, 2.3, 0.0
A, B, C	6014.8583, 1285.2297, 1073.0330
A_s, B_s, C_s	5997.4152, 1281.5025, 1069.9212
Charge, Multiplicity	0, 1
Predicted log column density	11.021±3.861
Electronic energy	-361.47476

geom901



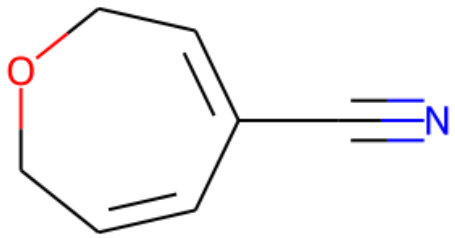
SMILES: N#CC1=CCC=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (3.95)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	
$\mu_{a,b,c}$	4.6, 0.4, 1.0
A, B, C	3113.0972, 1219.4091, 961.3422
A_s, B_s, C_s	3104.0693, 1215.8729, 958.5543
Charge, Multiplicity	0, 1
Predicted log column density	10.346±3.045
Electronic energy	-364.85580

geom902



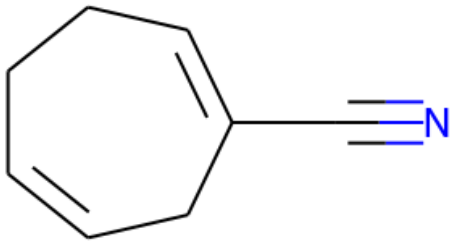
SMILES: N#CC1=CCOCC=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.13)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	4.1, 0.3, 1.1
A, B, C	3507.4382, 1191.1658, 919.1897
A_s, B_s, C_s	3497.2666, 1187.7114, 916.5240
Charge, Multiplicity	0, 1
Predicted log column density	13.531±4.392
Electronic energy	-400.73615

geom903



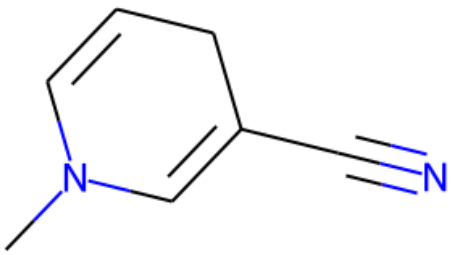
SMILES: N#CC1=CCCC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.51)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	cyclohepta-1,5-diene-1-carbonitrile
$\mu_{a,b,c}$	4.9, 0.6, 0.2
A, B, C	3321.2317, 1183.1368, 922.9800
A_s, B_s, C_s	3311.6001, 1179.7057, 920.3033
Charge, Multiplicity	0, 1
Predicted log column density	11.674±3.457
Electronic energy	-364.85514

geom904



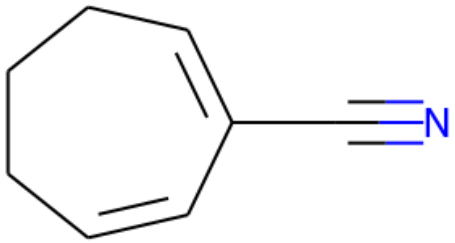
SMILES: CN1C=CCC(C#N)=C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (4.72)

Is DFT optimized?: True

Property	Value
Formula	C7H8N2
Molecular weight	120.155
IUPAC name	1-methyl-4H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	6.4, 0.2, 0.0
A, B, C	3114.6634, 1209.7197, 882.1942
A_s, B_s, C_s	3105.6309, 1206.2115, 879.6358
Charge, Multiplicity	0, 1
Predicted log column density	15.519±5.065
Electronic energy	-380.89805

geom905



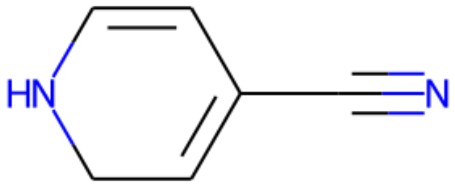
SMILES: N#CC1=CCCCC=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (3.86)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	cyclohepta-1,6-diene-1-carbonitrile
$\mu_{a,b,c}$	5.5, 0.6, 0.5
A, B, C	3320.1361, 1159.3651, 900.8943
A_s, B_s, C_s	3310.5077, 1156.0029, 898.2817
Charge, Multiplicity	0, 1
Predicted log column density	11.390±3.581
Electronic energy	-364.86122

geom906



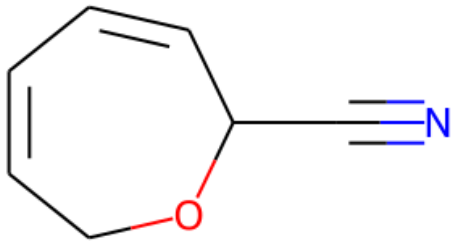
SMILES: N#CC1=CCNC=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.70)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	1,2-dihydropyridine-4-carbonitrile
$\mu_{a,b,c}$	6.4, 0.5, 0.3
A, B, C	5295.4227, 1489.5795, 1189.5345
A_s, B_s, C_s	5280.0660, 1485.2598, 1186.0849
Charge, Multiplicity	0, 1
Predicted log column density	10.949±5.525
Electronic energy	-341.59046

geom907



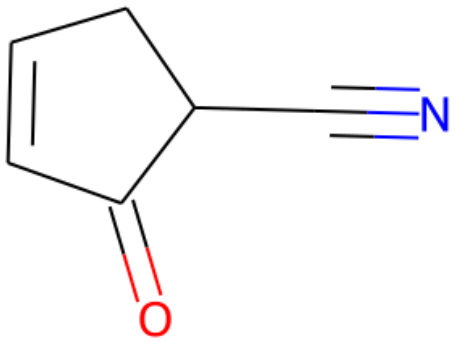
SMILES: N#CC1C=CC=CCO1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (4.90)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	3.5, 0.9, 0.7
A, B, C	3058.2849, 1374.1521, 1107.3300
A_s, B_s, C_s	3049.4158, 1370.1671, 1104.1187
Charge, Multiplicity	0, 1
Predicted log column density	10.429±4.828
Electronic energy	-400.72963

geom908



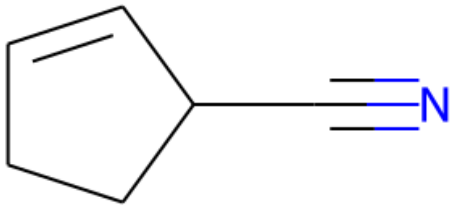
SMILES: N#CC1CC=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.12)

Is DFT optimized?: False

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	2-oxocyclopent-3-ene-1-carbonitrile
$\mu_{a,b,c}$	1.4, 3.8, 4.3
A, B, C	3064.3060, 2010.4783, 1451.1903
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.931±4.073
Electronic energy	-361.44379

geom909



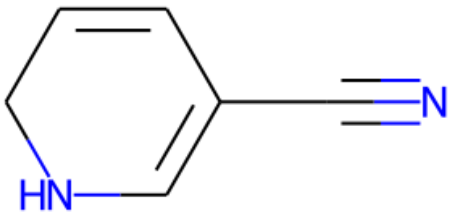
SMILES: N#CC1C=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (3.95)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	cyclopent-2-ene-1-carbonitrile
$\mu_{a,b,c}$	4.4, 0.3, 1.2
A, B, C	6600.9839, 1915.1999, 1602.8166
A_s, B_s, C_s	6581.8410, 1909.6458, 1598.1685
Charge, Multiplicity	0, 1
Predicted log column density	10.024±3.415
Electronic energy	-287.47829

geom910



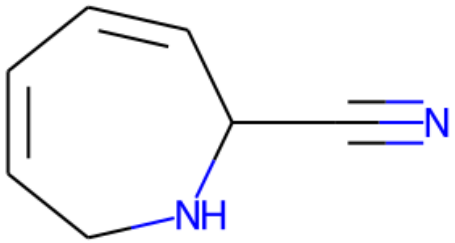
SMILES: N#CC1=CNCC=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.65)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	1,2-dihydropyridine-5-carbonitrile
$\mu_{a,b,c}$	6.6, 1.7, 0.0
A, B, C	5311.8263, 1482.5010, 1177.8791
A_s, B_s, C_s	5296.4220, 1478.2017, 1174.4632
Charge, Multiplicity	0, 1
Predicted log column density	10.026±5.313
Electronic energy	-341.59592

geom911



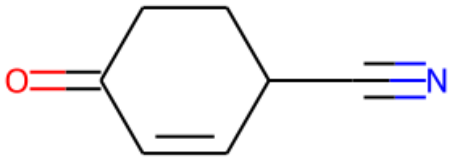
SMILES: N#CC1C=CC=CCN1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (4.96)

Is DFT optimized?: True

Property	Value
Formula	C7H8N2
Molecular weight	120.155
IUPAC name	
$\mu_{a,b,c}$	2.3, 0.3, 1.8
A, B, C	2718.3228, 1419.6127, 1148.6907
A_s, B_s, C_s	2710.4396, 1415.4958, 1145.3595
Charge, Multiplicity	0, 1
Predicted log column density	8.907±5.002
Electronic energy	-380.87319

geom912



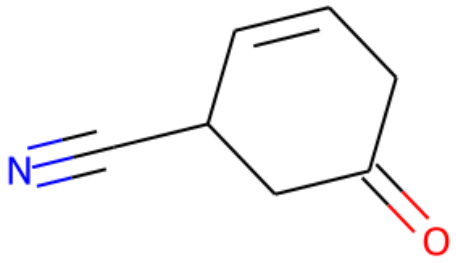
SMILES: N#CC1C=CC(=O)CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.47)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	4-oxocyclohex-2-ene-1-carbonitrile
$\mu_{a,b,c}$	0.6, 0.7, 3.8
A, B, C	3217.4718, 1176.2178, 1074.5322
A_s, B_s, C_s	3208.1412, 1172.8068, 1071.4160
Charge, Multiplicity	0, 1
Predicted log column density	8.974±4.009
Electronic energy	-400.78169

geom913



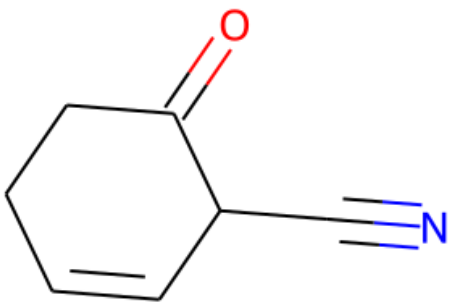
SMILES: N#CC1C=CCC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.83)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	1.5, 4.5, 3.0
A, B, C	2322.4001, 1517.7303, 1150.9278
A_s, B_s, C_s	2315.6651, 1513.3289, 1147.5901
Charge, Multiplicity	0, 1
Predicted log column density	9.825±4.068
Electronic energy	-400.77581

geom914



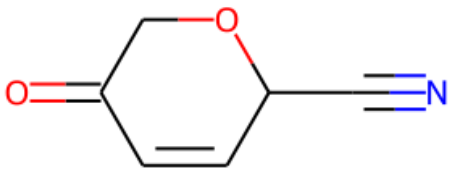
SMILES: N#CC1C=CCCC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.48)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	6-oxocyclohex-2-ene-1-carbonitrile
$\mu_{a,b,c}$	4.3, 2.2, 0.6
A, B, C	2271.4143, 1567.8434, 1172.0428
A_s, B_s, C_s	2264.8272, 1563.2967, 1168.6439
Charge, Multiplicity	0, 1
Predicted log column density	8.848±4.059
Electronic energy	-400.77386

geom915



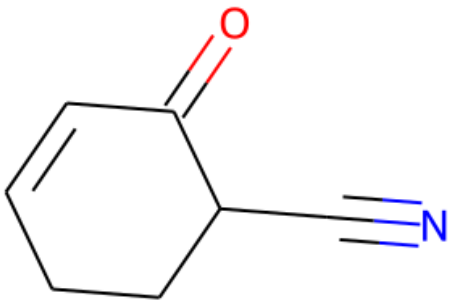
SMILES: N#CC1C=CC(=O)CO1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.89)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.3, 2.2, 2.4
A, B, C	3275.6770, 1227.5176, 1127.2337
A_s, B_s, C_s	3266.1776, 1223.9578, 1123.9647
Charge, Multiplicity	0, 1
Predicted log column density	10.232±4.499
Electronic energy	-436.65122

geom916



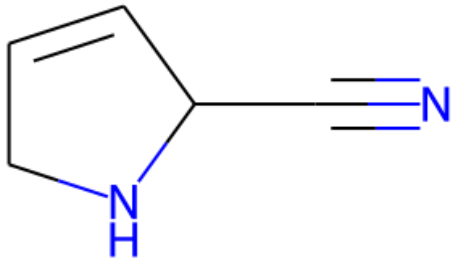
SMILES: N#CC1CCC=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.50)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	3.4, 3.7, 1.9
A, B, C	1980.5644, 1831.3566, 1260.1009
A_s, B_s, C_s	1974.8208, 1826.0456, 1256.4466
Charge, Multiplicity	0, 1
Predicted log column density	9.912±3.984
Electronic energy	-400.78204

geom917



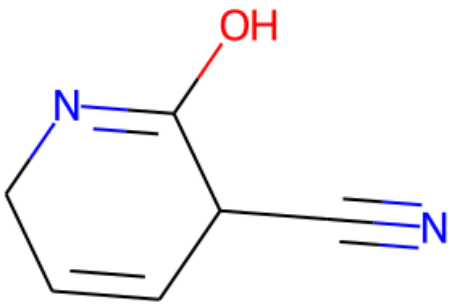
SMILES: N#CC1C=CCN1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.61)

Is DFT optimized?: True

Property	Value
Formula	C5H6N2
Molecular weight	94.117
IUPAC name	2,5-dihydro-1H-pyrrole-2-carbonitrile
$\mu_{a,b,c}$	3.4, 0.2, 0.5
A, B, C	5666.6148, 2147.5847, 1875.2040
A_s, B_s, C_s	5650.1816, 2141.3567, 1869.7659
Charge, Multiplicity	0, 1
Predicted log column density	8.839±4.855
Electronic energy	-303.49636

geom918



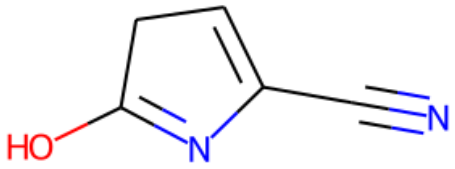
SMILES: N#CC1C=CCN=C1O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.92)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	4.0, 0.4, 1.7
A, B, C	2467.0040, 1601.5581, 1090.9433
A_s, B_s, C_s	2459.8497, 1596.9136, 1087.7795
Charge, Multiplicity	0, 1
Predicted log column density	7.963±5.108
Electronic energy	-416.80389

geom919



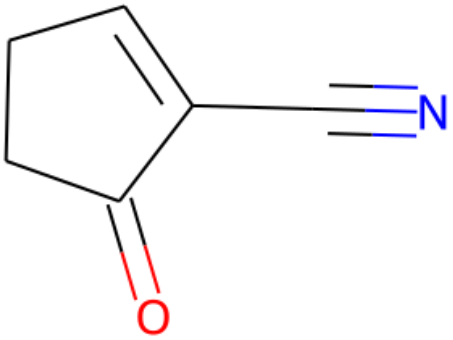
SMILES: N#CC1=CCC(O)=N1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.29)

Is DFT optimized?: True

Property	Value
Formula	C5H4N2O
Molecular weight	108.100
IUPAC name	
$\mu_{a,b,c}$	6.2, 5.1, 0.0
A, B, C	6018.7721, 1355.1112, 1113.7966
A_s, B_s, C_s	6001.3177, 1351.1813, 1110.5665
Charge, Multiplicity	0, 1
Predicted log column density	10.615±5.332
Electronic energy	-377.49413

geom920



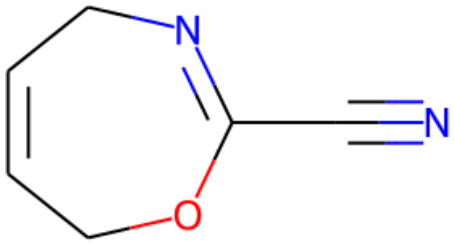
SMILES: N#CC1=CCCC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.08)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	5-oxocyclopentene-1-carbonitrile
$\mu_{a,b,c}$	5.8, 3.9, 0.0
A, B, C	3692.9708, 1799.2597, 1228.4371
A_s, B_s, C_s	3682.2612, 1794.0419, 1224.8746
Charge, Multiplicity	0, 1
Predicted log column density	11.351±4.415
Electronic energy	-361.47834

geom921



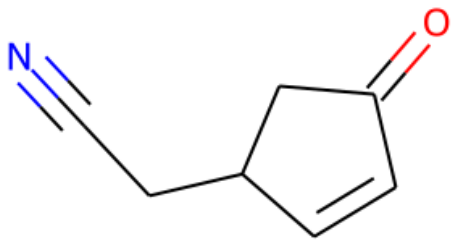
SMILES: N#CC1=NCC=CCO1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.20)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	5.7, 0.9, 0.0
A, B, C	3512.1775, 1281.1637, 985.7099
A_s, B_s, C_s	3501.9922, 1277.4483, 982.8513
Charge, Multiplicity	0, 1
Predicted log column density	10.346±5.848
Electronic energy	-416.76758

geom922



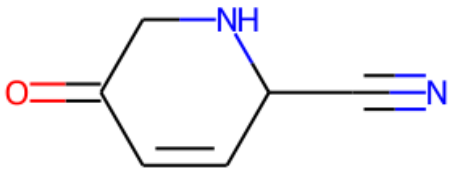
SMILES: N#CCC1C=CC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.81)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	2-(4-oxocyclopent-2-en-1-yl)acetonitrile
$\mu_{a,b,c}$	0.4, 4.8, 0.1
A, B, C	3805.7554, 966.8298, 806.5184
A_s, B_s, C_s	3794.7187, 964.0260, 804.1795
Charge, Multiplicity	0, 1
Predicted log column density	10.456±4.089
Electronic energy	-400.78179

geom923



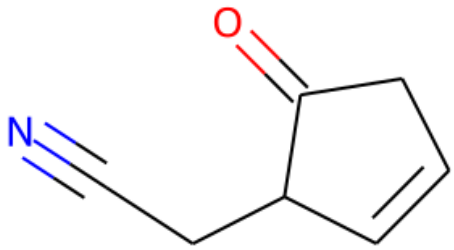
SMILES: N#CC1C=CC(=O)CN1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.20)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	1.1, 0.8, 3.0
A, B, C	3261.5530, 1205.2844, 1102.9765
A_s, B_s, C_s	3252.0945, 1201.7891, 1099.7778
Charge, Multiplicity	0, 1
Predicted log column density	9.957±4.563
Electronic energy	-416.79790

geom924



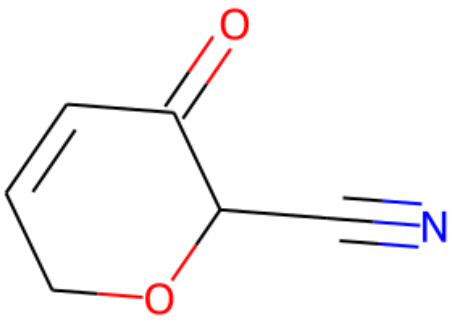
SMILES: N#CCC1C=CCC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.91)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	3.5, 1.5, 0.6
A, B, C	3226.5706, 1130.9286, 872.4637
A_s, B_s, C_s	3217.2135, 1127.6489, 869.9335
Charge, Multiplicity	0, 1
Predicted log column density	9.144±3.795
Electronic energy	-400.77618

geom925



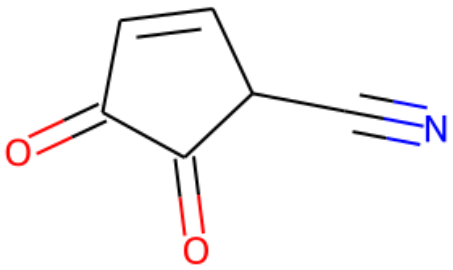
SMILES: N#CC1OCC=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.87)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	5-oxo-2H-pyran-6-carbonitrile
$\mu_{a,b,c}$	3.5, 3.1, 0.0
A, B, C	2071.3462, 1882.1974, 1287.9851
A_s, B_s, C_s	2065.3393, 1876.7390, 1284.2500
Charge, Multiplicity	0, 1
Predicted log column density	11.434±4.466
Electronic energy	-436.65159

geom926



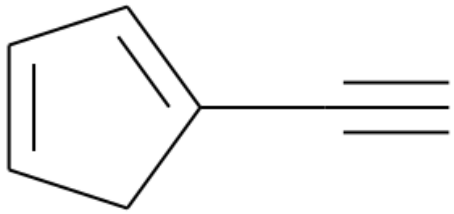
SMILES: N#CC1C=CC(=O)C1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.09)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	0.5, 4.7, 2.6
A, B, C	3126.8759, 1366.5071, 1035.3150
A_s, B_s, C_s	3117.8079, 1362.5442, 1032.3126
Charge, Multiplicity	0, 1
Predicted log column density	10.071±4.067
Electronic energy	-435.44173

geom927



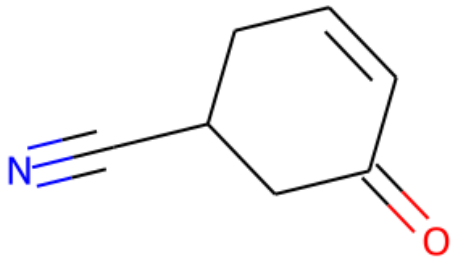
SMILES: C#CC1=CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.42)

Is DFT optimized?: True

Property	Value
Formula	C7H6
Molecular weight	90.125
IUPAC name	1-ethynylcyclopenta-1,3-diene
$\mu_{a,b,c}$	0.7, 0.4, 0.0
A, B, C	8417.1120, 1877.9350, 1550.1163
A_s, B_s, C_s	8392.7024, 1872.4889, 1545.6209
Charge, Multiplicity	0, 1
Predicted log column density	11.957±2.015
Electronic energy	-270.16151

geom928



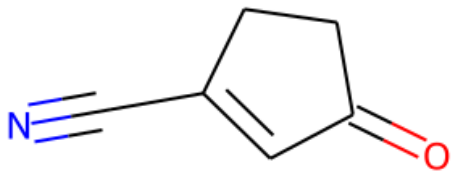
SMILES: N#CC1CC=CC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.81)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	5-oxocyclohex-3-ene-1-carbonitrile
$\mu_{a,b,c}$	0.6, 4.7, 3.4
A, B, C	2341.8932, 1506.8736, 1223.7568
A_s, B_s, C_s	2335.1017, 1502.5037, 1220.2079
Charge, Multiplicity	0, 1
Predicted log column density	10.302±4.493
Electronic energy	-400.78274

geom929



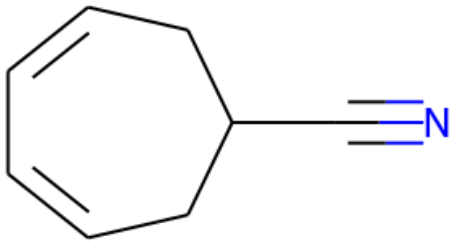
SMILES: N#CC1=CC(=O)CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.39)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	3-oxocyclopentene-1-carbonitrile
$\mu_{a,b,c}$	0.8, 2.6, 0.0
A, B, C	5658.2918, 1313.1326, 1080.0346
A_s, B_s, C_s	5641.8827, 1309.3245, 1076.9025
Charge, Multiplicity	0, 1
Predicted log column density	9.490±4.298
Electronic energy	-361.47900

geom930



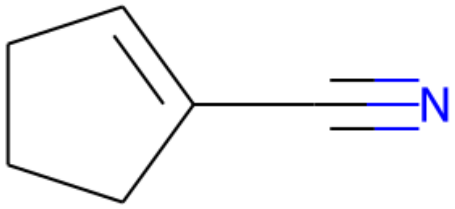
SMILES: N#CC1CC=CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.19)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	
$\mu_{a,b,c}$	3.9, 0.1, 0.0
A, B, C	3267.9336, 1198.8815, 914.9752
A_s, B_s, C_s	3258.4566, 1195.4047, 912.3218
Charge, Multiplicity	0, 1
Predicted log column density	10.288±4.547
Electronic energy	-364.85800

geom931



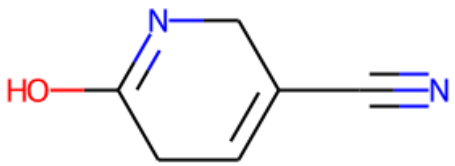
SMILES: N#CC1=CCCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.98)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	cyclopentene-1-carbonitrile
$\mu_{a,b,c}$	4.9, 0.2, 0.2
A, B, C	7207.4891, 1808.5598, 1494.5877
A_s, B_s, C_s	7186.5874, 1803.3150, 1490.2534
Charge, Multiplicity	0, 1
Predicted log column density	10.574±3.702
Electronic energy	-287.48435

geom932



SMILES: N#CC1=CCC(O)=NC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.48)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	3.4, 4.1, 0.0
A, B, C	5034.5926, 982.4394, 830.4070
A_s, B_s, C_s	5019.9923, 979.5903, 827.9989
Charge, Multiplicity	0, 1
Predicted log column density	10.274±6.157
Electronic energy	-416.80370

geom933

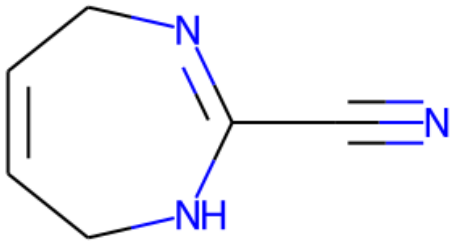
SMILES: N#CNC(=O)C1=CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.36)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2O
Molecular weight	134.138
IUPAC name	
$\mu_{a,b,c}$	6.6, 3.2, 0.7
A, B, C	4374.2171, 716.5976, 621.0165
A_s, B_s, C_s	4361.5319, 714.5195, 619.2156
Charge, Multiplicity	0, 1
Predicted log column density	10.058±4.310
Electronic energy	-454.89278

geom934



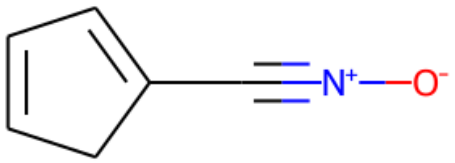
SMILES: N#CC1=NCC=CCN1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.50)

Is DFT optimized?: True

Property	Value
Formula	C6H7N3
Molecular weight	121.143
IUPAC name	4,7-dihydro-1H-1,3-diazepine-2-carbonitrile
$\mu_{a,b,c}$	4.9, 2.3, 0.2
A, B, C	3469.9163, 1231.5495, 931.3762
A_s, B_s, C_s	3459.8536, 1227.9780, 928.6752
Charge, Multiplicity	0, 1
Predicted log column density	8.959±6.382
Electronic energy	-396.91499

geom935



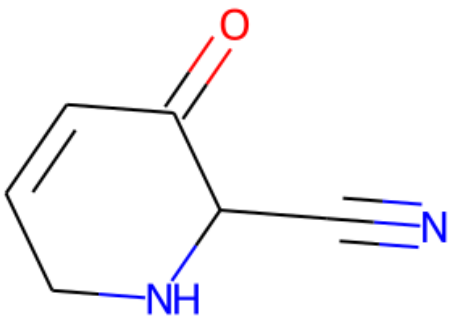
SMILES: [O-][N+]#CC1=CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.50)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	cyclopenta-1,3-diene-1-carbonitrile oxide
$\mu_{a,b,c}$	4.9, 0.3, 0.0
A, B, C	8370.7773, 1023.3857, 917.0852
A_s, B_s, C_s	8346.5020, 1020.4179, 914.4256
Charge, Multiplicity	0, 1
Predicted log column density	11.274±3.905
Electronic energy	-361.38042

geom936



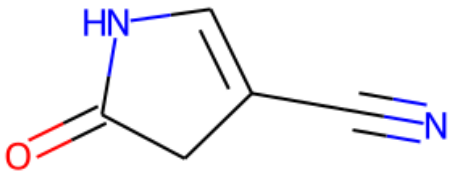
SMILES: N#CC1NCC=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.09)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	3-oxo-2,6-dihydro-1H-pyridine-2-carbonitrile
$\mu_{a,b,c}$	4.6, 2.7, 1.4
A, B, C	2031.4781, 1851.8936, 1274.7038
A_s, B_s, C_s	2025.5868, 1846.5231, 1271.0071
Charge, Multiplicity	0, 1
Predicted log column density	8.611±5.023
Electronic energy	-416.79675

geom937



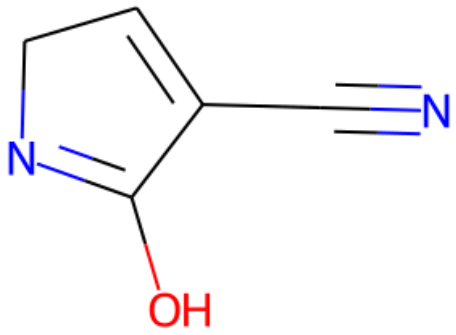
SMILES: N#CC1=CNC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.52)

Is DFT optimized?: True

Property	Value
Formula	C5H4N2O
Molecular weight	108.100
IUPAC name	2-oxo-1,3-dihydropyrrole-4-carbonitrile
$\mu_{a,b,c}$	2.0, 2.9, 0.0
A, B, C	6838.2144, 1279.8969, 1085.3969
A_s, B_s, C_s	6818.3836, 1276.1852, 1082.2492
Charge, Multiplicity	0, 1
Predicted log column density	10.827±4.833
Electronic energy	-377.53263

geom938



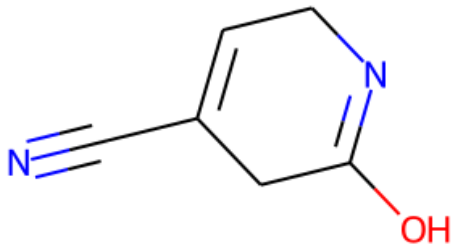
SMILES: N#CC1=CCN=C1O

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.55)

Is DFT optimized?: True

Property	Value
Formula	C5H4N2O
Molecular weight	108.100
IUPAC name	5-oxo-1,2-dihydropyrrole-4-carbonitrile
$\mu_{a,b,c}$	3.9, 1.8, 0.0
A, B, C	3736.3238, 1889.6961, 1264.8041
A_s, B_s, C_s	3725.4885, 1884.2160, 1261.1362
Charge, Multiplicity	0, 1
Predicted log column density	10.320±5.166
Electronic energy	-377.50563

geom939



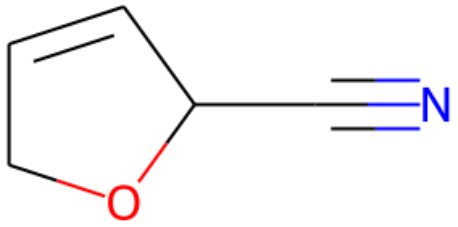
SMILES: N#CC1=CCN=C(O)C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	6-oxo-2,5-dihydro-1H-pyridine-4-carbonitrile
$\mu_{a,b,c}$	3.1, 1.7, 0.0
A, B, C	3337.2772, 1156.7079, 868.0888
A_s, B_s, C_s	3327.5991, 1153.3535, 865.5713
Charge, Multiplicity	0, 1
Predicted log column density	8.575±5.741
Electronic energy	-416.81579

geom940



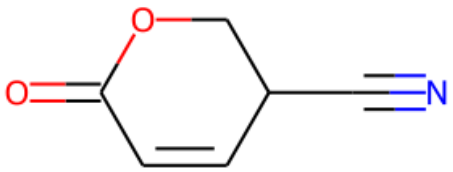
SMILES: N#CC1C=CCO1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.82)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	2,5-dihydrofuran-2-carbonitrile
$\mu_{a,b,c}$	4.3, 1.7, 0.9
A, B, C	6033.9322, 2148.0849, 1854.4362
A_s, B_s, C_s	6016.4338, 2141.8554, 1849.0583
Charge, Multiplicity	0, 1
Predicted log column density	10.363±4.644
Electronic energy	-323.35309

geom941



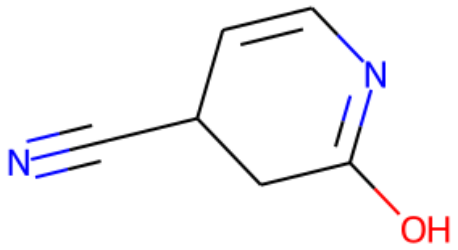
SMILES: N#CC1C=CC(=O)OC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.30)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	1.3, 2.8, 5.1
A, B, C	3152.6645, 1237.2474, 1160.8585
A_s, B_s, C_s	3143.5218, 1233.6594, 1157.4921
Charge, Multiplicity	0, 1
Predicted log column density	10.451±4.231
Electronic energy	-436.67772

geom942



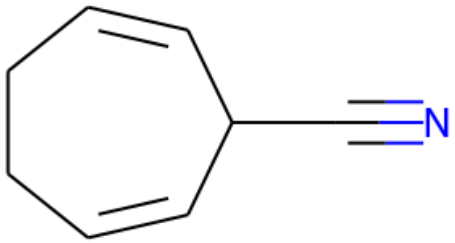
SMILES: N#CC1C=CN=C(O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.45)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	2-oxo-3,4-dihydro-1H-pyridine-4-carbonitrile
$\mu_{a,b,c}$	2.1, 1.6, 3.1
A, B, C	2506.8083, 1484.2276, 1162.6661
A_s, B_s, C_s	2499.5385, 1479.9233, 1159.2944
Charge, Multiplicity	0, 1
Predicted log column density	8.555±5.827
Electronic energy	-416.81126

geom943



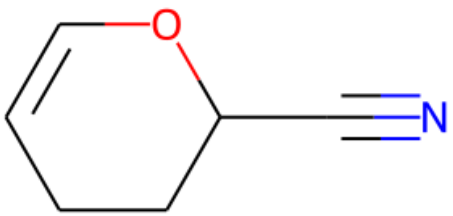
SMILES: N#CC1C=CCCC=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.89)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	
$\mu_{a,b,c}$	3.5, 0.2, 2.3
A, B, C	2382.5178, 1475.6288, 1268.7257
A_s, B_s, C_s	2375.6085, 1471.3495, 1265.0464
Charge, Multiplicity	0, 1
Predicted log column density	10.508±4.308
Electronic energy	-364.84638

geom944



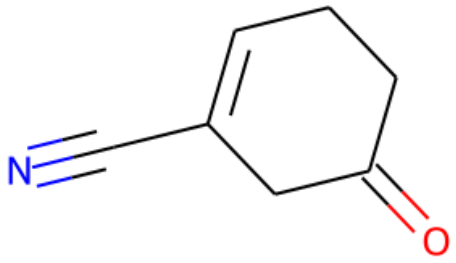
SMILES: N#CC1CCC=CO1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.24)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	3,4-dihydro-2H-pyran-2-carbonitrile
$\mu_{a,b,c}$	3.0, 1.2, 2.1
A, B, C	3169.4930, 1954.1258, 1724.8133
A_s, B_s, C_s	3160.3015, 1948.4589, 1719.8113
Charge, Multiplicity	0, 1
Predicted log column density	11.978±5.314
Electronic energy	-362.67127

geom945



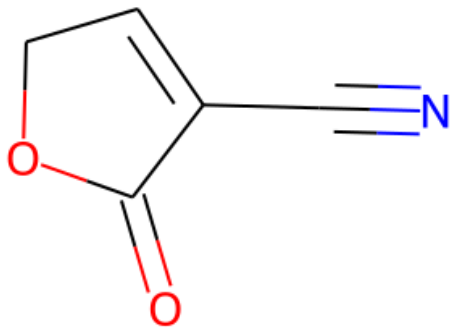
SMILES: N#CC1=CCCC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.58)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	2.3, 3.5, 0.8
A, B, C	3184.6104, 1157.8311, 883.2373
A_s, B_s, C_s	3175.3750, 1154.4734, 880.6760
Charge, Multiplicity	0, 1
Predicted log column density	10.052±4.579
Electronic energy	-400.78387

geom946



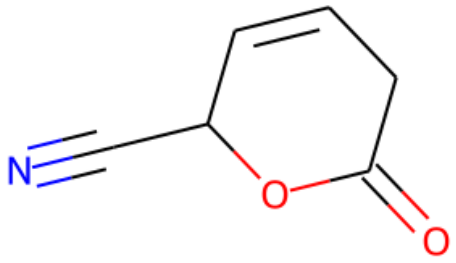
SMILES: N#CC1=CCOC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.37)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	5-oxo-2H-furan-4-carbonitrile
$\mu_{a,b,c}$	3.9, 5.6, 0.0
A, B, C	3938.7942, 1851.1584, 1269.4232
A_s, B_s, C_s	3927.3717, 1845.7901, 1265.7418
Charge, Multiplicity	0, 1
Predicted log column density	12.321±4.347
Electronic energy	-397.37943

geom947



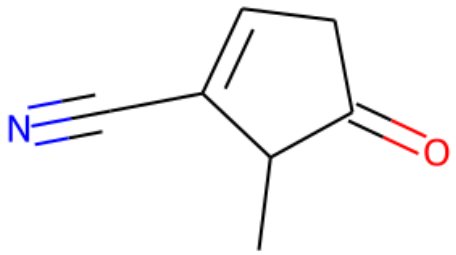
SMILES: N#CC1C=CCC(=O)O1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.28)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.2, 5.0, 1.1
A, B, C	2604.6813, 1488.1999, 1187.4946
A_s, B_s, C_s	2597.1277, 1483.8841, 1184.0509
Charge, Multiplicity	0, 1
Predicted log column density	10.385±5.024
Electronic energy	-436.67161

geom948



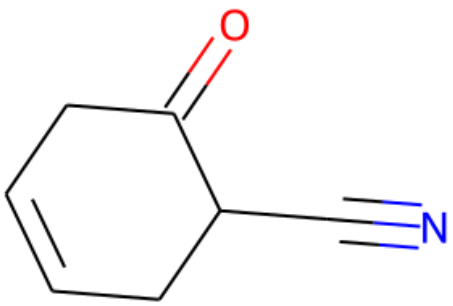
SMILES: CC1C(=O)CC=C1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.44)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	1.7, 2.0, 0.5
A, B, C	3184.9427, 1247.2194, 945.7558
A_s, B_s, C_s	3175.7063, 1243.6024, 943.0131
Charge, Multiplicity	0, 1
Predicted log column density	11.159±4.412
Electronic energy	-400.78147

geom949



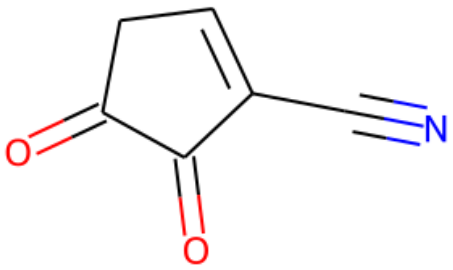
SMILES: N#CC1CC=CCC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.06)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	2.1, 2.7, 1.4
A, B, C	1968.3371, 1763.8683, 1342.1606
A_s, B_s, C_s	1962.6289, 1758.7531, 1338.2683
Charge, Multiplicity	0, 1
Predicted log column density	9.128±4.712
Electronic energy	-400.77582

geom950



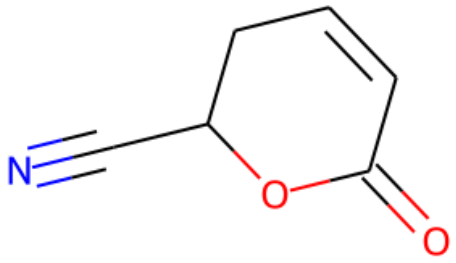
SMILES: N#CC1=CCC(=O)C1=O

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.65)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	2.0, 5.8, 0.0
A, B, C	3508.0909, 1274.9358, 940.5451
A_s, B_s, C_s	3497.9174, 1271.2384, 937.8175
Charge, Multiplicity	0, 1
Predicted log column density	12.269±5.005
Electronic energy	-435.44938

geom951



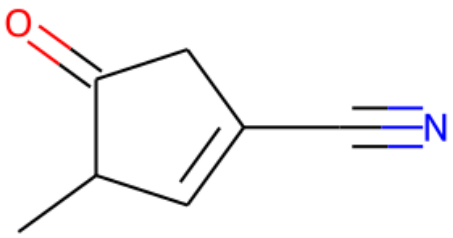
SMILES: N#CC1CC=CC(=O)O1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.08)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	1.3, 5.4, 1.8
A, B, C	2526.0694, 1541.0677, 1259.1197
A_s, B_s, C_s	2518.7438, 1536.5986, 1255.4682
Charge, Multiplicity	0, 1
Predicted log column density	10.520±4.777
Electronic energy	-436.67719

geom952



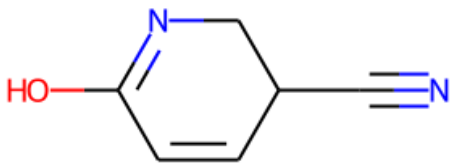
SMILES: CC1C=C(C#N)CC1=O

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.68)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	2.3, 1.9, 0.6
A, B, C	3469.5017, 1080.7538, 865.2849
A_s, B_s, C_s	3459.4401, 1077.6197, 862.7756
Charge, Multiplicity	0, 1
Predicted log column density	8.847±5.120
Electronic energy	-400.78061

geom953



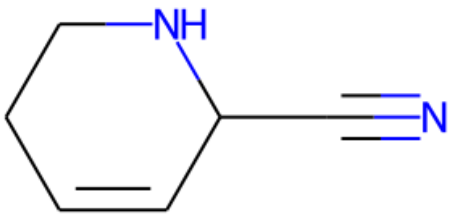
SMILES: N#CC1C=CC(O)=NC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.44)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	1.4, 4.5, 3.3
A, B, C	2965.6655, 1224.1628, 1183.5003
A_s, B_s, C_s	2957.0651, 1220.6127, 1180.0682
Charge, Multiplicity	0, 1
Predicted log column density	8.649±5.958
Electronic energy	-416.79526

geom954



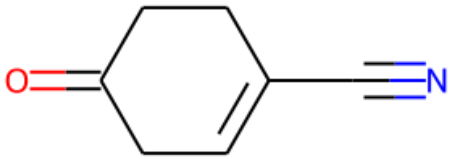
SMILES: N#CC1C=CCCN1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.07)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	1,2,3,6-tetrahydropyridine-6-carbonitrile
$\mu_{a,b,c}$	3.2, 0.2, 1.2
A, B, C	3744.6622, 1698.9967, 1441.9126
A_s, B_s, C_s	3733.8026, 1694.0696, 1437.7310
Charge, Multiplicity	0, 1
Predicted log column density	10.011±4.842
Electronic energy	-342.80872

geom955



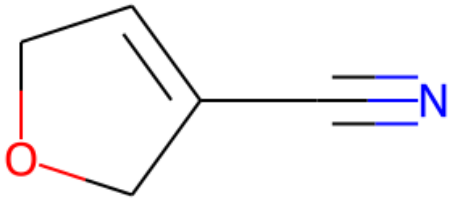
SMILES: N#CC1=CCC(=O)CC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.70)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	4-oxocyclohexene-1-carbonitrile
$\mu_{a,b,c}$	1.7, 0.4, 1.3
A, B, C	4461.6925, 997.6708, 848.9272
A_s, B_s, C_s	4448.7536, 994.7776, 846.4653
Charge, Multiplicity	0, 1
Predicted log column density	9.512±4.881
Electronic energy	-400.78417

geom956



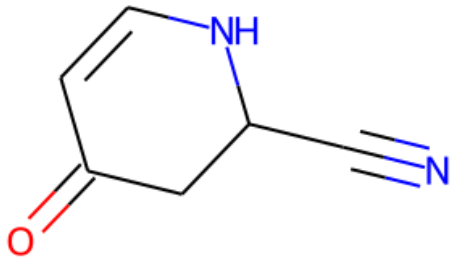
SMILES: N#CC1=CCOC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.58)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	2,5-dihydrofuran-3-carbonitrile
$\mu_{a,b,c}$	3.0, 1.5, 0.1
A, B, C	7942.0214, 1833.0741, 1518.0015
A_s, B_s, C_s	7918.9896, 1827.7582, 1513.5993
Charge, Multiplicity	0, 1
Predicted log column density	13.618±4.319
Electronic energy	-323.35987

geom957



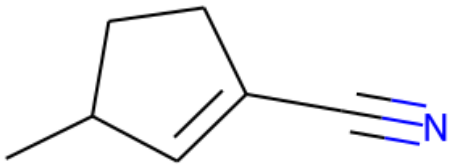
SMILES: N#CC1CC(=O)C=CN1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.72)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	4-oxo-2,3-dihydro-1H-pyridine-2-carbonitrile
$\mu_{a,b,c}$	2.0, 4.9, 3.0
A, B, C	2437.7961, 1512.9255, 1217.5752
A_s, B_s, C_s	2430.7265, 1508.5380, 1214.0442
Charge, Multiplicity	0, 1
Predicted log column density	11.103±4.942
Electronic energy	-416.81613

geom958



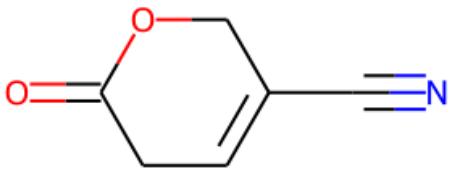
SMILES: CC1C=C(C#N)CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	3-methylcyclopentene-1-carbonitrile
$\mu_{a,b,c}$	4.9, 0.8, 0.5
A, B, C	4935.0790, 1262.1074, 1056.7964
A_s, B_s, C_s	4920.7673, 1258.4473, 1053.7316
Charge, Multiplicity	0, 1
Predicted log column density	8.170±4.450
Electronic energy	-326.79010

geom959



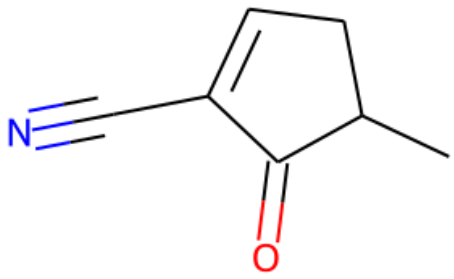
SMILES: N#CC1=CCC(=O)OC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.75)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.2, 1.9, 0.1
A, B, C	4977.9399, 1007.8704, 846.9505
A_s, B_s, C_s	4963.5039, 1004.9476, 844.4943
Charge, Multiplicity	0, 1
Predicted log column density	12.195±4.763
Electronic energy	-436.68113

geom960



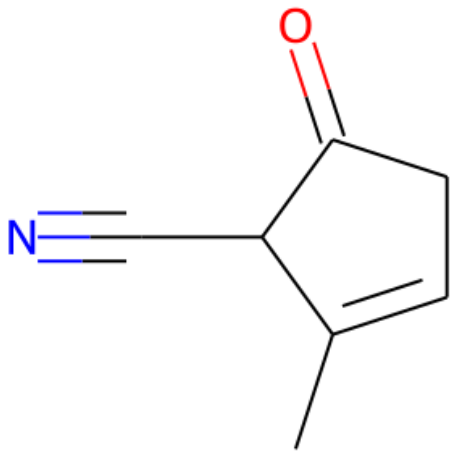
SMILES: CC1CC=C(C#N)C1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.50)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	4-methyl-5-oxocyclopentene-1-carbonitrile
$\mu_{a,b,c}$	5.2, 4.6, 0.3
A, B, C	3205.5331, 1244.2133, 944.3218
A_s, B_s, C_s	3196.2371, 1240.6051, 941.5832
Charge, Multiplicity	0, 1
Predicted log column density	10.619±4.725
Electronic energy	-400.78413

geom961



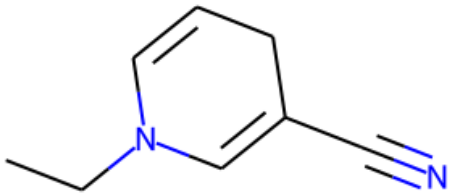
SMILES: CC1=CCC(=O)C1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.61)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	0.9, 5.4, 1.0
A, B, C	1979.2340, 1814.5675, 1041.9203
A_s, B_s, C_s	1973.4942, 1809.3052, 1038.8987
Charge, Multiplicity	0, 1
Predicted log column density	10.511±4.924
Electronic energy	-400.77640

geom962



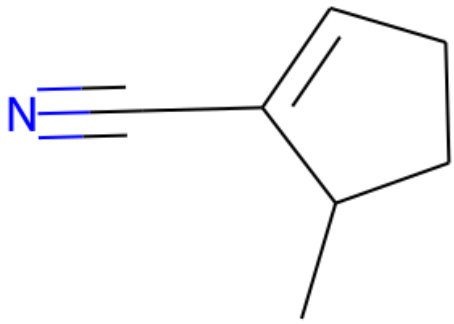
SMILES: CCN1C=CCC(C#N)=C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.76)

Is DFT optimized?: True

Property	Value
Formula	C8H10N2
Molecular weight	134.182
IUPAC name	1-ethyl-4H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	6.4, 1.5, 0.3
A, B, C	2306.9286, 897.3430, 693.3578
A_s, B_s, C_s	2300.2385, 894.7407, 691.3471
Charge, Multiplicity	0, 1
Predicted log column density	13.562±5.930
Electronic energy	-420.20541

geom963



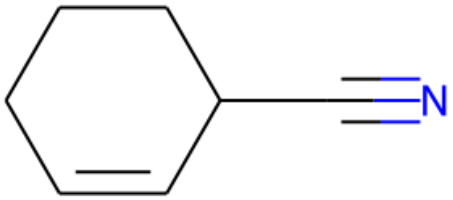
SMILES: CC1CCC=C1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.21)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	5-methylcyclopentene-1-carbonitrile
$\mu_{a,b,c}$	4.8, 0.3, 0.2
A, B, C	3420.5645, 1686.5889, 1258.1920
A_s, B_s, C_s	3410.6449, 1681.6977, 1254.5433
Charge, Multiplicity	0, 1
Predicted log column density	11.511±4.316
Electronic energy	-326.79045

geom964



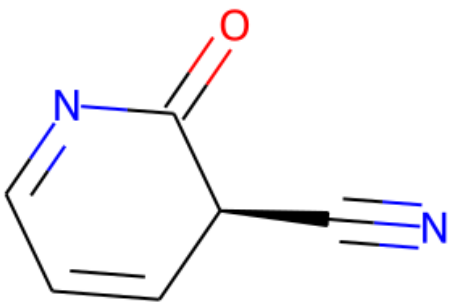
SMILES: N#CC1C=CCCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.83)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	cyclohex-2-ene-1-carbonitrile
$\mu_{a,b,c}$	3.9, 0.0, 2.1
A, B, C	3575.6955, 1667.7529, 1419.5195
A_s, B_s, C_s	3565.3260, 1662.9164, 1415.4029
Charge, Multiplicity	0, 1
Predicted log column density	9.724±4.103
Electronic energy	-326.78968

geom965



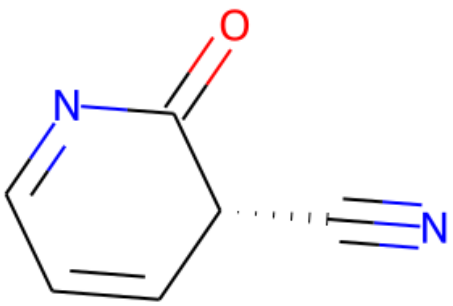
SMILES: N#C[C@H]1C=CC=NC1=O

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.25)

Is DFT optimized?: True

Property	Value
Formula	C6H4N2O
Molecular weight	120.111
IUPAC name	(3R)-2-oxo-3H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	2.9, 4.8, 2.6
A, B, C	2315.5317, 1744.5036, 1247.4271
A_s, B_s, C_s	2308.8167, 1739.4446, 1243.8096
Charge, Multiplicity	0, 1
Predicted log column density	10.701±5.288
Electronic energy	-415.57849

geom966



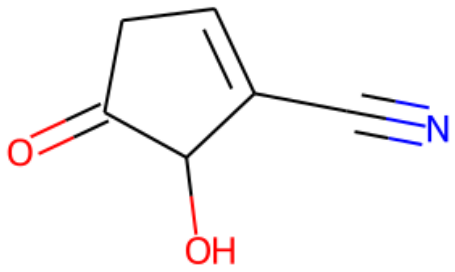
SMILES: N#C[C@@H]1C=CC=NC1=O

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.25)

Is DFT optimized?: True

Property	Value
Formula	C6H4N2O
Molecular weight	120.111
IUPAC name	(3S)-2-oxo-3H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	2.9, 4.8, 2.6
A, B, C	2314.4672, 1744.9342, 1248.1629
A_s, B_s, C_s	2307.7553, 1739.8739, 1244.5432
Charge, Multiplicity	0, 1
Predicted log column density	10.701±5.288
Electronic energy	-415.57849

geom967



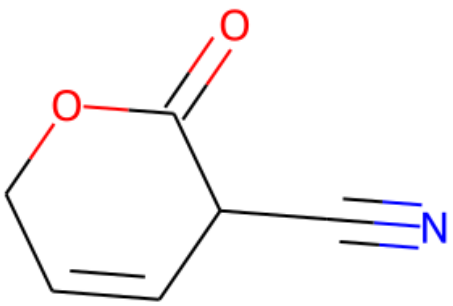
SMILES: N#CC1=CCC(=O)C1O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.69)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	3.1, 2.9, 1.0
A, B, C	3301.3932, 1269.9689, 950.0991
A_s, B_s, C_s	3291.8191, 1266.2860, 947.3438
Charge, Multiplicity	0, 1
Predicted log column density	11.050±4.385
Electronic energy	-436.66272

geom968



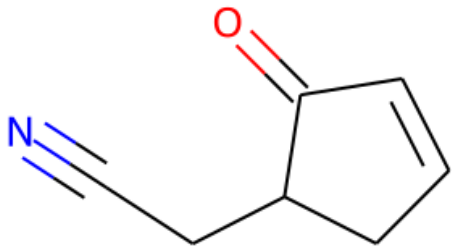
SMILES: N#CC1C=CCOC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.23)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	6-oxo-2,5-dihydropyran-5-carbonitrile
$\mu_{a,b,c}$	2.7, 4.4, 1.9
A, B, C	2104.9717, 1818.9165, 1296.6483
A_s, B_s, C_s	2098.8672, 1813.6416, 1292.8880
Charge, Multiplicity	0, 1
Predicted log column density	11.355±4.457
Electronic energy	-436.67062

geom969



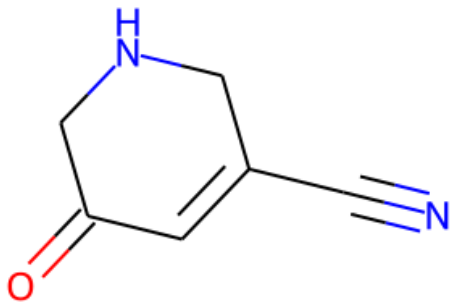
SMILES: N#CCC1CC=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.12)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	2-(2-oxocyclopent-3-en-1-yl)acetonitrile
$\mu_{a,b,c}$	3.0, 2.6, 0.6
A, B, C	3225.3177, 1138.6871, 872.8216
A_s, B_s, C_s	3215.9643, 1135.3849, 870.2904
Charge, Multiplicity	0, 1
Predicted log column density	10.581±4.362
Electronic energy	-400.78420

geom970



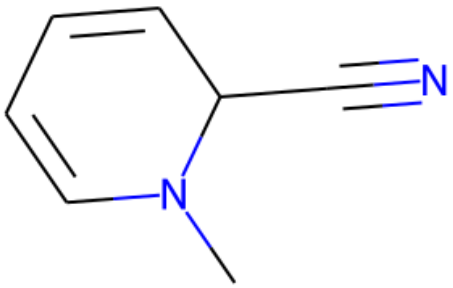
SMILES: N#CC1=CC(=O)CNC1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.84)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	5-oxo-2,6-dihydro-1H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	1.2, 2.4, 0.3
A, B, C	3173.8663, 1188.6509, 887.8409
A_s, B_s, C_s	3164.6620, 1185.2038, 885.2662
Charge, Multiplicity	0, 1
Predicted log column density	10.567±5.264
Electronic energy	-416.80393

geom971



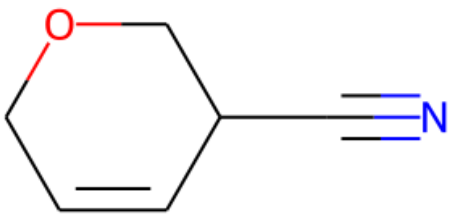
SMILES: CN1C=CC=CC1C#N

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.60)

Is DFT optimized?: True

Property	Value
Formula	C7H8N2
Molecular weight	120.155
IUPAC name	1-methyl-2H-pyridine-2-carbonitrile
$\mu_{a,b,c}$	2.0, 2.6, 2.0
A, B, C	2218.3888, 1732.3351, 1232.5743
A_s, B_s, C_s	2211.9555, 1727.3113, 1228.9999
Charge, Multiplicity	0, 1
Predicted log column density	13.726±4.903
Electronic energy	-380.88398

geom972



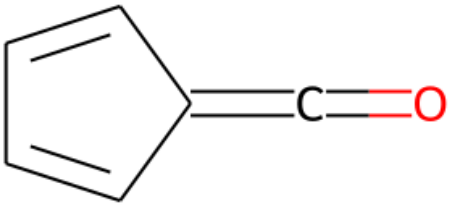
SMILES: N#CC1C=CCOC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.31)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	3.9, 1.5, 2.9
A, B, C	3785.2222, 1709.9071, 1453.2945
A_s, B_s, C_s	3774.2451, 1704.9484, 1449.0799
Charge, Multiplicity	0, 1
Predicted log column density	11.699±4.905
Electronic energy	-362.66496

geom973



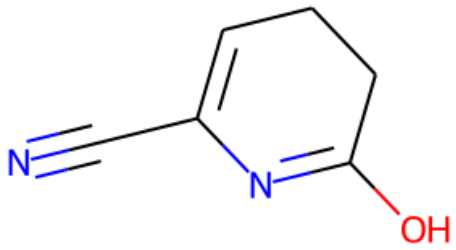
SMILES: O=C=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.54)

Is DFT optimized?: True

Property	Value
Formula	C6H4O
Molecular weight	92.097
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	8508.1992, 1935.1499, 1576.5730
A_s, B_s, C_s	8483.5254, 1929.5380, 1572.0009
Charge, Multiplicity	0, 1
Predicted log column density	11.553±2.250
Electronic energy	-306.10798

geom974



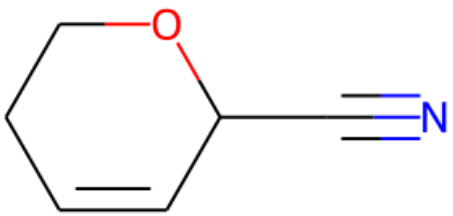
SMILES: N#CC1=CCCC(O)=N1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.65)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	7.0, 4.7, 0.6
A, B, C	3093.9729, 1241.5821, 911.3329
A_s, B_s, C_s	3085.0004, 1237.9815, 908.6900
Charge, Multiplicity	0, 1
Predicted log column density	9.656±5.457
Electronic energy	-416.80481

geom975



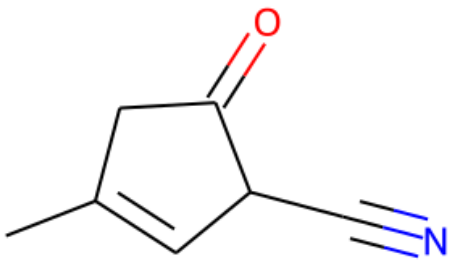
SMILES: N#CC1C=CCCO1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.15)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	3,6-dihydro-2H-pyran-6-carbonitrile
$\mu_{a,b,c}$	4.1, 1.1, 0.6
A, B, C	3870.8033, 1717.7251, 1455.4171
A_s, B_s, C_s	3859.5779, 1712.7437, 1451.1964
Charge, Multiplicity	0, 1
Predicted log column density	10.849±4.871
Electronic energy	-362.66416

geom976



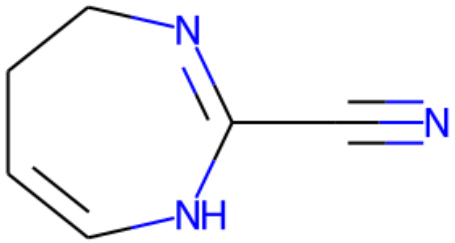
SMILES: CC1=CC(C#N)C(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.77)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	5.8, 0.3, 1.6
A, B, C	2604.5103, 1307.9267, 951.8320
A_s, B_s, C_s	2596.9573, 1304.1337, 949.0717
Charge, Multiplicity	0, 1
Predicted log column density	8.842±5.560
Electronic energy	-400.77598

geom977



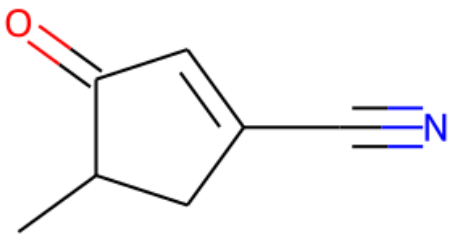
SMILES: N#CC1=NCCC=CN1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.92)

Is DFT optimized?: True

Property	Value
Formula	C6H7N3
Molecular weight	121.143
IUPAC name	4,5-dihydro-1H-1,3-diazepine-2-carbonitrile
$\mu_{a,b,c}$	4.5, 2.4, 0.7
A, B, C	3515.0437, 1232.4700, 956.3487
A_s, B_s, C_s	3504.8501, 1228.8959, 953.5753
Charge, Multiplicity	0, 1
Predicted log column density	11.455±7.080
Electronic energy	-396.93003

geom978



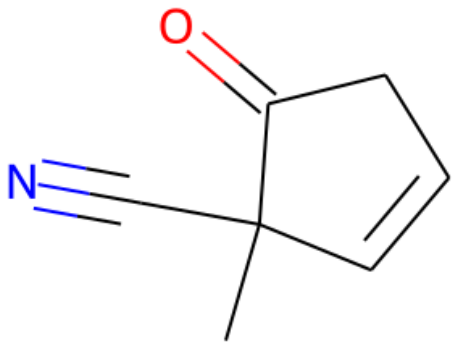
SMILES: CC1CC(C#N)=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.93)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	1.5, 2.4, 0.6
A, B, C	3523.9195, 1076.2812, 859.2911
A_s, B_s, C_s	3513.7002, 1073.1600, 856.7992
Charge, Multiplicity	0, 1
Predicted log column density	10.273±4.973
Electronic energy	-400.78472

geom979



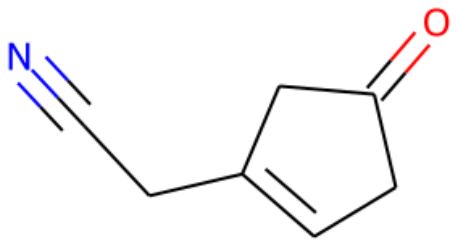
SMILES: CC1(C#N)C=CCC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.79)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	4.0, 2.6, 2.3
A, B, C	2228.4742, 1575.5217, 1368.9174
A_s, B_s, C_s	2222.0116, 1570.9527, 1364.9475
Charge, Multiplicity	0, 1
Predicted log column density	10.821±5.756
Electronic energy	-400.77182

geom980



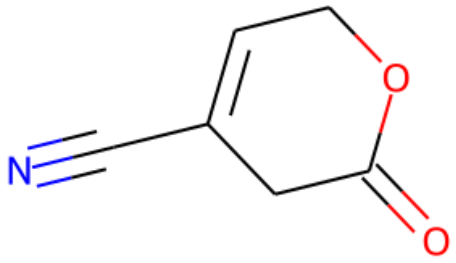
SMILES: N#CCC1=CCC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.78)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	0.3, 4.3, 1.8
A, B, C	3659.1465, 953.4736, 820.7402
A_s, B_s, C_s	3648.5350, 950.7085, 818.3600
Charge, Multiplicity	0, 1
Predicted log column density	9.694±4.614
Electronic energy	-400.77853

geom981



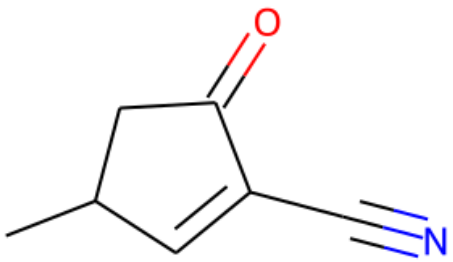
SMILES: N#CC1=CCOC(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.94)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.0, 3.7, 0.0
A, B, C	3416.9151, 1160.4138, 875.5746
A_s, B_s, C_s	3407.0061, 1157.0486, 873.0354
Charge, Multiplicity	0, 1
Predicted log column density	11.824±4.800
Electronic energy	-436.68173

geom982



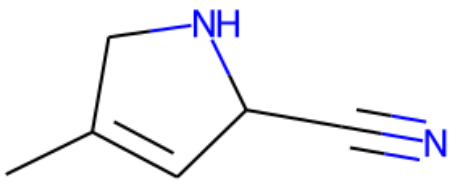
SMILES: CC1C=C(C#N)C(=O)C1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (5.94)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	6.8, 1.9, 1.0
A, B, C	2828.9376, 1246.1017, 912.3655
A_s, B_s, C_s	2820.7337, 1242.4880, 909.7196
Charge, Multiplicity	0, 1
Predicted log column density	9.799±5.226
Electronic energy	-400.78377

geom983



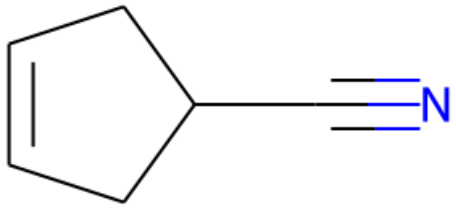
SMILES: CC1=CC(C#N)NC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.83)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	
$\mu_{a,b,c}$	5.0, 1.3, 2.4
A, B, C	4651.1709, 1340.3613, 1133.3133
A_s, B_s, C_s	4637.6825, 1336.4742, 1130.0267
Charge, Multiplicity	0, 1
Predicted log column density	9.524±4.995
Electronic energy	-342.80610

geom984



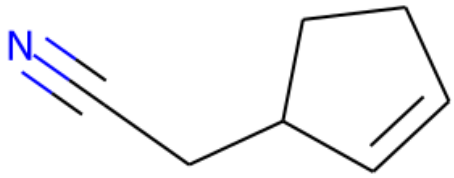
SMILES: N#CC1CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (4.96)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	cyclopent-3-ene-1-carbonitrile
$\mu_{a,b,c}$	3.8, 0.0, 2.1
A, B, C	5190.4564, 2155.8466, 1896.6029
A_s, B_s, C_s	5175.4041, 2149.5946, 1891.1028
Charge, Multiplicity	0, 1
Predicted log column density	10.213±4.340
Electronic energy	-287.47834

geom985



SMILES: N#CCC1C=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.15)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	2-cyclopent-2-en-1-ylacetonitrile
$\mu_{a,b,c}$	3.8, 1.7, 0.4
A, B, C	5416.6394, 1217.4962, 1040.2581
A_s, B_s, C_s	5400.9311, 1213.9655, 1037.2414
Charge, Multiplicity	0, 1
Predicted log column density	10.339±4.440
Electronic energy	-326.78429

geom986

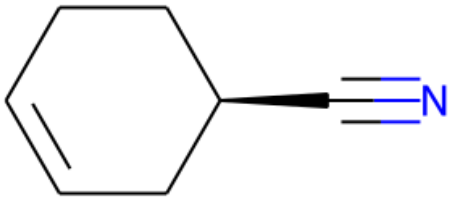
SMILES: N#C[C@@H]1CC=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.24)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	(1S)-cyclohex-3-ene-1-carbonitrile
$\mu_{a,b,c}$	3.1, 0.3, 2.7
A, B, C	3014.9598, 1872.1170, 1663.3930
A_s, B_s, C_s	3006.2164, 1866.6879, 1658.5692
Charge, Multiplicity	0, 1
Predicted log column density	10.198±4.214
Electronic energy	-326.79106

geom987



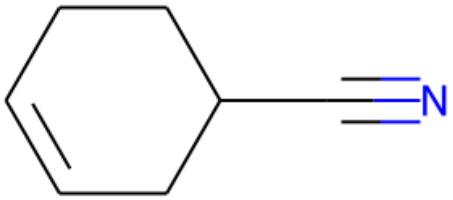
SMILES: N#C[C@H]1CC=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.24)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	(1R)-cyclohex-3-ene-1-carbonitrile
$\mu_{a,b,c}$	3.1, 0.3, 2.7
A, B, C	3013.4333, 1872.6516, 1664.2105
A_s, B_s, C_s	3004.6944, 1867.2209, 1659.3843
Charge, Multiplicity	0, 1
Predicted log column density	10.198±4.214
Electronic energy	-326.79106

geom988



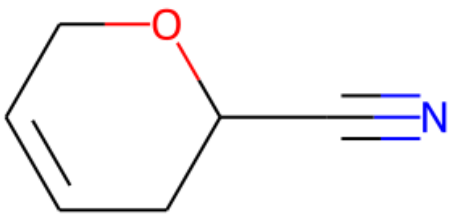
SMILES: N#CC1CC=CCC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.24)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	cyclohex-3-ene-1-carbonitrile
$\mu_{a,b,c}$	3.1, 0.3, 2.7
A, B, C	3010.5370, 1873.2822, 1665.8341
A_s, B_s, C_s	3001.8065, 1867.8497, 1661.0032
Charge, Multiplicity	0, 1
Predicted log column density	10.198±4.214
Electronic energy	-326.79106

geom989



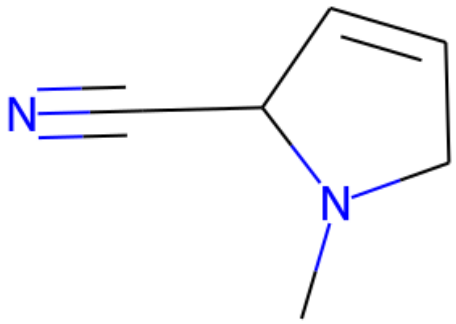
SMILES: N#CC1CC=CCO1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.30)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	3,6-dihydro-2H-pyran-2-carbonitrile
$\mu_{a,b,c}$	3.1, 1.2, 1.1
A, B, C	3134.7947, 1955.0510, 1749.0519
A_s, B_s, C_s	3125.7038, 1949.3814, 1743.9797
Charge, Multiplicity	0, 1
Predicted log column density	10.334±4.914
Electronic energy	-362.66492

geom990



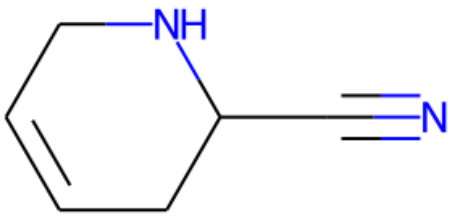
SMILES: CN1CC=CC1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.35)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	1-methyl-2,5-dihydropyrrole-2-carbonitrile
$\mu_{a,b,c}$	4.6, 0.0, 1.8
A, B, C	3214.1093, 1919.4455, 1304.1663
A_s, B_s, C_s	3204.7884, 1913.8791, 1300.3842
Charge, Multiplicity	0, 1
Predicted log column density	12.753±4.863
Electronic energy	-342.79519

geom991



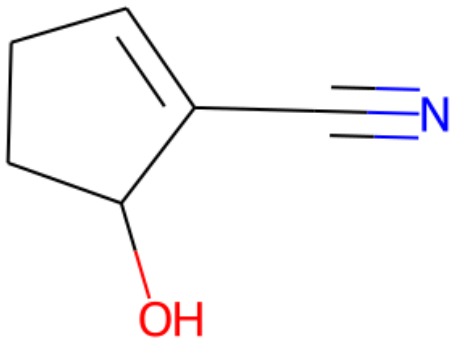
SMILES: N#CC1CC=CCN1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.36)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	1,2,3,6-tetrahydropyridine-2-carbonitrile
$\mu_{a,b,c}$	2.4, 0.0, 1.9
A, B, C	3082.5042, 1919.0551, 1711.1047
A_s, B_s, C_s	3073.5649, 1913.4898, 1706.1425
Charge, Multiplicity	0, 1
Predicted log column density	8.009±5.313
Electronic energy	-342.81001

geom992



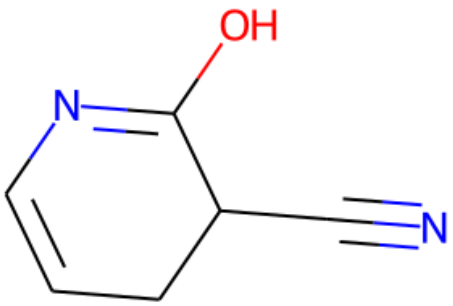
SMILES: N#CC1=CCCC1O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.45)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	5-hydroxycyclopentene-1-carbonitrile
$\mu_{a,b,c}$	5.2, 2.0, 0.7
A, B, C	3366.5323, 1778.8443, 1218.9280
A_s, B_s, C_s	3356.7693, 1773.6857, 1215.3931
Charge, Multiplicity	0, 1
Predicted log column density	11.137±4.764
Electronic energy	-362.67747

geom993



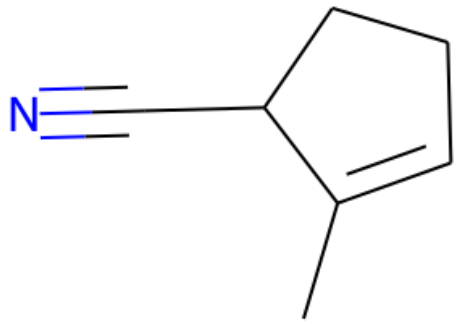
SMILES: N#CC1CC=CN=C1O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.46)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	2-oxo-3,4-dihydro-1H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	2.7, 0.1, 2.7
A, B, C	2064.3416, 1830.4158, 1255.4380
A_s, B_s, C_s	2058.3550, 1825.1076, 1251.7972
Charge, Multiplicity	0, 1
Predicted log column density	8.467±5.729
Electronic energy	-416.80742

geom994



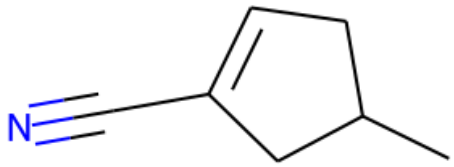
SMILES: CC1=CCCC1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.47)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	
$\mu_{a,b,c}$	4.1, 0.4, 1.3
A, B, C	3021.2133, 1894.1423, 1245.4485
A_s, B_s, C_s	3012.4518, 1888.6493, 1241.8367
Charge, Multiplicity	0, 1
Predicted log column density	10.209±4.408
Electronic energy	-326.78952

geom995



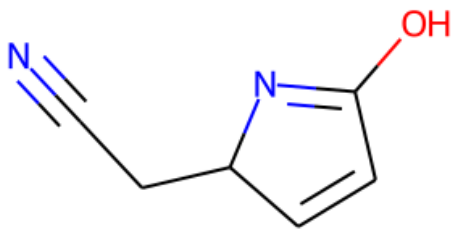
SMILES: CC1CC=C(C#N)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.50)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	
$\mu_{a,b,c}$	4.8, 1.0, 0.7
A, B, C	4570.0602, 1323.3173, 1164.4046
A_s, B_s, C_s	4556.8070, 1319.4797, 1161.0278
Charge, Multiplicity	0, 1
Predicted log column density	10.772±4.464
Electronic energy	-326.78999

geom996



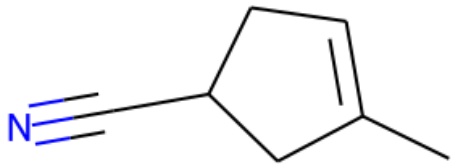
SMILES: N#CCC1C=CC(O)=N1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.51)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	3.5, 2.4, 1.0
A, B, C	5473.5259, 901.3291, 806.9406
A_s, B_s, C_s	5457.6527, 898.7153, 804.6005
Charge, Multiplicity	0, 1
Predicted log column density	9.299±5.010
Electronic energy	-416.80402

geom997



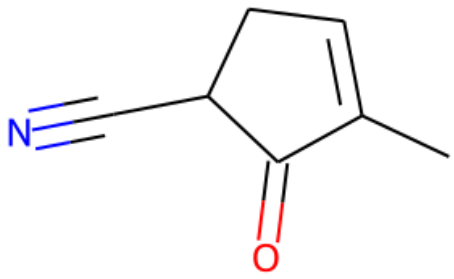
SMILES: CC1=CCC(C#N)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.59)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	3-methylcyclopent-3-ene-1-carbonitrile
$\mu_{a,b,c}$	3.5, 1.7, 2.2
A, B, C	3751.1708, 1462.9553, 1283.6082
A_s, B_s, C_s	3740.2924, 1458.7127, 1279.8857
Charge, Multiplicity	0, 1
Predicted log column density	10.484±4.978
Electronic energy	-326.78889

geom998



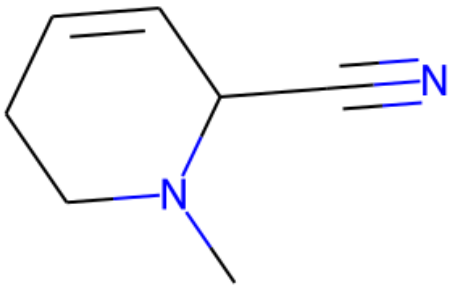
SMILES: CC1=CCC(C#N)C1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	4.3, 4.5, 1.4
A, B, C	3025.4877, 1290.2902, 981.3654
A_s, B_s, C_s	3016.7138, 1286.5484, 978.5194
Charge, Multiplicity	0, 1
Predicted log column density	9.080±4.752
Electronic energy	-400.78484

geom999



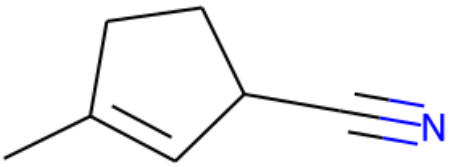
SMILES: CN1CCC=CC1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.63)

Is DFT optimized?: True

Property	Value
Formula	C7H10N2
Molecular weight	122.171
IUPAC name	1-methyl-3,6-dihydro-2H-pyridine-6-carbonitrile
$\mu_{a,b,c}$	4.8, 0.4, 0.2
A, B, C	2985.1903, 1374.3205, 1107.1275
A_s, B_s, C_s	2976.5332, 1370.3349, 1103.9169
Charge, Multiplicity	0, 1
Predicted log column density	12.416±4.757
Electronic energy	-382.10246

geom1000



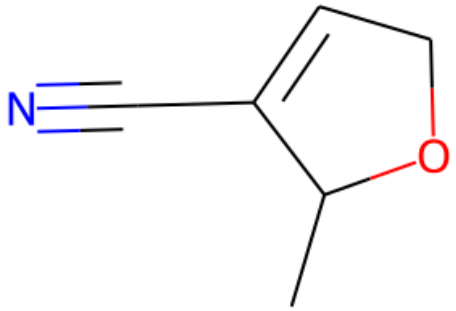
SMILES: CC1=CC(C#N)CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.64)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	3-methylcyclopent-2-ene-1-carbonitrile
$\mu_{a,b,c}$	3.9, 1.7, 1.7
A, B, C	3950.5067, 1420.2304, 1239.2978
A_s, B_s, C_s	3939.0502, 1416.1117, 1235.7038
Charge, Multiplicity	0, 1
Predicted log column density	8.529±4.924
Electronic energy	-326.78921

geom1001



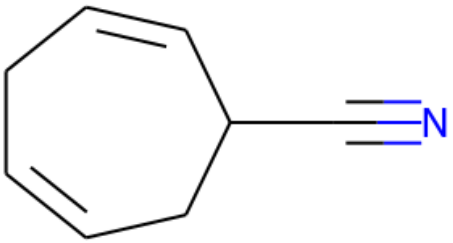
SMILES: CC1OCC=C1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.65)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	3.0, 1.3, 0.2
A, B, C	3528.0484, 1770.1972, 1244.9982
A_s, B_s, C_s	3517.8171, 1765.0637, 1241.3877
Charge, Multiplicity	0, 1
Predicted log column density	12.453±5.082
Electronic energy	-362.67085

geom1002



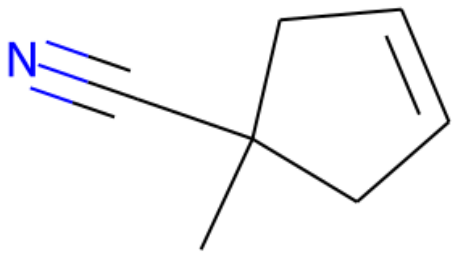
SMILES: N#CC1C=CCC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.65)

Is DFT optimized?: True

Property	Value
Formula	C8H9N
Molecular weight	119.167
IUPAC name	
$\mu_{a,b,c}$	2.4, 0.1, 3.0
A, B, C	2085.4641, 1639.6480, 1477.7130
A_s, B_s, C_s	2079.4163, 1634.8930, 1473.4276
Charge, Multiplicity	0, 1
Predicted log column density	9.504±4.806
Electronic energy	-364.84832

geom1003



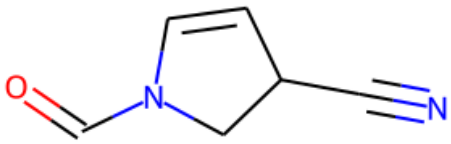
SMILES: CC1(C#N)CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.70)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	1-methylcyclopent-3-ene-1-carbonitrile
$\mu_{a,b,c}$	4.0, 1.5, 0.0
A, B, C	3662.3776, 1591.0385, 1561.0024
A_s, B_s, C_s	3651.7567, 1586.4244, 1556.4755
Charge, Multiplicity	0, 1
Predicted log column density	9.470±5.768
Electronic energy	-326.78542

geom1004



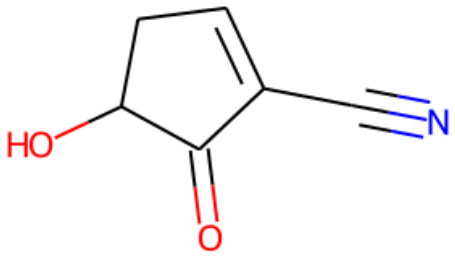
SMILES: N#CC1C=CN(C=O)C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.71)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	1.0, 4.2, 1.5
A, B, C	3807.5171, 1026.9426, 864.3743
A_s, B_s, C_s	3796.4753, 1023.9645, 861.8676
Charge, Multiplicity	0, 1
Predicted log column density	8.826±5.148
Electronic energy	-416.81539

geom1005



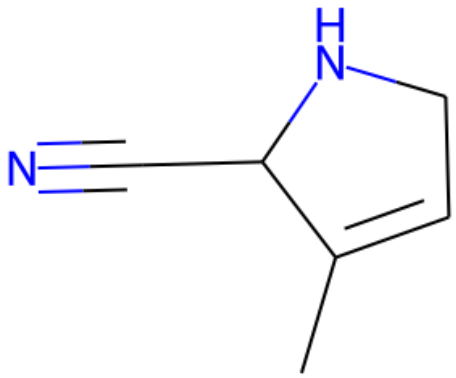
SMILES: N#CC1=CCC(O)C1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.71)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	3.3, 3.9, 1.0
A, B, C	3383.9865, 1238.7003, 933.2841
A_s, B_s, C_s	3374.1730, 1235.1080, 930.5776
Charge, Multiplicity	0, 1
Predicted log column density	10.256±4.722
Electronic energy	-436.66946

geom1006



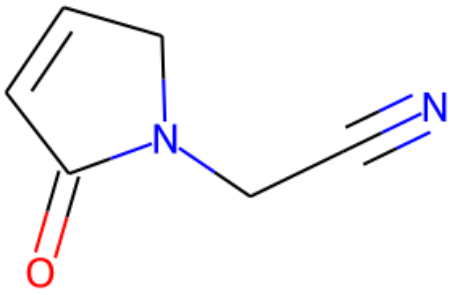
SMILES: CC1=CCNC1C#N

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.72)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	
$\mu_{a,b,c}$	3.2, 0.5, 0.5
A, B, C	2696.3936, 2109.9810, 1381.4535
A_s, B_s, C_s	2688.5740, 2103.8620, 1377.4473
Charge, Multiplicity	0, 1
Predicted log column density	8.910±5.110
Electronic energy	-342.80794

geom1007



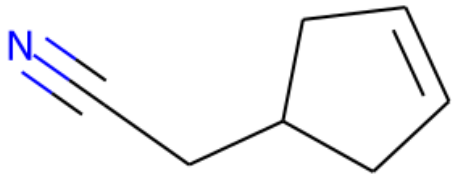
SMILES: N#CCN1CC=CC1=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.73)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	2-(5-oxo-2H-pyrrol-1-yl)acetonitrile
$\mu_{a,b,c}$	2.4, 3.4, 2.7
A, B, C	2966.7899, 1278.4202, 999.8543
A_s, B_s, C_s	2958.1862, 1274.7128, 996.9547
Charge, Multiplicity	0, 1
Predicted log column density	10.932±4.534
Electronic energy	-416.82514

geom1008



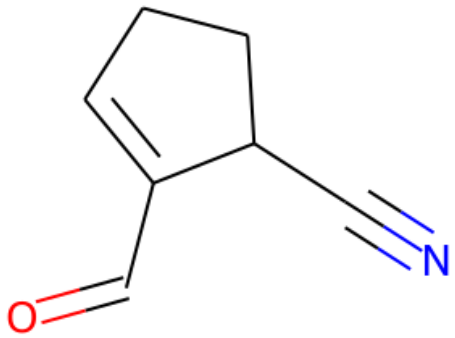
SMILES: N#CCC1CC=CC1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.73)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	2-cyclopent-3-en-1-ylacetonitrile
$\mu_{a,b,c}$	3.9, 1.7, 0.2
A, B, C	4888.6952, 1300.9303, 1148.6575
A_s, B_s, C_s	4874.5180, 1297.1576, 1145.3264
Charge, Multiplicity	0, 1
Predicted log column density	9.560±4.727
Electronic energy	-326.78447

geom1009



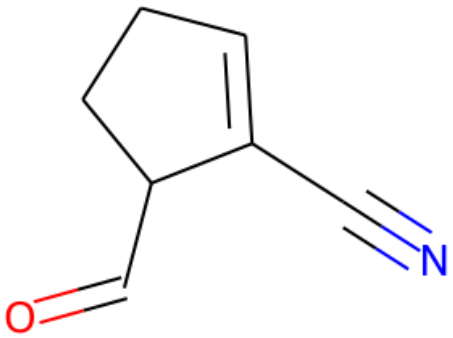
SMILES: N#CC1CCC=C1C=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.76)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	3.4, 5.4, 0.6
A, B, C	2054.9042, 1647.0015, 1067.6971
A_s, B_s, C_s	2048.9450, 1642.2252, 1064.6008
Charge, Multiplicity	0, 1
Predicted log column density	8.524±4.556
Electronic energy	-400.77061

geom1010



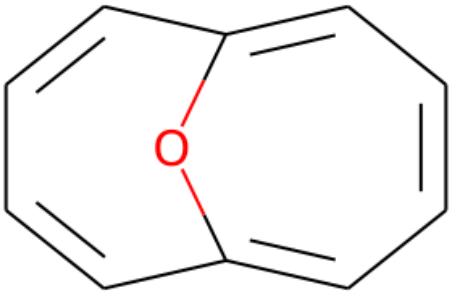
SMILES: N#CC1=CCCC1C=O

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (5.76)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	6.6, 0.3, 1.7
A, B, C	2180.7123, 1641.5680, 1032.6570
A_s, B_s, C_s	2174.3882, 1636.8075, 1029.6623
Charge, Multiplicity	0, 1
Predicted log column density	9.368±4.345
Electronic energy	-400.76470

geom1011



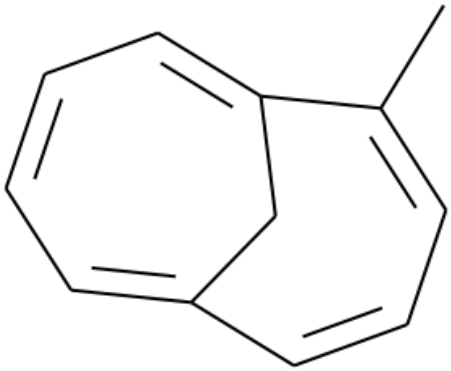
SMILES: C1=CC=C2C=CC=CC(=C1)O2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (6.51)

Is DFT optimized?: False

Property	Value
Formula	C10H8O
Molecular weight	144.173
IUPAC name	11-oxabicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	0.8, 0.1, 0.1
A, B, C	2312.9815, 1231.8729, 916.7861
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.958±3.012
Electronic energy	-460.35908

geom1012



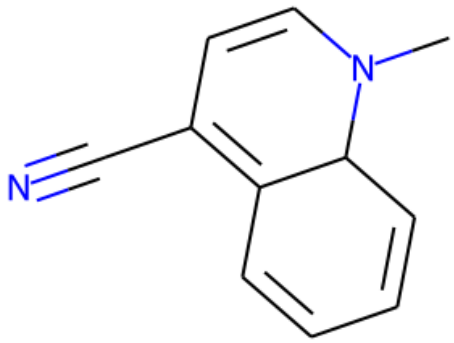
SMILES: CC1=CC=CC2=CC=CC=C1C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (6.58)

Is DFT optimized?: True

Property	Value
Formula	C12H12
Molecular weight	156.228
IUPAC name	2-methylbicyclo[4.4.1]undeca-1(10),2,4,6,8-pentaene
$\mu_{a,b,c}$	0.6, 1.6, 0.2
A, B, C	1613.6946, 981.2594, 685.4624
A_s, B_s, C_s	1609.0149, 978.4137, 683.4745
Charge, Multiplicity	0, 1
Predicted log column density	12.844±3.570
Electronic energy	-464.19240

geom1013



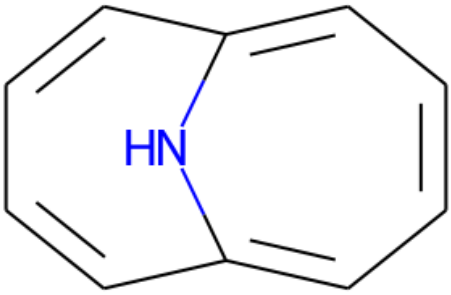
SMILES: CN1C=CC(C#N)=C2C=CC=CC21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (6.28)

Is DFT optimized?: True

Property	Value
Formula	C11H10N2
Molecular weight	170.215
IUPAC name	1-methyl-8aH-quinoline-4-carbonitrile
$\mu_{a,b,c}$	6.8, 3.4, 0.6
A, B, C	1145.8212, 806.6693, 492.7900
A_s, B_s, C_s	1142.4983, 804.3300, 491.3609
Charge, Multiplicity	0, 1
Predicted log column density	13.468±4.385
Electronic energy	-534.32746

geom1014



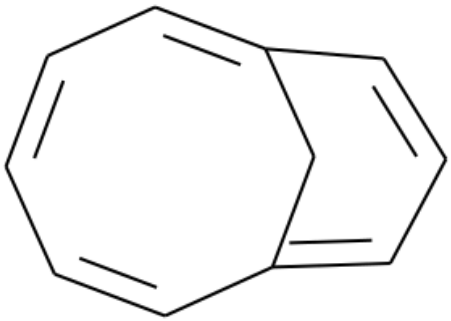
SMILES: C1=CC=C2C=CC=CC(=C1)N2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (6.97)

Is DFT optimized?: True

Property	Value
Formula	C10H9N
Molecular weight	143.189
IUPAC name	11-azabicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	0.5, 1.3, 1.0
A, B, C	2325.8270, 1170.1955, 876.4469
A_s, B_s, C_s	2319.0821, 1166.8020, 873.9052
Charge, Multiplicity	0, 1
Predicted log column density	12.583±3.361
Electronic energy	-440.91425

geom1015



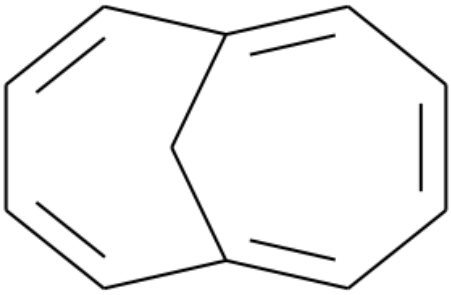
SMILES: C1=CC=C2C=CC=C(C=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (7.07)

Is DFT optimized?: True

Property	Value
Formula	C11H10
Molecular weight	142.201
IUPAC name	bicyclo[5.3.1]undeca-1(10),2,4,6,8-pentaene
$\mu_{a,b,c}$	0.5, 0.0, 0.4
A, B, C	1825.3008, 1293.1759, 1100.4722
A_s, B_s, C_s	1820.0074, 1289.4257, 1097.2808
Charge, Multiplicity	0, 1
Predicted log column density	13.718±3.530
Electronic energy	-424.90155

geom1016



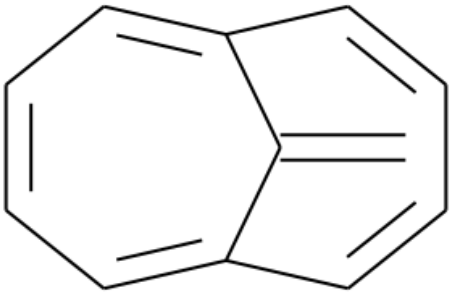
SMILES: C1=CC=C2C=CC=CC(=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (7.07)

Is DFT optimized?: True

Property	Value
Formula	C11H10
Molecular weight	142.201
IUPAC name	bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	0.1, 0.5, 0.5
A, B, C	1853.1820, 1280.7151, 996.4928
A_s, B_s, C_s	1847.8078, 1277.0010, 993.6030
Charge, Multiplicity	0, 1
Predicted log column density	13.718±3.530
Electronic energy	-424.77524

geom1017



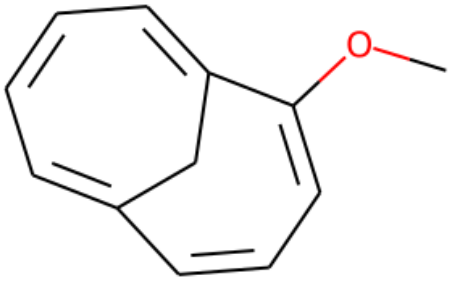
SMILES: C=C1C2=CC=CC=C1C=CC=C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (7.24)

Is DFT optimized?: True

Property	Value
Formula	C12H10
Molecular weight	154.212
IUPAC name	11-methylidenebicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	0.2, 0.7, 0.2
A, B, C	1486.1391, 1078.4552, 995.6128
A_s, B_s, C_s	1481.8293, 1075.3277, 992.7255
Charge, Multiplicity	0, 1
Predicted log column density	12.302±3.497
Electronic energy	-462.79211

geom1018



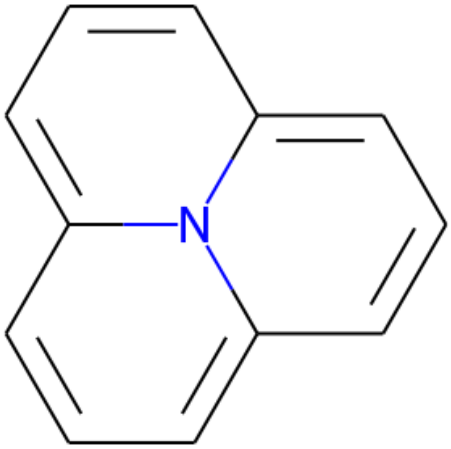
SMILES: COC1=CC=CC2=CC=CC=C1C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (7.26)

Is DFT optimized?: False

Property	Value
Formula	C12H12O
Molecular weight	172.227
IUPAC name	2-methoxybicyclo[4.4.1]undeca-1(10),2,4,6,8-pentaene
$\mu_{a,b,c}$	2.2, 0.1, 0.1
A, B, C	1303.2253, 787.6289, 551.5404
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	16.149±4.973
Electronic energy	-539.32440

geom1019



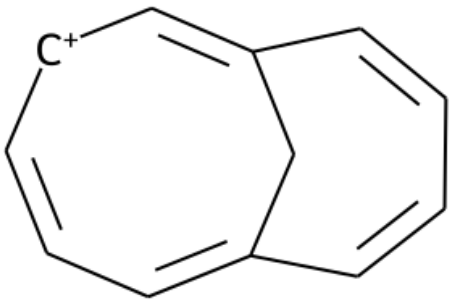
SMILES: C1=CC2=CC=CC3=CC=CC(=C1)N23

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.51)

Is DFT optimized?: True

Property	Value
Formula	C12H9N
Molecular weight	167.211
IUPAC name	13-azatricyclo[7.3.1.05,13]trideca-1(12),2,4,6,8,10-hexaene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	1131.4049, 1131.3782, 565.6958
A_s, B_s, C_s	1128.1239, 1128.0972, 564.0553
Charge, Multiplicity	0, 1
Predicted log column density	12.924±3.649
Electronic energy	-517.25264

geom1020



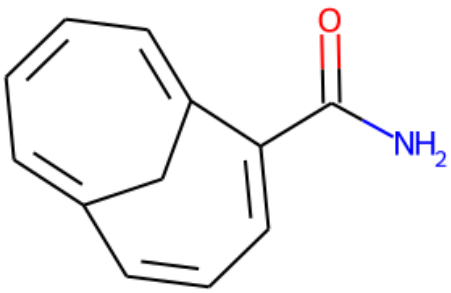
SMILES: C1=C[CH+]C=C2C=CC=CC(=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.54)

Is DFT optimized?: True

Property	Value
Formula	C12H11+
Molecular weight	155.220
IUPAC name	
$\mu_{a,b,c}$	0.3, 0.1, 0.8
A, B, C	1661.4001, 952.6994, 787.4431
A_s, B_s, C_s	1656.5820, 949.9366, 785.1595
Charge, Multiplicity	1, 1
Predicted log column density	13.469±4.140
Electronic energy	-463.36100

geom1021



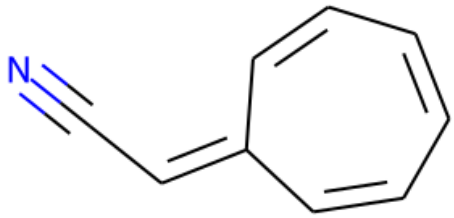
SMILES: NC(=O)C1=CC=CC2=CC=CC=C1C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.51)

Is DFT optimized?: False

Property	Value
Formula	C12H11NO
Molecular weight	185.226
IUPAC name	bicyclo[4.4.1]undeca-1(10),2,4,6,8-pentaene-2-carboxamide
$\mu_{a,b,c}$	3.6, 0.5, 1.8
A, B, C	1294.8265, 576.5782, 432.9628
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	13.627±4.856
Electronic energy	-593.50265

geom1022



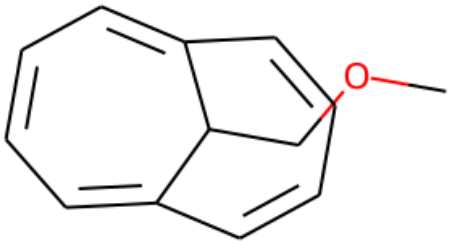
SMILES: N#CC=C1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.91)

Is DFT optimized?: False

Property	Value
Formula	C9H7N
Molecular weight	129.162
IUPAC name	2-cyclohepta-2,4,6-trien-1-ylideneacetonitrile
$\mu_{a,b,c}$	2.4, 0.6, 5.8
A, B, C	3163.4559, 846.2758, 667.6976
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.962±4.026
Electronic energy	-401.69139

geom1023



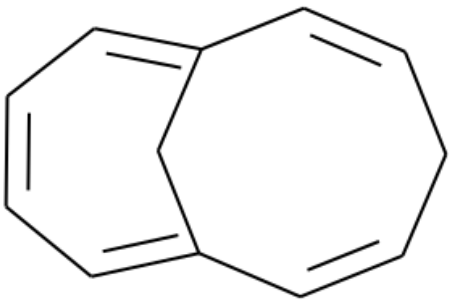
SMILES: COCC1C2=CC=CC=C1C=CC=C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (7.85)

Is DFT optimized?: False

Property	Value
Formula	C13H14O
Molecular weight	186.254
IUPAC name	11-(methoxymethyl)bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	2.2, 0.8, 0.5
A, B, C	925.9242, 691.6271, 536.6243
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.257±5.536
Electronic energy	-578.53467

geom1024



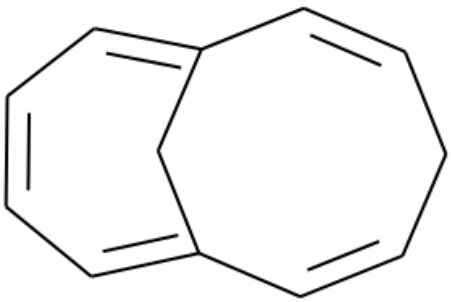
SMILES: C1=CC=C2/C=C/CC=CC(=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.72)

Is DFT optimized?: True

Property	Value
Formula	C12H12
Molecular weight	156.228
IUPAC name	(5E)-bicyclo[5.4.1]dodeca-1(11),2,5,7,9-pentaene
$\mu_{a,b,c}$	1.6, 0.0, 0.5
A, B, C	1727.4506, 928.6117, 767.0980
A_s, B_s, C_s	1722.4410, 925.9187, 764.8734
Charge, Multiplicity	0, 1
Predicted log column density	13.172±3.785
Electronic energy	-464.18776

geom1025



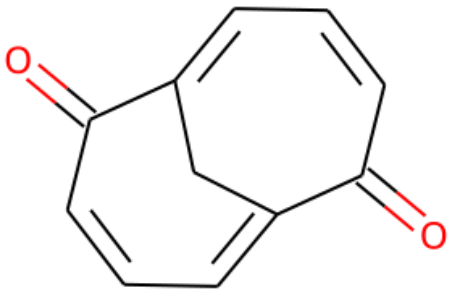
SMILES: C1=CC=C2C=CCC=CC(=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.72)

Is DFT optimized?: True

Property	Value
Formula	C12H12
Molecular weight	156.228
IUPAC name	bicyclo[5.4.1]dodeca-1(11),2,5,7,9-pentaene
$\mu_{a,b,c}$	1.6, 0.0, 0.5
A, B, C	1727.0373, 928.9701, 767.0879
A_s, B_s, C_s	1722.0289, 926.2761, 764.8634
Charge, Multiplicity	0, 1
Predicted log column density	13.172±3.785
Electronic energy	-464.18777

geom1026



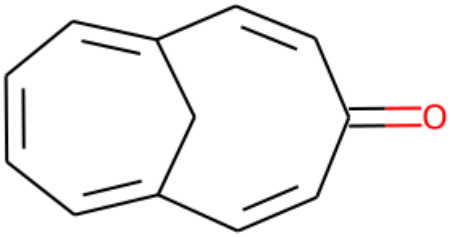
SMILES: O=C1C=CC=C2CC1=CC=CC2=O

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.65)

Is DFT optimized?: True

Property	Value
Formula	C11H8O2
Molecular weight	172.183
IUPAC name	bicyclo[4.4.1]undeca-1(10),3,5,8-tetraene-2,7-dione
$\mu_{a,b,c}$	0.0, 0.0, 0.7
A, B, C	1448.7321, 767.4194, 548.6715
A_s, B_s, C_s	1444.5308, 765.1939, 547.0803
Charge, Multiplicity	0, 1
Predicted log column density	12.709±5.498
Electronic energy	-574.17775

geom1027



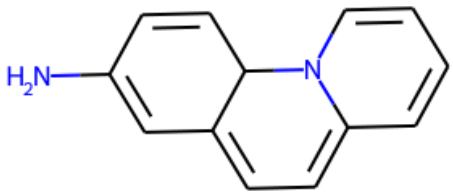
SMILES: O=C1C=CC2=CC=CC=C(C=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.70)

Is DFT optimized?: False

Property	Value
Formula	C12H10O
Molecular weight	170.211
IUPAC name	bicyclo[5.4.1]dodeca-1(11),2,5,7,9-pentaen-4-one
$\mu_{a,b,c}$	1.2, 3.6, 1.4
A, B, C	1637.1083, 693.0500, 553.4026
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.804±4.560
Electronic energy	-538.06669

geom1028



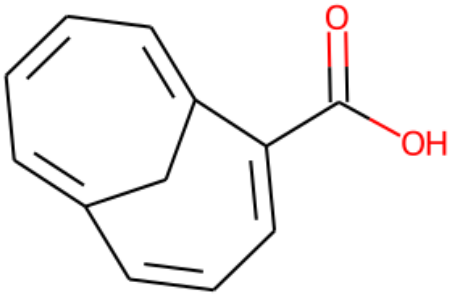
SMILES: NC1=CC2=CC=C3C=CC=CN3C2C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.97)

Is DFT optimized?: True

Property	Value
Formula	C13H12N2
Molecular weight	196.253
IUPAC name	10aH-benzo[c]quinolizin-8-amine
$\mu_{a,b,c}$	0.4, 1.2, 1.0
A, B, C	1576.8715, 403.8587, 328.6535
A_s, B_s, C_s	1572.2986, 402.6875, 327.7004
Charge, Multiplicity	0, 1
Predicted log column density	11.941±5.684
Electronic energy	-611.85345

geom1029



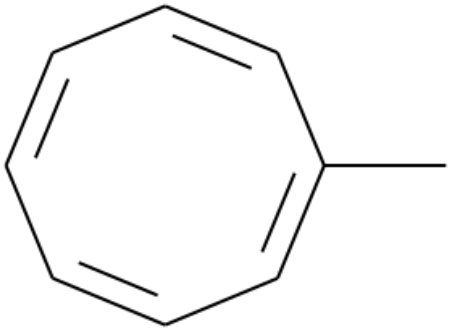
SMILES: O=C(O)C1=CC=CC2=CC=CC=C1C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.10)

Is DFT optimized?: False

Property	Value
Formula	C12H10O2
Molecular weight	186.210
IUPAC name	bicyclo[4.4.1]undeca-1(10),2,4,6,8-pentaene-2-carboxylic acid
$\mu_{a,b,c}$	3.0, 3.0, 3.9
A, B, C	1269.6677, 584.8574, 441.3992
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	12.133±5.135
Electronic energy	-613.33498

geom1030



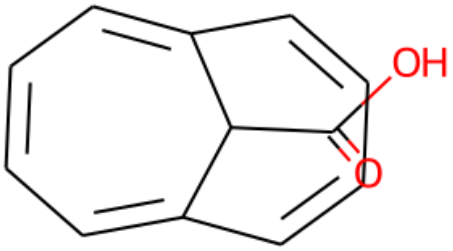
SMILES: CC1=C/C=C\C=C\C=C/1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.31)

Is DFT optimized?: True

Property	Value
Formula	C9H10
Molecular weight	118.179
IUPAC name	
$\mu_{a,b,c}$	0.3, 0.1, 0.1
A, B, C	2538.2563, 1552.2489, 1111.5809
A_s, B_s, C_s	2530.8954, 1547.7474, 1108.3574
Charge, Multiplicity	0, 1
Predicted log column density	12.642±3.289
Electronic energy	-348.79326

geom1031



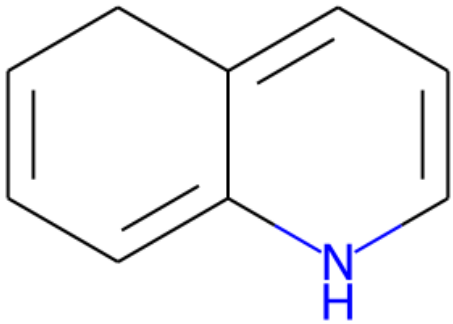
SMILES: O=C(O)C1C2=CC=CC=C1C=CC=C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.79)

Is DFT optimized?: False

Property	Value
Formula	C12H10O2
Molecular weight	186.210
IUPAC name	bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene-11-carboxylic acid
$\mu_{a,b,c}$	1.4, 1.7, 1.6
A, B, C	1053.9891, 697.9308, 611.5641
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	11.688±4.792
Electronic energy	-613.35846

geom1032



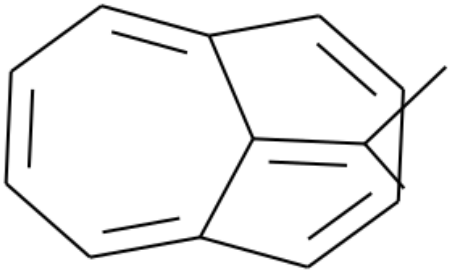
SMILES: C1=CCC2=CC=CNC2=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (8.18)

Is DFT optimized?: True

Property	Value
Formula	C9H9N
Molecular weight	131.178
IUPAC name	1,5-dihydroquinoline
$\mu_{a,b,c}$	2.3, 0.8, 0.0
A, B, C	2985.5263, 1190.6785, 855.6463
A_s, B_s, C_s	2976.8683, 1187.2255, 853.1650
Charge, Multiplicity	0, 1
Predicted log column density	12.345±5.361
Electronic energy	-402.95702

geom1033



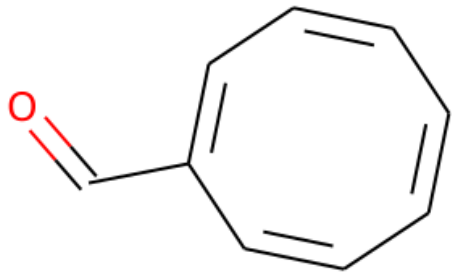
SMILES: CC(C)=C1C2=CC=CC=C1C=CC=C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.92)

Is DFT optimized?: False

Property	Value
Formula	C14H14
Molecular weight	182.266
IUPAC name	11-propan-2-ylidenebicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	0.3, 1.3, 0.0
A, B, C	969.7080, 749.7100, 602.0154
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.248±5.200
Electronic energy	-541.41041

geom1034



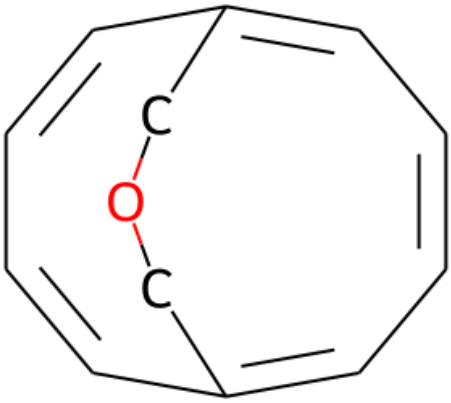
SMILES: O=CC1=CC=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.76)

Is DFT optimized?: False

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	cyclooctatetraenecarbaldehyde
$\mu_{a,b,c}$	1.8, 2.9, 0.0
A, B, C	2356.9194, 1067.9383, 853.4485
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.412±3.057
Electronic energy	-422.77277

geom1035



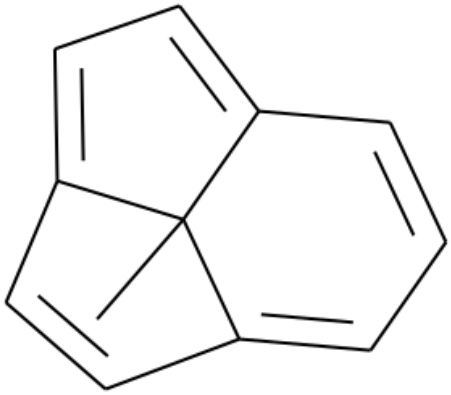
SMILES: C1=CC=C2C=CC=CC(=C1)COC2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (8.30)

Is DFT optimized?: False

Property	Value
Formula	C12H12O
Molecular weight	172.227
IUPAC name	12-oxabicyclo[4.4.3]trideca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	0.3, 0.1, 1.0
A, B, C	1025.2875, 959.7776, 809.6611
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	15.901±5.191
Electronic energy	-539.17072

geom1036



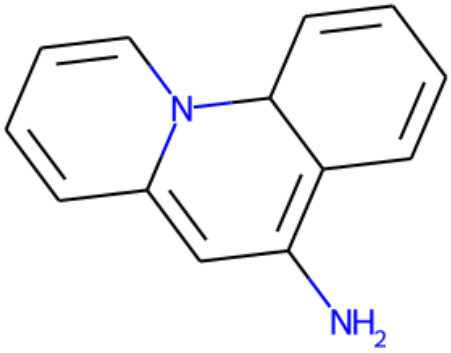
SMILES: CC12C3=CC=CC1=CC=C2C=C3

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.21)

Is DFT optimized?: False

Property	Value
Formula	C12H10
Molecular weight	154.212
IUPAC name	11-methyltricyclo[5.3.1.04,11]undeca-1(10),2,4,6,8-pentaene
$\mu_{a,b,c}$	0.2, 1.2, 0.1
A, B, C	1471.9804, 1226.9231, 906.3370
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.172±6.493
Electronic energy	-463.05109

geom1037



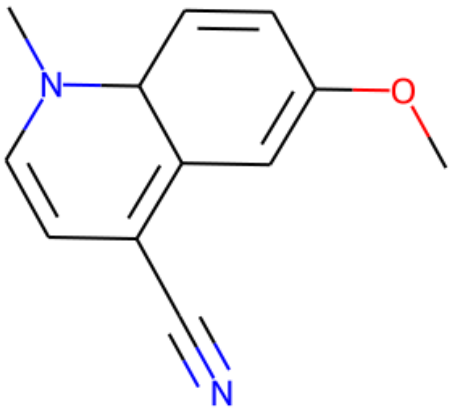
SMILES: NC1=C2C=CC=CC2N2C=CC=CC2=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.14)

Is DFT optimized?: False

Property	Value
Formula	C13H12N2
Molecular weight	196.253
IUPAC name	10aH-benzo[c]quinolizin-6-amine
$\mu_{a,b,c}$	0.6, 1.9, 3.9
A, B, C	1129.0898, 480.0544, 351.8871
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	11.738±5.205
Electronic energy	-611.57253

geom1038



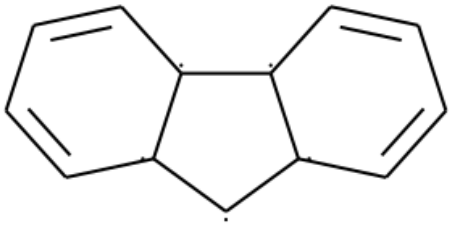
SMILES: COC1=CC2=C(C#N)C=CN(C)C2C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.64)

Is DFT optimized?: False

Property	Value
Formula	C12H12N2O
Molecular weight	200.241
IUPAC name	6-methoxy-1-methyl-8aH-quinoline-4-carbonitrile
$\mu_{a,b,c}$	6.8, 3.4, 1.4
A, B, C	859.8531, 483.0014, 332.7554
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	15.198±5.516
Electronic energy	-648.92601

geom1039



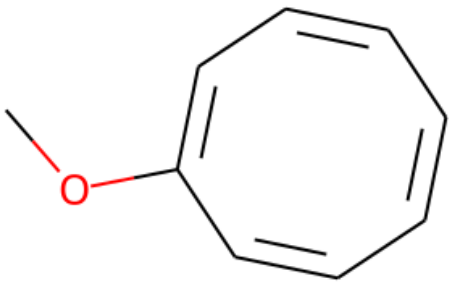
SMILES: [CH]1[C]2C=CC=C[C]2[C]2C=CC=C[C]12

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.09)

Is DFT optimized?: True

Property	Value
Formula	C13H9
Molecular weight	165.215
IUPAC name	4b,8a,9,9a-tetrahydro-4aH-fluorene
$\mu_{a,b,c}$	0.2, 0.1, 0.0
A, B, C	2193.0897, 573.3649, 454.5323
A_s, B_s, C_s	2186.7298, 571.7022, 453.2141
Charge, Multiplicity	0, 6
Predicted log column density	13.998±4.102
Electronic energy	-500.34174

geom1040



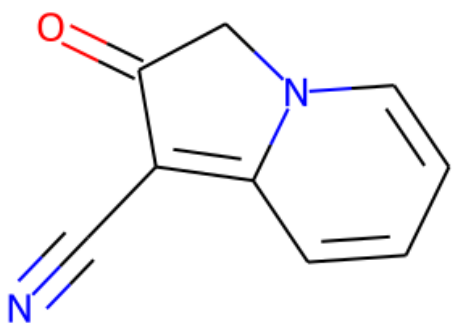
SMILES: COC1=CC=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.04)

Is DFT optimized?: True

Property	Value
Formula	C9H10O
Molecular weight	134.178
IUPAC name	methoxycyclooctatetraene
$\mu_{a,b,c}$	0.2, 1.5, 0.4
A, B, C	2270.2066, 1095.1852, 856.4028
A_s, B_s, C_s	2263.6230, 1092.0092, 853.9192
Charge, Multiplicity	0, 1
Predicted log column density	14.662±4.741
Electronic energy	-423.97648

geom1041



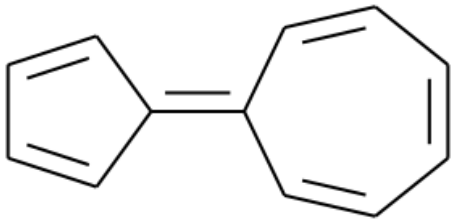
SMILES: N#CC1=C2C=CC=CN2CC1=O

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.56)

Is DFT optimized?: True

Property	Value
Formula	C9H6N2O
Molecular weight	158.160
IUPAC name	2-oxo-3H-indolizine-1-carbonitrile
$\mu_{a,b,c}$	10.3, 2.7, 0.0
A, B, C	1646.4929, 839.0812, 557.8015
A_s, B_s, C_s	1641.7180, 836.6479, 556.1839
Charge, Multiplicity	0, 1
Predicted log column density	13.732±5.705
Electronic energy	-531.10469

geom1042



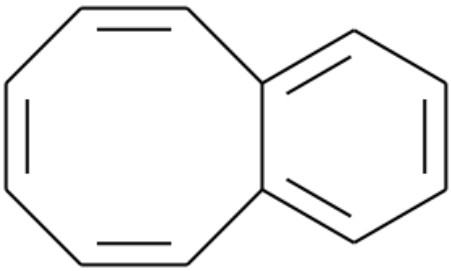
SMILES: C1=CC=CC(=C2C=CC=C2)C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.46)

Is DFT optimized?: True

Property	Value
Formula	C12H10
Molecular weight	154.212
IUPAC name	7-cyclopenta-2,4-dien-1-ylidenecyclohepta-1,3,5-triene
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	2630.3817, 563.6613, 464.1912
A_s, B_s, C_s	2622.7536, 562.0267, 462.8451
Charge, Multiplicity	0, 1
Predicted log column density	13.105±5.158
Electronic energy	-463.05792

geom1043



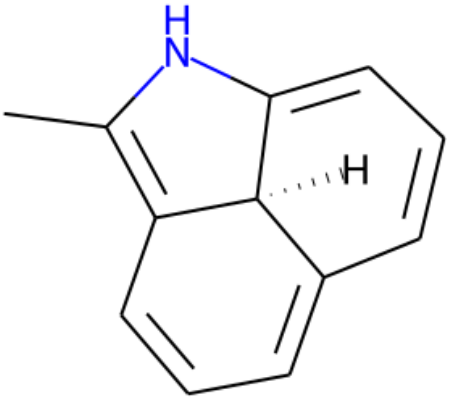
SMILES: C1=CC=Cc2ccccc2C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (7.99)

Is DFT optimized?: False

Property	Value
Formula	C12H10
Molecular weight	154.212
IUPAC name	benzo[8]annulene
$\mu_{a,b,c}$	0.3, 0.7, 0.9
A, B, C	2601.4071, 599.2662, 506.1365
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.727±2.894
Electronic energy	-462.81534

geom1044



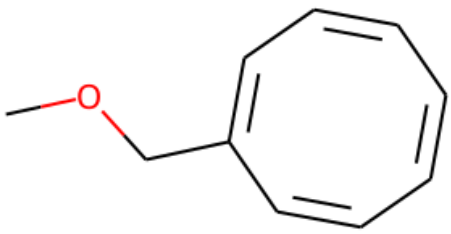
SMILES: CC1=C2C=CC=C3C=CC=C(N1)[C@@H]32

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.40)

Is DFT optimized?: True

Property	Value
Formula	C12H11N
Molecular weight	169.227
IUPAC name	(9S)-2-methyl-1,9-dihydrobenzo[cd]indole
$\mu_{a,b,c}$	1.6, 1.0, 1.0
A, B, C	1223.5043, 916.9763, 539.6478
A_s, B_s, C_s	1219.9561, 914.3170, 538.0829
Charge, Multiplicity	0, 1
Predicted log column density	14.713±7.588
Electronic energy	-518.42899

geom1045



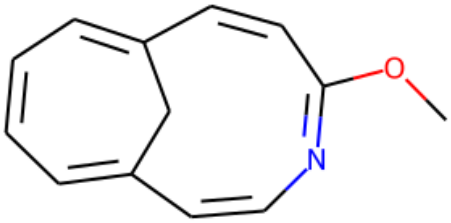
SMILES: COCC1=CC=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.31)

Is DFT optimized?: True

Property	Value
Formula	C10H12O
Molecular weight	148.205
IUPAC name	methoxymethylcyclooctatetraene
$\mu_{a,b,c}$	0.8, 1.2, 0.2
A, B, C	2202.8762, 649.9241, 561.8028
A_s, B_s, C_s	2196.4879, 648.0393, 560.1736
Charge, Multiplicity	0, 1
Predicted log column density	11.604±4.546
Electronic energy	-463.27543

geom1046



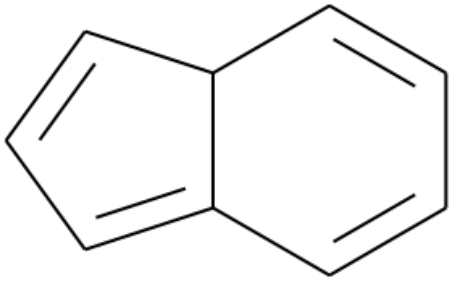
SMILES: COC1=NC=CC2=CC=CC=C(C=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.56)

Is DFT optimized?: False

Property	Value
Formula	C13H13NO
Molecular weight	199.253
IUPAC name	5-methoxy-4-azabicyclo[6.4.1]trideca-1(12),2,4,6,8,10-hexaene
$\mu_{a,b,c}$	0.3, 0.7, 1.3
A, B, C	1324.5588, 413.4909, 354.3809
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.740±5.951
Electronic energy	-632.70286

geom1047



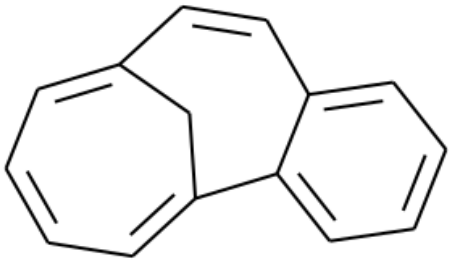
SMILES: C1=CC2=CC=CC2C=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.25)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	3aH-indene
$\mu_{a,b,c}$	0.1, 0.3, 0.3
A, B, C	3630.8511, 1623.2611, 1155.3641
A_s, B_s, C_s	3620.3216, 1618.5537, 1152.0136
Charge, Multiplicity	0, 1
Predicted log column density	12.881±4.542
Electronic energy	-347.59512

geom1048



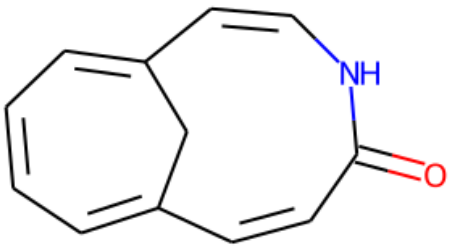
SMILES: C1=CC=C2CC(=C1)C=Cc1ccccc12

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.49)

Is DFT optimized?: False

Property	Value
Formula	C15H12
Molecular weight	192.261
IUPAC name	tricyclo[8.4.1.02,7]pentadeca-1(14),2,4,6,8,10,12-heptaene
$\mu_{a,b,c}$	0.1, 0.9, 0.1
A, B, C	1410.7026, 502.5536, 409.7661
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.170±3.023
Electronic energy	-578.47239

geom1049



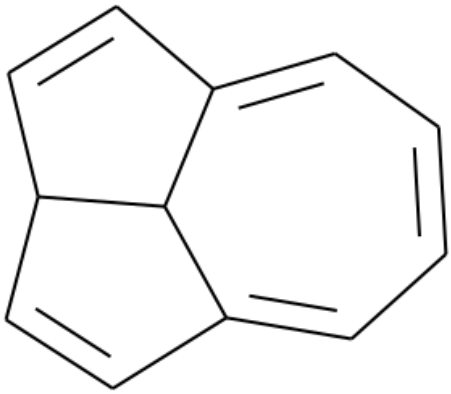
SMILES: O=C1C=CC2=CC=CC=C(C=CN1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (8.69)

Is DFT optimized?: True

Property	Value
Formula	C12H11NO
Molecular weight	185.226
IUPAC name	4-azabicyclo[6.4.1]trideca-1(12),2,6,8,10-pentaen-5-one
$\mu_{a,b,c}$	2.3, 2.9, 0.1
A, B, C	1407.2293, 550.9480, 427.5995
A_s, B_s, C_s	1403.1483, 549.3502, 426.3594
Charge, Multiplicity	0, 1
Predicted log column density	14.654±5.711
Electronic energy	-593.59335

geom1050



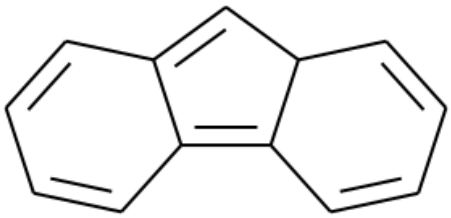
SMILES: C1=CC=C2C=CC3C=CC(=C1)C23

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.22)

Is DFT optimized?: True

Property	Value
Formula	C12H10
Molecular weight	154.212
IUPAC name	tricyclo[5.4.1.04,12]dodeca-1(11),2,5,7,9-pentaene
$\mu_{a,b,c}$	2.3, 0.0, 0.4
A, B, C	1545.3972, 1174.4247, 726.5552
A_s, B_s, C_s	1540.9155, 1171.0189, 724.4481
Charge, Multiplicity	0, 1
Predicted log column density	14.334±6.646
Electronic energy	-462.99571

geom1051



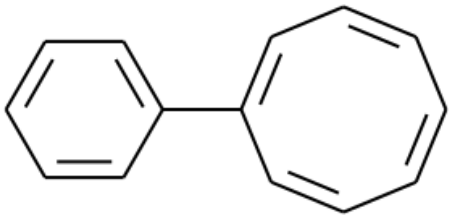
SMILES: C1=CC2=c3ccccc3=CC2C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.10)

Is DFT optimized?: False

Property	Value
Formula	C13H10
Molecular weight	166.223
IUPAC name	8aH-fluorene
$\mu_{a,b,c}$	0.2, 1.4, 0.6
A, B, C	1928.4890, 646.8887, 517.2865
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.968±4.551
Electronic energy	-500.99231

geom1052



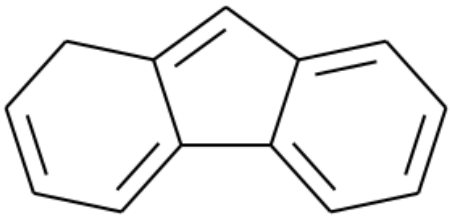
SMILES: C1=CC=CC(c2ccccc2)=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.77)

Is DFT optimized?: True

Property	Value
Formula	C14H12
Molecular weight	180.250
IUPAC name	phenylcyclooctatetraene
$\mu_{a,b,c}$	0.0, 0.0, 0.1
A, B, C	1675.1396, 400.3327, 376.3944
A_s, B_s, C_s	1670.2817, 399.1717, 375.3029
Charge, Multiplicity	0, 1
Predicted log column density	12.739±3.859
Electronic energy	-540.46855

geom1053



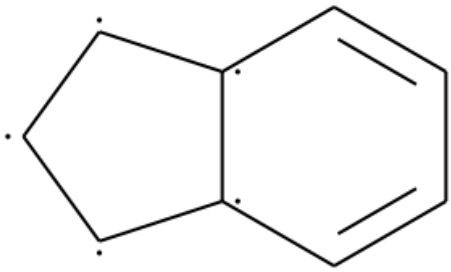
SMILES: C1=CCC2=Cc3ccccc3C2=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (7.66)

Is DFT optimized?: False

Property	Value
Formula	C13H10
Molecular weight	166.223
IUPAC name	1H-fluorene
$\mu_{a,b,c}$	0.3, 0.2, 1.1
A, B, C	2216.9799, 585.8005, 475.9253
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.868±2.787
Electronic energy	-501.19781

geom1054



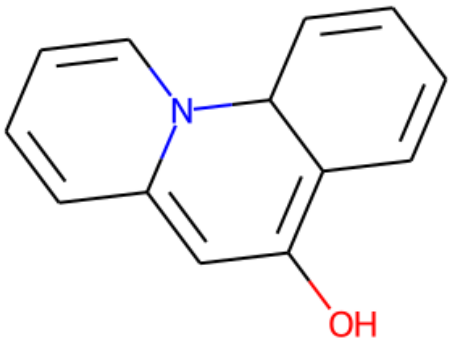
SMILES: [CH]1[CH][C]2C=CC=C[C]2[CH]1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.46)

Is DFT optimized?: False

Property	Value
Formula	C9H7
Molecular weight	115.155
IUPAC name	2,3,3a,7a-tetrahydro-1H-indene
$\mu_{a,b,c}$	0.6, 0.1, 0.2
A, B, C	3682.0584, 1597.7608, 1133.2169
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 6
Predicted log column density	15.512±4.689
Electronic energy	-346.65805

geom1055



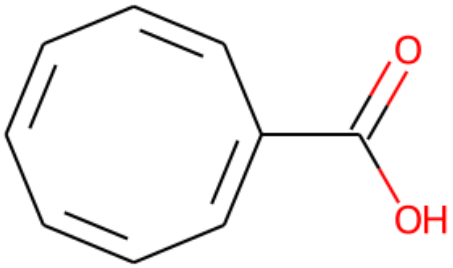
SMILES: OC1=C2C=CC=CC2N2C=CC=CC2=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.62)

Is DFT optimized?: True

Property	Value
Formula	C13H11NO
Molecular weight	197.237
IUPAC name	10aH-benzo[c]quinolizin-6-ol
$\mu_{a,b,c}$	1.5, 1.5, 0.1
A, B, C	1087.1190, 536.1899, 367.9408
A_s, B_s, C_s	1083.9663, 534.6350, 366.8738
Charge, Multiplicity	0, 1
Predicted log column density	10.186±4.987
Electronic energy	-631.71566

geom1056



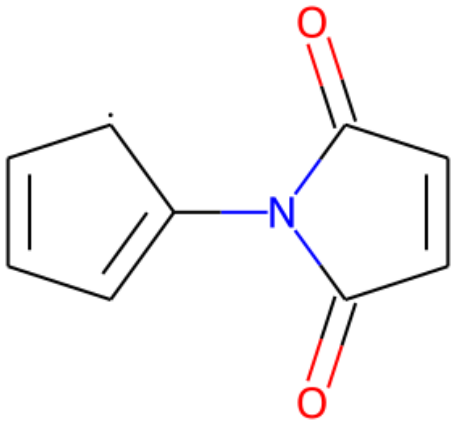
SMILES: O=C(O)C1=CC=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.48)

Is DFT optimized?: True

Property	Value
Formula	C9H8O2
Molecular weight	148.161
IUPAC name	cyclooctatetraenecarboxylic acid
$\mu_{a,b,c}$	5.1, 1.9, 1.0
A, B, C	2011.5681, 855.3119, 672.1975
A_s, B_s, C_s	2005.7345, 852.8315, 670.2481
Charge, Multiplicity	0, 1
Predicted log column density	11.700±4.684
Electronic energy	-498.00337

geom1057



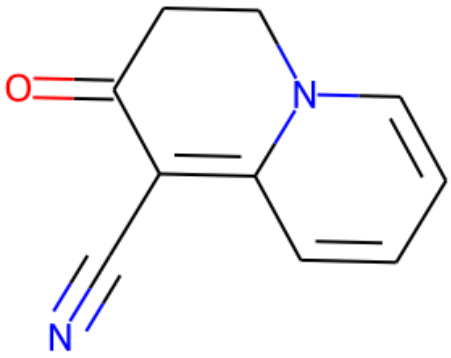
SMILES: O=C1C=CC(=O)N1C1=CC=C[CH]1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.34)

Is DFT optimized?: False

Property	Value
Formula	C9H6NO2
Molecular weight	160.152
IUPAC name	1-cyclopenta-1,3-dien-1-ylpyrrole-2,5-dione
$\mu_{a,b,c}$	0.1, 1.1, 0.2
A, B, C	1894.5286, 812.5707, 568.9465
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 2
Predicted log column density	13.804±5.561
Electronic energy	-551.51743

geom1058



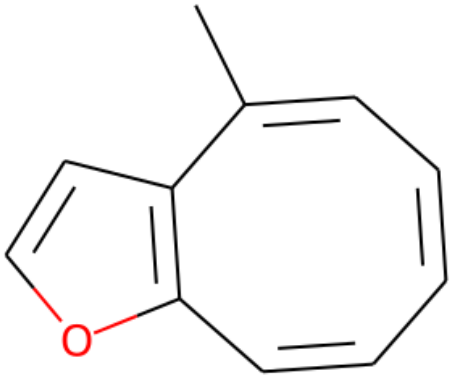
SMILES: N#CC1=C2C=CC=CN2CCC1=O

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.55)

Is DFT optimized?: False

Property	Value
Formula	C10H8N2O
Molecular weight	172.187
IUPAC name	2-oxo-3,4-dihydroquinolizine-1-carbonitrile
$\mu_{a,b,c}$	0.9, 5.4, 8.9
A, B, C	1229.1846, 751.9016, 473.8332
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.337±6.114
Electronic energy	-570.37285

geom1059



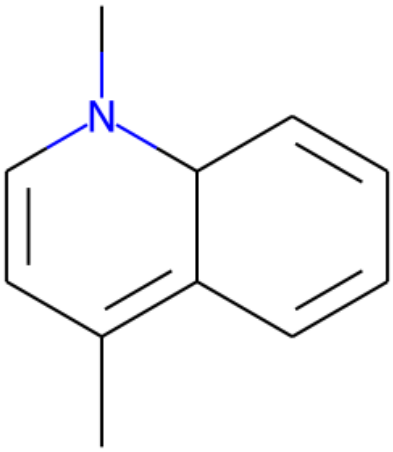
SMILES: CC1=CC=CC=Cc2occc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (7.77)

Is DFT optimized?: True

Property	Value
Formula	C11H10O
Molecular weight	158.200
IUPAC name	4-methylcycloocta[b]furan
$\mu_{a,b,c}$	0.0, 2.0, 0.3
A, B, C	1376.0936, 1035.5989, 654.2468
A_s, B_s, C_s	1372.1029, 1032.5956, 652.3495
Charge, Multiplicity	0, 1
Predicted log column density	13.400±5.386
Electronic energy	-500.06380

geom1060



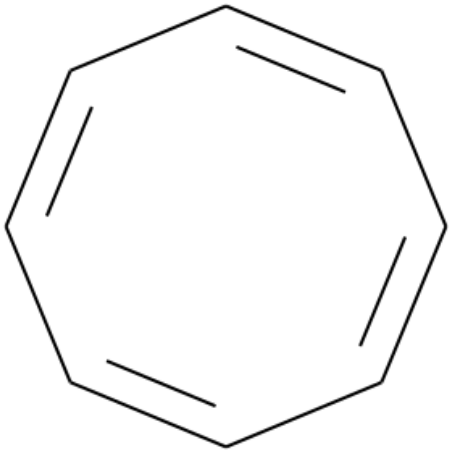
SMILES: CC1=C2C=CC=CC2N(C)C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.43)

Is DFT optimized?: False

Property	Value
Formula	C11H13N
Molecular weight	159.232
IUPAC name	1,4-dimethyl-8aH-quinoline
$\mu_{a,b,c}$	0.9, 0.2, 0.6
A, B, C	1243.4157, 1041.2495, 605.2136
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	13.385±4.851
Electronic energy	-481.53459

geom1061



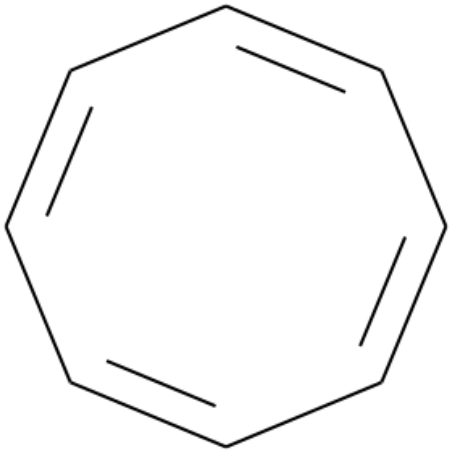
SMILES: C1=C/C=C\C=C/C=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.02)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	cyclooctatetraene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	2701.6075, 2700.0024, 1530.5394
A_s, B_s, C_s	2693.7728, 2692.1724, 1526.1008
Charge, Multiplicity	0, 1
Predicted log column density	12.708±4.502
Electronic energy	-309.48483

geom1062



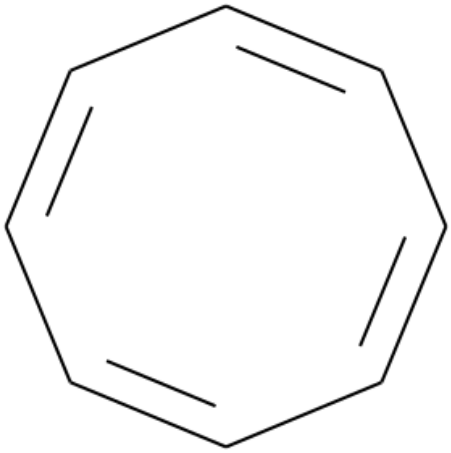
SMILES: C1=C\C=C/C=C\C=C/1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.02)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	cyclooctatetraene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	2698.8926, 2698.5864, 1525.9674
A_s, B_s, C_s	2691.0658, 2690.7604, 1521.5421
Charge, Multiplicity	0, 1
Predicted log column density	12.708±4.502
Electronic energy	-309.48485

geom1063



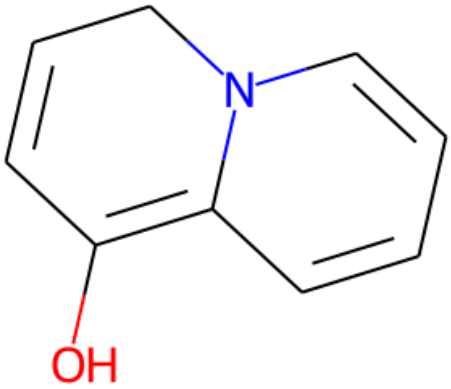
SMILES: C1=CC=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.02)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	cyclooctatetraene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	2700.8191, 2699.8729, 1529.5796
A_s, B_s, C_s	2692.9868, 2692.0433, 1525.1438
Charge, Multiplicity	0, 1
Predicted log column density	12.708±4.502
Electronic energy	-309.48483

geom1064



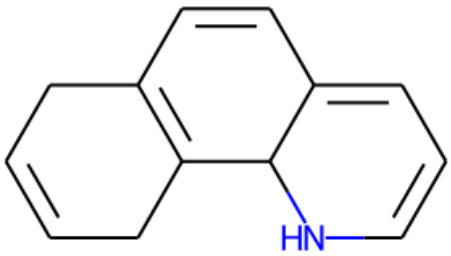
SMILES: OC1=C2C=CC=CN2CC=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (8.40)

Is DFT optimized?: False

Property	Value
Formula	C9H9NO
Molecular weight	147.177
IUPAC name	4H-quinolizin-1-ol
$\mu_{a,b,c}$	0.0, 1.5, 1.7
A, B, C	1879.4476, 1109.0626, 700.5515
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.628±4.845
Electronic energy	-478.13459

geom1065



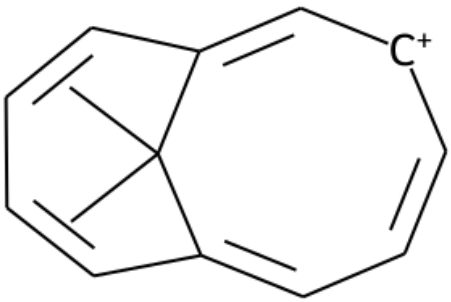
SMILES: C1=CNC2C(=C1)C=CC1=C2CC=CC1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.93)

Is DFT optimized?: True

Property	Value
Formula	C13H13N
Molecular weight	183.254
IUPAC name	1,7,10,10b-tetrahydrobenzo[h]quinoline
$\mu_{a,b,c}$	1.1, 1.1, 1.4
A, B, C	1426.7033, 575.3590, 432.6544
A_s, B_s, C_s	1422.5659, 573.6905, 431.3997
Charge, Multiplicity	0, 1
Predicted log column density	13.261±6.463
Electronic energy	-557.60328

geom1066



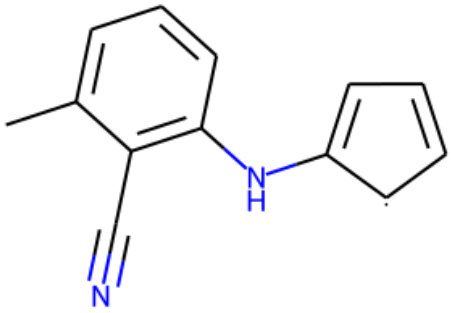
SMILES: CC1(C)C2=CC=C[CH+]C=C1C=CC=C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.06)

Is DFT optimized?: True

Property	Value
Formula	C14H15+
Molecular weight	183.274
IUPAC name	
$\mu_{a,b,c}$	1.0, 1.6, 1.4
A, B, C	1058.7230, 697.5653, 674.3457
A_s, B_s, C_s	1055.6527, 695.5424, 672.3901
Charge, Multiplicity	1, 1
Predicted log column density	12.809±5.816
Electronic energy	-541.94862

geom1067



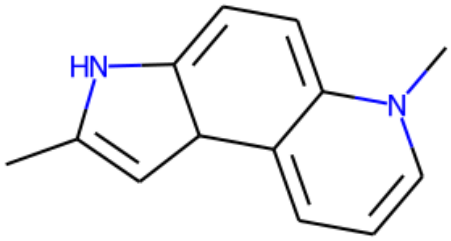
SMILES: Cc1cccc(NC2=CC=C[CH]2)c1C#N

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.83)

Is DFT optimized?: False

Property	Value
Formula	C13H11N2
Molecular weight	195.245
IUPAC name	
$\mu_{a,b,c}$	0.6, 3.7, 2.7
A, B, C	1183.9799, 415.7296, 342.1449
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	14.772±6.938
Electronic energy	-611.22416

geom1068



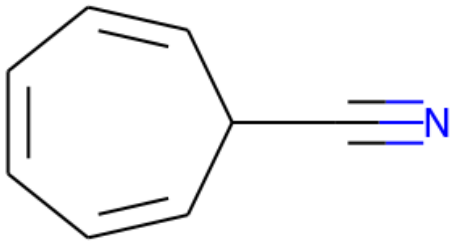
SMILES: CC1=CC2C(=CC=C3C2=CC=CN3C)N1

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (9.21)

Is DFT optimized?: False

Property	Value
Formula	C13H14N2
Molecular weight	198.269
IUPAC name	2,6-dimethyl-3,9b-dihydropyrrolo[3,2-f]quinoline
$\mu_{a,b,c}$	0.7, 2.6, 0.8
A, B, C	1252.4431, 427.8822, 347.0300
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.683±8.276
Electronic energy	-613.05843

geom1069



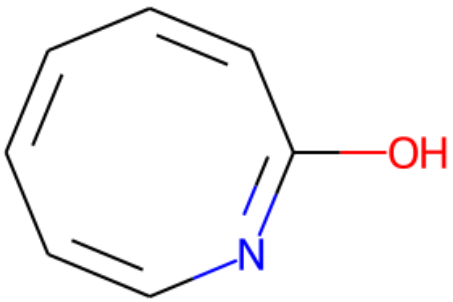
SMILES: N#CC1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (4.01)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	cyclohepta-2,4,6-triene-1-carbonitrile
$\mu_{a,b,c}$	2.9, 0.0, 3.0
A, B, C	2258.1775, 1673.2815, 1531.6826
A_s, B_s, C_s	2251.6288, 1668.4289, 1527.2407
Charge, Multiplicity	0, 1
Predicted log column density	10.766±4.000
Electronic energy	-363.62707

geom1070



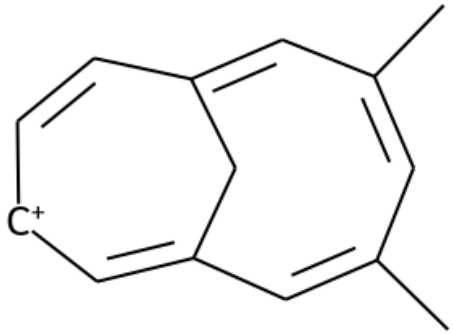
SMILES: OC1=NC=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.50)

Is DFT optimized?: False

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	1H-azocin-2-one
$\mu_{a,b,c}$	0.2, 1.0, 0.6
A, B, C	2590.4111, 1758.3572, 1232.2786
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.170±4.572
Electronic energy	-400.73703

geom1071



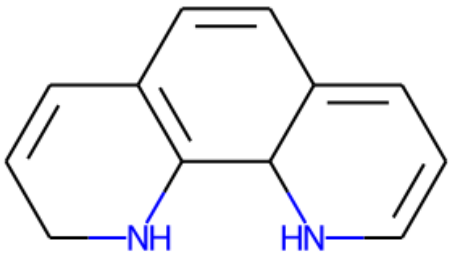
SMILES: CC1=CC(C)=CC2=C[CH+]C=CC(=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.85)

Is DFT optimized?: False

Property	Value
Formula	C14H15+
Molecular weight	183.274
IUPAC name	
$\mu_{a,b,c}$	0.3, 1.1, 1.4
A, B, C	1071.0676, 625.0529, 447.7183
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 1
Predicted log column density	12.688±6.650
Electronic energy	-541.99408

geom1072



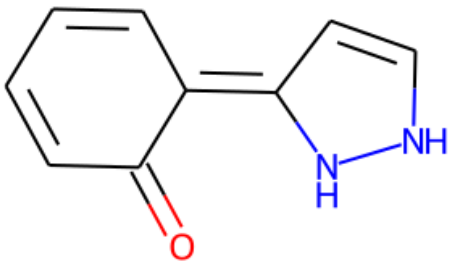
SMILES: C1=CNC2C(=C1)C=CC1=C2NCC=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.17)

Is DFT optimized?: False

Property	Value
Formula	C12H12N2
Molecular weight	184.242
IUPAC name	1,2,10,10a-tetrahydro-1,10-phenanthroline
$\mu_{a,b,c}$	0.0, 0.9, 0.5
A, B, C	1426.3269, 571.8530, 426.5708
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	12.765±8.467
Electronic energy	-573.70950

geom1073



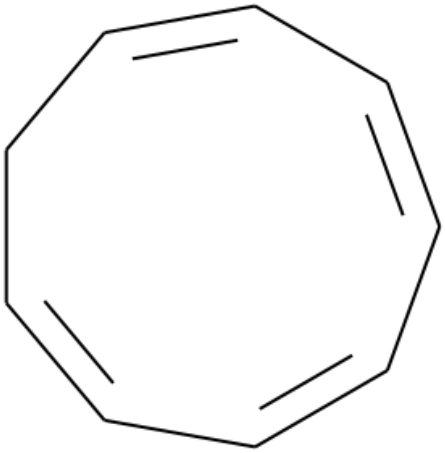
SMILES: O=C1C=CC=C/C1=C1\C=CNN1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.04)

Is DFT optimized?: False

Property	Value
Formula	C9H8N2O
Molecular weight	160.176
IUPAC name	2-(1H-pyrazol-5-yl)phenol
$\mu_{a,b,c}$	0.3, 5.7, 0.1
A, B, C	2229.2263, 674.4200, 518.8458
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.120±7.225
Electronic energy	-532.27533

geom1074



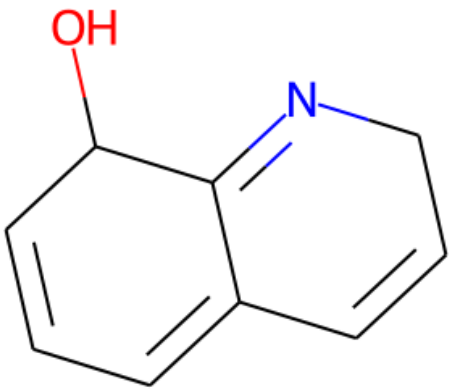
SMILES: C1=C\C=C/C/C=C\C=C/1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.43)

Is DFT optimized?: True

Property	Value
Formula	C9H10
Molecular weight	118.179
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.9, 0.1
A, B, C	2746.6216, 1698.2581, 1166.7061
A_s, B_s, C_s	2738.6564, 1693.3332, 1163.3226
Charge, Multiplicity	0, 1
Predicted log column density	12.165±5.048
Electronic energy	-348.69222

geom1075



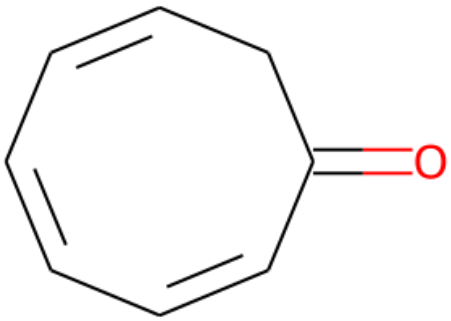
SMILES: OC1C=CC=C2C=CCN=C21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (8.17)

Is DFT optimized?: True

Property	Value
Formula	C9H9NO
Molecular weight	147.177
IUPAC name	2,8-dihydroquinolin-8-ol
$\mu_{a,b,c}$	2.2, 2.4, 0.3
A, B, C	1892.3440, 1104.5077, 712.9448
A_s, B_s, C_s	1886.8562, 1101.3047, 710.8772
Charge, Multiplicity	0, 1
Predicted log column density	8.949±5.019
Electronic energy	-478.14774

geom1076



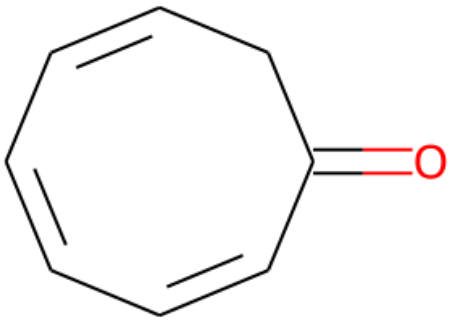
SMILES: O=C1/C=C\C=C/C=C\C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.91)

Is DFT optimized?: False

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	(2Z,4Z,6Z)-cycloocta-2,4,6-trien-1-one
$\mu_{a,b,c}$	0.6, 1.3, 2.8
A, B, C	2850.0856, 1559.2423, 1111.3415
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.390±3.637
Electronic energy	-384.57259

geom1077



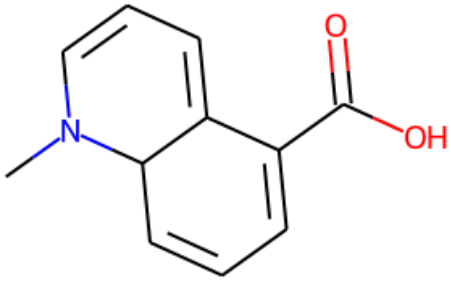
SMILES: O=C1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.91)

Is DFT optimized?: True

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	cycloocta-2,4,6-trien-1-one
$\mu_{a,b,c}$	3.5, 0.6, 0.6
A, B, C	2857.4099, 1579.3414, 1146.8110
A_s, B_s, C_s	2849.1234, 1574.7613, 1143.4852
Charge, Multiplicity	0, 1
Predicted log column density	12.390±3.637
Electronic energy	-384.58743

geom1078



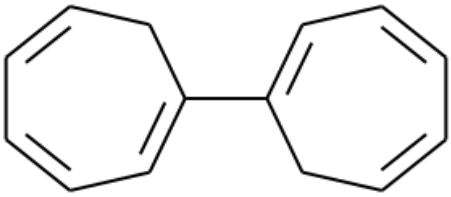
SMILES: CN1C=CC=C2C(C(=O)O)=CC=CC21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.15)

Is DFT optimized?: False

Property	Value
Formula	C11H11NO2
Molecular weight	189.214
IUPAC name	1-methyl-8aH-quinoline-5-carboxylic acid
$\mu_{a,b,c}$	4.1, 2.3, 3.1
A, B, C	1115.7115, 569.9469, 449.7372
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	11.977±6.349
Electronic energy	-630.72630

geom1079



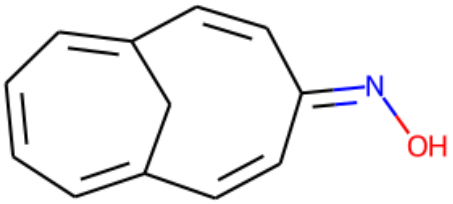
SMILES: C1=CC=C(C2=CC=CC=CC2)CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (9.47)

Is DFT optimized?: False

Property	Value
Formula	C14H14
Molecular weight	182.266
IUPAC name	1-cyclohepta-1,3,5-trien-1-ylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.1, 0.0, 0.9
A, B, C	1840.9692, 360.1768, 302.4283
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.695±6.111
Electronic energy	-541.61766

geom1080



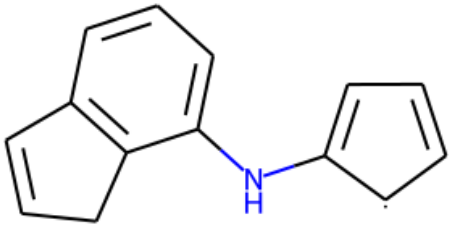
SMILES: ON=C1C=CC2=CC=CC=C(C=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.24)

Is DFT optimized?: True

Property	Value
Formula	C12H11NO
Molecular weight	185.226
IUPAC name	N-(4-bicyclo[5.4.1]dodeca-1(11),2,5,7,9-pentaenylidene)hydroxylamine
$\mu_{a,b,c}$	1.2, 0.3, 0.2
A, B, C	1755.8424, 476.3756, 426.3084
A_s, B_s, C_s	1750.7505, 474.9941, 425.0722
Charge, Multiplicity	0, 1
Predicted log column density	10.731±6.304
Electronic energy	-593.33538

geom1081



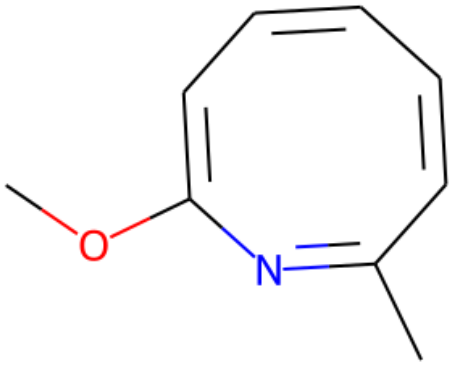
SMILES: [CH]1C=CC=C1Nc1cccc2c1CC=C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.18)

Is DFT optimized?: False

Property	Value
Formula	C14H12N
Molecular weight	194.257
IUPAC name	
$\mu_{a,b,c}$	0.2, 1.8, 0.9
A, B, C	1557.4935, 334.0762, 275.6244
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	14.675±4.549
Electronic energy	-595.18856

geom1082



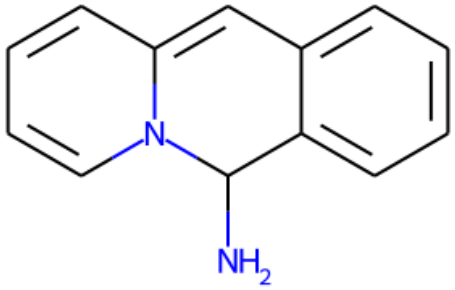
SMILES: COC1=CC=CC=CC(C)=N1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.03)

Is DFT optimized?: False

Property	Value
Formula	C9H11NO
Molecular weight	149.193
IUPAC name	2-methoxy-8-methylazocine
$\mu_{a,b,c}$	2.0, 1.1, 0.3
A, B, C	1608.2539, 966.0504, 730.4839
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.854±4.901
Electronic energy	-479.32005

geom1083



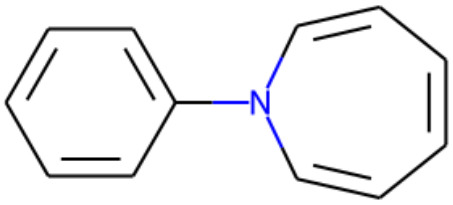
SMILES: NC1c2ccccc2C=C2C=CC=CN21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.90)

Is DFT optimized?: False

Property	Value
Formula	C13H12N2
Molecular weight	196.253
IUPAC name	6H-benzo[b]quinolizin-6-amine
$\mu_{a,b,c}$	2.1, 1.5, 0.3
A, B, C	1430.4308, 438.9562, 345.7165
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.584±4.512
Electronic energy	-611.88553

geom1084



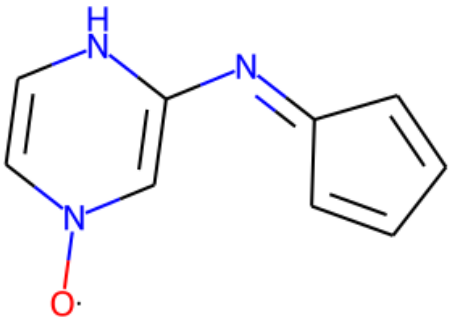
SMILES: C1=CC=CN(c2ccccc2)C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.22)

Is DFT optimized?: True

Property	Value
Formula	C12H11N
Molecular weight	169.227
IUPAC name	1-phenylazepine
$\mu_{a,b,c}$	1.0, 0.0, 0.5
A, B, C	2058.3000, 510.7995, 434.8129
A_s, B_s, C_s	2052.3309, 509.3182, 433.5519
Charge, Multiplicity	0, 1
Predicted log column density	14.070±4.775
Electronic energy	-518.42962

geom1085



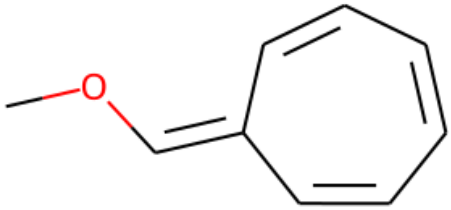
SMILES: [O]N1C=CNC(N=C2C=CC=C2)=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.10)

Is DFT optimized?: True

Property	Value
Formula	C9H8N3O
Molecular weight	174.183
IUPAC name	
$\mu_{a,b,c}$	3.4, 4.1, 0.9
A, B, C	1975.0998, 460.4831, 385.5258
A_s, B_s, C_s	1969.3720, 459.1477, 384.4078
Charge, Multiplicity	0, 2
Predicted log column density	13.476±6.620
Electronic energy	-586.92613

geom1086



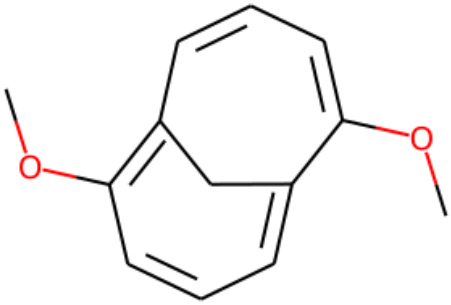
SMILES: COC=C1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.13)

Is DFT optimized?: False

Property	Value
Formula	C9H10O
Molecular weight	134.178
IUPAC name	7-(methoxymethylidene)cyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.4, 0.6, 1.6
A, B, C	3402.4920, 748.0425, 615.6669
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.135±5.813
Electronic energy	-423.98645

geom1087



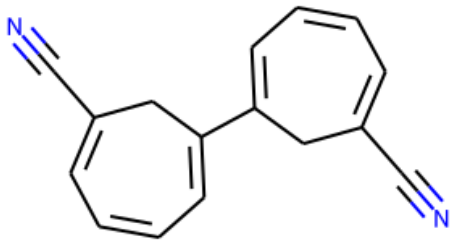
SMILES: COC1=CC=CC2=C(OC)C=CC=C1C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.51)

Is DFT optimized?: False

Property	Value
Formula	C13H14O2
Molecular weight	202.253
IUPAC name	2,7-dimethoxybicyclo[4.4.1]undeca-1,3,5,7,9-pentaene
$\mu_{a,b,c}$	3.5, 0.1, 2.6
A, B, C	1193.7188, 447.2610, 360.0598
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	16.756±7.085
Electronic energy	-653.79369

geom1088



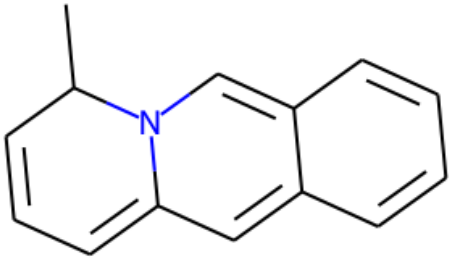
SMILES: N#CC1=CC=CC=C(C2=CC=CC=C(C#N)C2)C1

Nearest TMC-1 molecule (distance): C1=CC=C2C(=C1)C=CC=C2C#N (9.64)

Is DFT optimized?: False

Property	Value
Formula	C16H12N2
Molecular weight	232.286
IUPAC name	6-(6-cyanocyclohepta-1,3,5-trien-1-yl)cyclohepta-1,3,5-triene-1-carbonitrile
$\mu_{a,b,c}$	0.1, 1.7, 8.6
A, B, C	614.5951, 259.3717, 182.8377
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	11.529±4.976
Electronic energy	-726.02175

geom1089



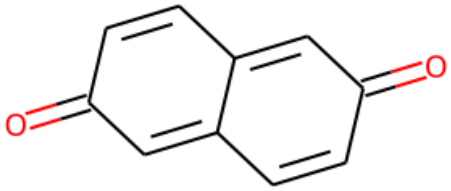
SMILES: CC1C=CC=C2C=c3ccccc3=CN21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.28)

Is DFT optimized?: True

Property	Value
Formula	C14H13N
Molecular weight	195.265
IUPAC name	4-methyl-4H-benzo[b]quinolizine
$\mu_{a,b,c}$	1.2, 1.8, 0.1
A, B, C	1577.5787, 402.6846, 343.9103
A_s, B_s, C_s	1573.0037, 401.5169, 342.9130
Charge, Multiplicity	0, 1
Predicted log column density	11.505±5.861
Electronic energy	-595.84419

geom1090



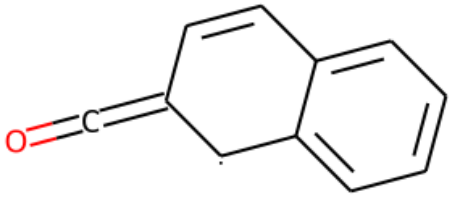
SMILES: O=C1C=CC2=CC(=O)C=CC2=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (8.56)

Is DFT optimized?: True

Property	Value
Formula	C10H6O2
Molecular weight	158.156
IUPAC name	naphthalene-2,6-dione
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	2639.5934, 613.8704, 498.0441
A_s, B_s, C_s	2631.9386, 612.0902, 496.5997
Charge, Multiplicity	0, 1
Predicted log column density	10.228±5.727
Electronic energy	-534.91545

geom1091



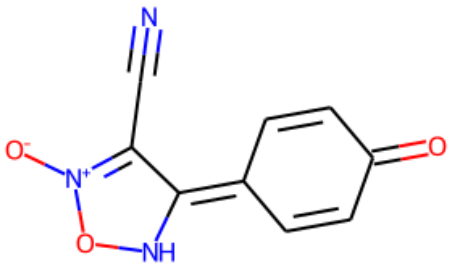
SMILES: O=C=C1[CH]c2ccccc2C=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.54)

Is DFT optimized?: True

Property	Value
Formula	C11H7O
Molecular weight	155.176
IUPAC name	
$\mu_{a,b,c}$	0.9, 0.5, 0.0
A, B, C	2702.7272, 583.6029, 479.9640
A_s, B_s, C_s	2694.8893, 581.9105, 478.5721
Charge, Multiplicity	0, 2
Predicted log column density	11.977±3.012
Electronic energy	-498.39279

geom1092



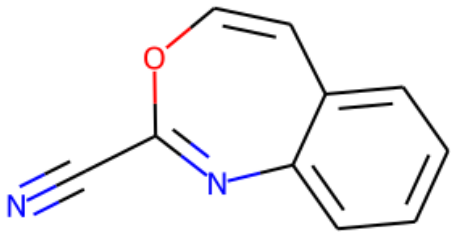
SMILES: N#CC1=[N+]([O-])ONC1=C1C=CC(=O)C=C1

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.06)

Is DFT optimized?: False

Property	Value
Formula	C9H5N3O3
Molecular weight	203.157
IUPAC name	4-(4-hydroxyphenyl)-2-oxido-1,2,5-oxadiazol-2-ium-3-carbonitrile
$\mu_{a,b,c}$	0.6, 1.1, 4.9
A, B, C	1360.3206, 357.7852, 285.6658
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	10.509±8.330
Electronic energy	-735.41771

geom1093



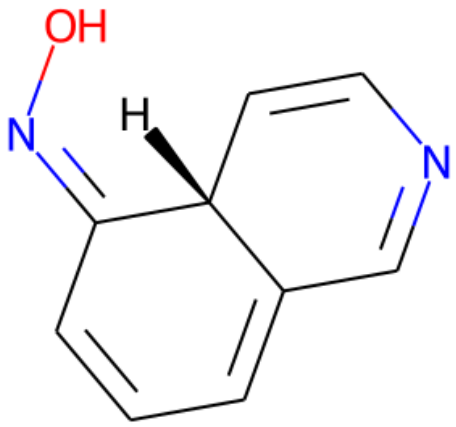
SMILES: N#CC1=Nc2ccccc2C=CO1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (8.49)

Is DFT optimized?: False

Property	Value
Formula	C10H6N2O
Molecular weight	170.171
IUPAC name	3,1-benzoxazepine-2-carbonitrile
$\mu_{a,b,c}$	0.7, 1.3, 5.5
A, B, C	1822.7517, 585.9219, 453.0630
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.574±6.928
Electronic energy	-569.14991

geom1094



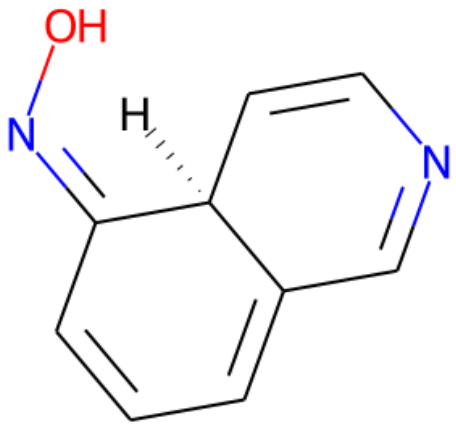
SMILES: O/N=C1/C=CC=C2C=NC=C[C@H]21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.12)

Is DFT optimized?: True

Property	Value
Formula	C9H8N2O
Molecular weight	160.176
IUPAC name	(NE)-N-[(4aR)-4aH-isoquinolin-5-ylidene]hydroxylamine
$\mu_{a,b,c}$	2.0, 1.3, 0.2
A, B, C	1408.9775, 972.2609, 603.1975
A_s, B_s, C_s	1404.8914, 969.4413, 601.4483
Charge, Multiplicity	0, 1
Predicted log column density	7.518±7.301
Electronic energy	-532.21750

geom1095



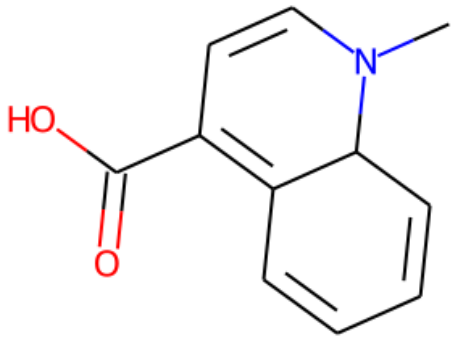
SMILES: O/N=C1/C=CC=C2C=NC=C[C@@H]21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.12)

Is DFT optimized?: False

Property	Value
Formula	C9H8N2O
Molecular weight	160.176
IUPAC name	(NE)-N-[(4aS)-4aH-isoquinolin-5-ylidene]hydroxylamine
$\mu_{a,b,c}$	1.6, 0.8, 1.6
A, B, C	1399.9252, 957.2790, 595.4972
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	7.518±7.301
Electronic energy	-532.21189

geom1096



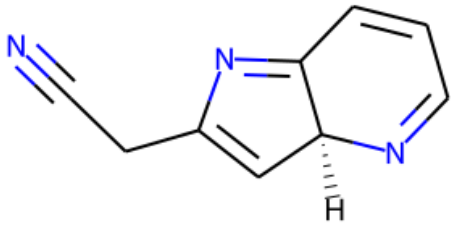
SMILES: CN1C=CC(C(=O)O)=C2C=CC=CC21

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.17)

Is DFT optimized?: True

Property	Value
Formula	C11H11NO2
Molecular weight	189.214
IUPAC name	1-methyl-8aH-quinoline-4-carboxylic acid
$\mu_{a,b,c}$	8.3, 0.7, 0.4
A, B, C	1057.7803, 634.2912, 411.3178
A_s, B_s, C_s	1054.7127, 632.4517, 410.1249
Charge, Multiplicity	0, 1
Predicted log column density	11.932±6.212
Electronic energy	-630.63905

geom1097



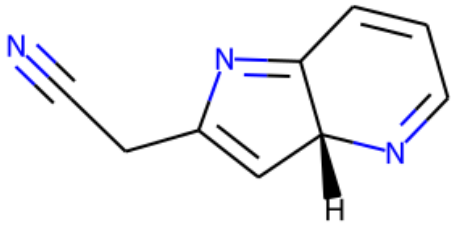
SMILES: N#CCC1=C[C@@H]2N=CC=CC2=N1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.85)

Is DFT optimized?: True

Property	Value
Formula	C9H7N3
Molecular weight	157.176
IUPAC name	2-[(3aS)-3aH-pyrrolo[3,2-b]pyridin-2-yl]acetonitrile
$\mu_{a,b,c}$	4.6, 0.9, 1.6
A, B, C	2830.8114, 536.7011, 481.4719
A_s, B_s, C_s	2822.6020, 535.1446, 480.0757
Charge, Multiplicity	0, 1
Predicted log column density	8.896±8.710
Electronic energy	-511.18125

geom1098



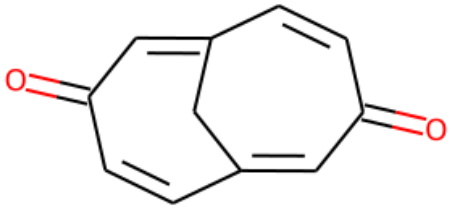
SMILES: N#CCC1=C[C@H]2N=CC=CC2=N1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.85)

Is DFT optimized?: True

Property	Value
Formula	C9H7N3
Molecular weight	157.176
IUPAC name	2-[(3aR)-3aH-pyrrolo[3,2-b]pyridin-2-yl]acetonitrile
$\mu_{a,b,c}$	4.6, 0.9, 1.6
A, B, C	2829.9960, 536.9908, 481.3164
A_s, B_s, C_s	2821.7890, 535.4335, 479.9206
Charge, Multiplicity	0, 1
Predicted log column density	8.896±8.710
Electronic energy	-511.18124

geom1099



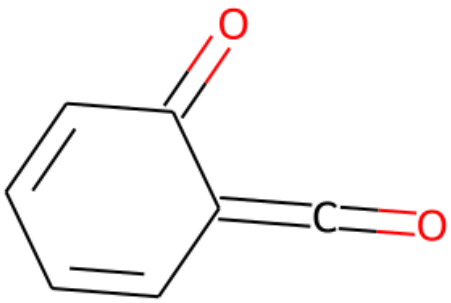
SMILES: O=C1C=CC2=CC(=O)C=CC(=C1)C2

Nearest TMC-1 molecule (distance): C1=CC=C2C=C(C=CC2=C1)C#N (9.28)

Is DFT optimized?: True

Property	Value
Formula	C11H8O2
Molecular weight	172.183
IUPAC name	bicyclo[4.4.1]undeca-1,4,6,9-tetraene-3,8-dione
$\mu_{a,b,c}$	0.0, 0.0, 0.4
A, B, C	1849.5379, 606.2121, 492.2275
A_s, B_s, C_s	1844.1742, 604.4541, 490.8000
Charge, Multiplicity	0, 1
Predicted log column density	11.385±6.774
Electronic energy	-574.16540

geom1100



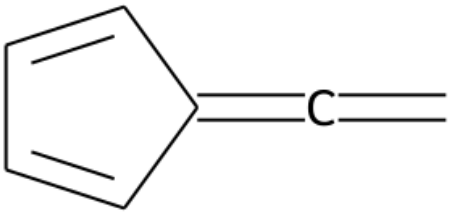
SMILES: O=C=C1C=CC=CC1=O

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.82)

Is DFT optimized?: False

Property	Value
Formula	C7H4O2
Molecular weight	120.107
IUPAC name	
$\mu_{a,b,c}$	0.0, 3.8, 2.1
A, B, C	2997.0349, 1489.3945, 994.9488
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	0, 1
Predicted log column density	11.014±3.172
Electronic energy	-419.41627

geom1101



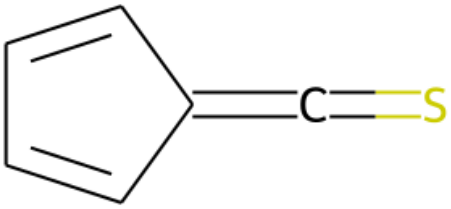
SMILES: C=C=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.59)

Is DFT optimized?: True

Property	Value
Formula	C7H6
Molecular weight	90.125
IUPAC name	
$\mu_{a,b,c}$	1.0, 0.0, 0.0
A, B, C	8203.8007, 1889.4171, 1552.2038
A_s, B_s, C_s	8180.0097, 1883.9377, 1547.7024
Charge, Multiplicity	0, 1
Predicted log column density	12.419±2.189
Electronic energy	-270.16854

geom1102



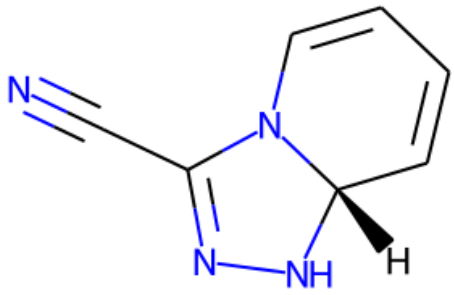
SMILES: S=C=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.88)

Is DFT optimized?: True

Property	Value
Formula	C6H4S
Molecular weight	108.165
IUPAC name	
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	8482.2057, 1186.7567, 1041.0959
A_s, B_s, C_s	8457.6073, 1183.3151, 1038.0767
Charge, Multiplicity	0, 1
Predicted log column density	14.165±2.450
Electronic energy	-629.05985

geom1103



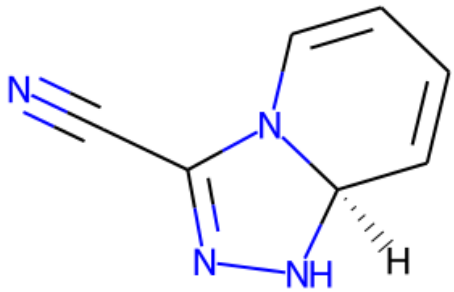
SMILES: N#CC1=NN[C@H]2C=CC=CN12

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.94)

Is DFT optimized?: True

Property	Value
Formula	C7H6N4
Molecular weight	146.153
IUPAC name	(8aS)-1,8a-dihydro-[1,2,4]triazolo[4,3-a]pyridine-3-carbonitrile
$\mu_{a,b,c}$	4.5, 0.9, 1.4
A, B, C	2154.7618, 1016.4499, 711.6191
A_s, B_s, C_s	2148.5130, 1013.5022, 709.5554
Charge, Multiplicity	0, 1
Predicted log column density	10.030±6.608
Electronic energy	-489.10608

geom1104



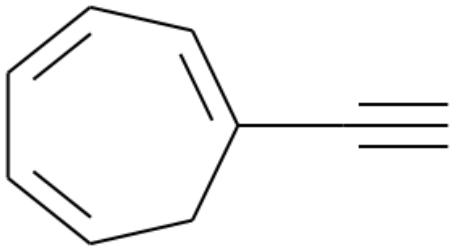
SMILES: N#CC1=NN[C@@H]2C=CC=CN12

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (5.94)

Is DFT optimized?: True

Property	Value
Formula	C7H6N4
Molecular weight	146.153
IUPAC name	(8aR)-1,8a-dihydro-[1,2,4]triazolo[4,3-a]pyridine-3-carbonitrile
$\mu_{a,b,c}$	4.5, 0.9, 1.4
A, B, C	2154.5005, 1016.3647, 711.7775
A_s, B_s, C_s	2148.2524, 1013.4172, 709.7134
Charge, Multiplicity	0, 1
Predicted log column density	10.030±6.608
Electronic energy	-489.10608

geom1105



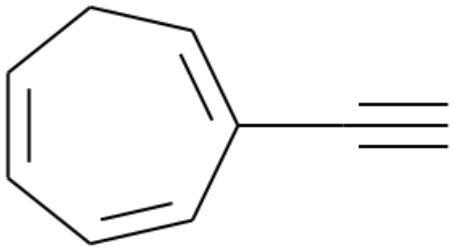
SMILES: C#CC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.30)

Is DFT optimized?: False

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	1-ethynylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.1, 0.4, 0.7
A, B, C	3600.1727, 1139.3487, 870.3315
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.004±2.304
Electronic energy	-347.51148

geom1106



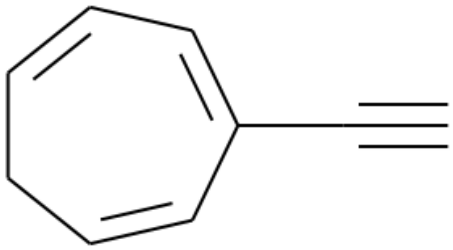
SMILES: C#CC1=CCC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.37)

Is DFT optimized?: False

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	2-ethynylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.1, 0.8, 1.2
A, B, C	3568.7550, 1142.2747, 869.9968
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.530±2.331
Electronic energy	-347.50832

geom1107



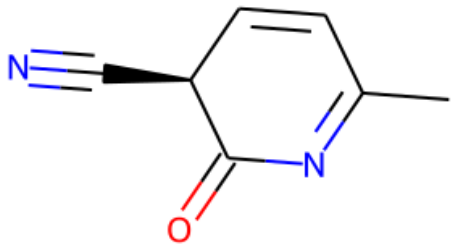
SMILES: C#CC1=CC=CCC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.61)

Is DFT optimized?: False

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	3-ethynylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.0, 0.1, 1.7
A, B, C	3647.1766, 1128.6517, 866.6861
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.427±2.586
Electronic energy	-347.51001

geom1108



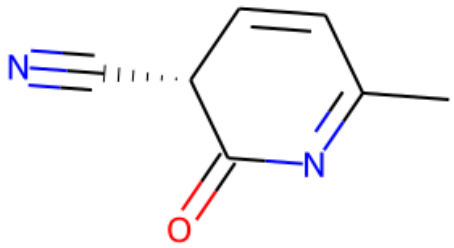
SMILES: CC1=NC(=O)[C@@H](C#N)C=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (6.44)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2O
Molecular weight	134.138
IUPAC name	(3R)-6-methyl-2-oxo-3H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	4.0, 3.6, 3.5
A, B, C	1988.1675, 1153.6590, 946.5375
A_s, B_s, C_s	1982.4018, 1150.3134, 943.7926
Charge, Multiplicity	0, 1
Predicted log column density	11.743±6.073
Electronic energy	-454.89430

geom1109



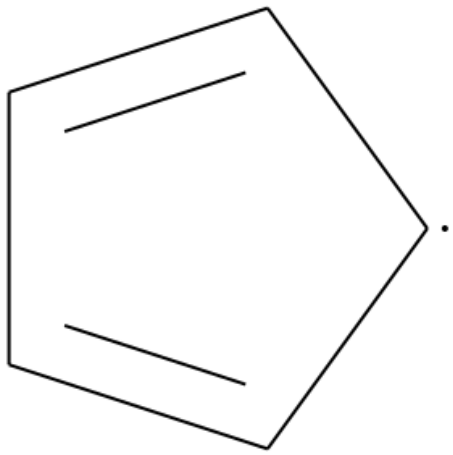
SMILES: CC1=NC(=O)[C@H](C#N)C=C1

Nearest TMC-1 molecule (distance): C1C=CC(=C1)C#N (6.44)

Is DFT optimized?: True

Property	Value
Formula	C7H6N2O
Molecular weight	134.138
IUPAC name	(3S)-6-methyl-2-oxo-3H-pyridine-3-carbonitrile
$\mu_{a,b,c}$	4.0, 3.7, 3.5
A, B, C	1989.9044, 1153.0813, 945.8401
A_s, B_s, C_s	1984.1337, 1149.7373, 943.0972
Charge, Multiplicity	0, 1
Predicted log column density	11.743±6.073
Electronic energy	-454.89430

geom1110



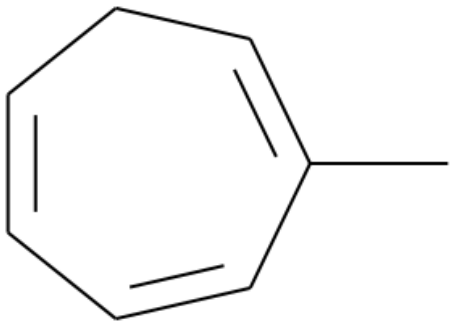
SMILES: [CH]1C=CC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (6.11)

Is DFT optimized?: True

Property	Value
Formula	C5H5
Molecular weight	65.095
IUPAC name	cyclopenta-1,3-diene
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	9303.9012, 8517.9072, 4446.7867
A_s, B_s, C_s	9276.9199, 8493.2053, 4433.8910
Charge, Multiplicity	0, 2
Predicted log column density	12.974±2.999
Electronic energy	-193.39913

geom1111



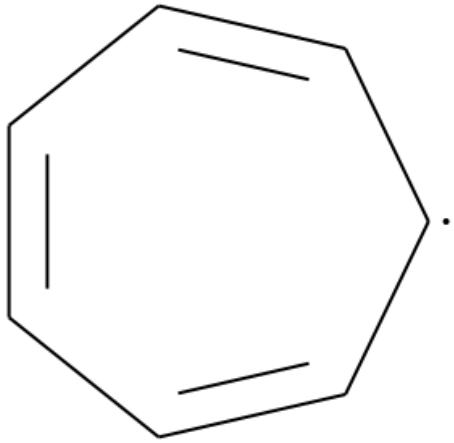
SMILES: CC1=CCC=CC=C1

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (6.48)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	2-methylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.2, 0.2, 0.2
A, B, C	3499.5289, 1904.8051, 1364.3033
A_s, B_s, C_s	3489.3802, 1899.2811, 1360.3468
Charge, Multiplicity	0, 1
Predicted log column density	12.140±3.119
Electronic energy	-310.73102

geom1112



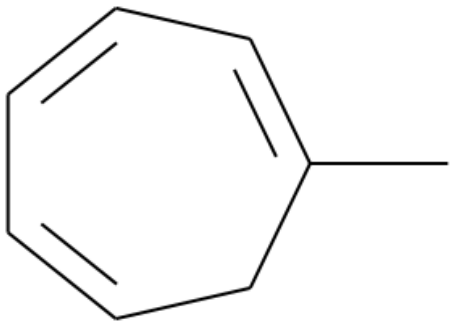
SMILES: [CH]1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.71)

Is DFT optimized?: True

Property	Value
Formula	C7H7
Molecular weight	91.133
IUPAC name	cyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	3719.2387, 3718.8801, 1859.5297
A_s, B_s, C_s	3708.4529, 3708.0953, 1854.1371
Charge, Multiplicity	0, 2
Predicted log column density	13.017±3.885
Electronic energy	-270.79666

geom1113



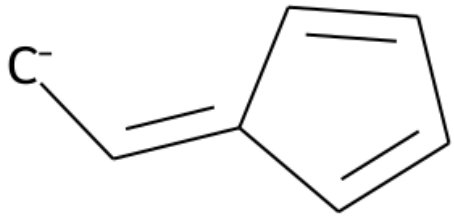
SMILES: CC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (6.65)

Is DFT optimized?: False

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	1-methylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.0, 0.5, 0.7
A, B, C	3533.4847, 1859.0987, 1237.4682
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.497±3.300
Electronic energy	-310.72056

geom1114



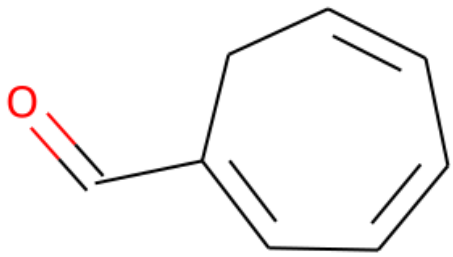
SMILES: `[CH2-]C=C1C=CC=C1`

Nearest TMC-1 molecule (distance): `C1=CC=C(C=C1)C#N` (6.85)

Is DFT optimized?: True

Property	Value
Formula	C7H7-
Molecular weight	91.133
IUPAC name	2-ethenylcyclopenta-1,3-diene
$\mu_{a,b,c}$	0.9, 0.4, 0.0
A, B, C	7718.2151, 1951.5263, 1557.6747
A_s, B_s, C_s	7695.8323, 1945.8669, 1553.1575
Charge, Multiplicity	-1, 1
Predicted log column density	12.771±3.723
Electronic energy	-270.84966

geom1115



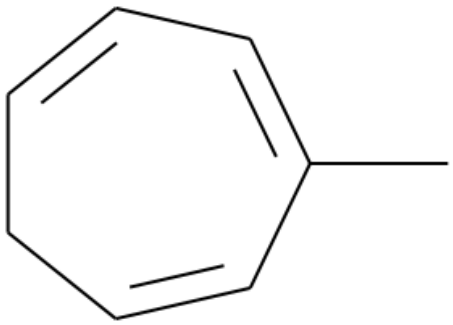
SMILES: O=CC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.87)

Is DFT optimized?: False

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	cyclohepta-1,3,5-triene-1-carbaldehyde
$\mu_{a,b,c}$	0.1, 3.3, 0.2
A, B, C	3410.8361, 1215.3930, 901.1659
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.816±2.767
Electronic energy	-384.70873

geom1116



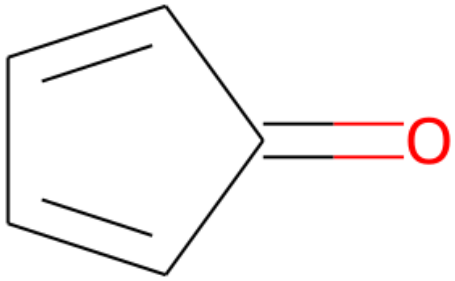
SMILES: CC1=CC=CCC=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.54)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	3-methylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.1, 0.3, 0.0
A, B, C	3572.1830, 1896.7287, 1346.4833
A_s, B_s, C_s	3561.8237, 1891.2282, 1342.5785
Charge, Multiplicity	0, 1
Predicted log column density	12.037±3.091
Electronic energy	-310.73128

geom1117



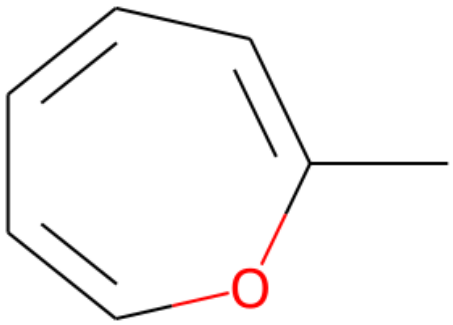
SMILES: O=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (5.95)

Is DFT optimized?: True

Property	Value
Formula	C5H4O
Molecular weight	80.086
IUPAC name	cyclopenta-2,4-dien-1-one
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	8155.0659, 3951.8683, 2661.9246
A_s, B_s, C_s	8131.4162, 3940.4079, 2654.2051
Charge, Multiplicity	0, 1
Predicted log column density	11.693±3.260
Electronic energy	-268.02054

geom1118



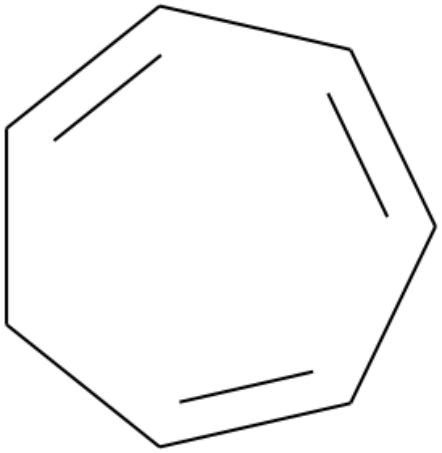
SMILES: CC1=CC=CC=CO1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.87)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	2-methyloxepine
$\mu_{a,b,c}$	0.3, 0.3, 1.3
A, B, C	3770.3112, 2025.3782, 1410.8832
A_s, B_s, C_s	3759.3773, 2019.5046, 1406.7916
Charge, Multiplicity	0, 1
Predicted log column density	14.832±4.225
Electronic energy	-346.61340

geom1119



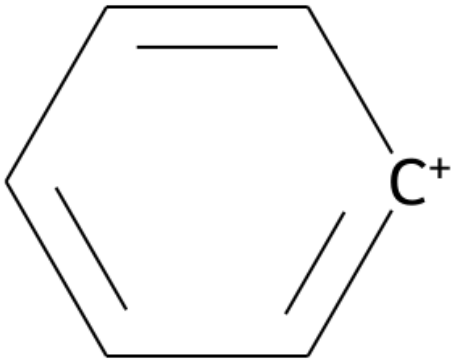
SMILES: C1=CC=CCC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.89)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	cyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.0, 0.3, 0.1
A, B, C	3688.1694, 3678.3081, 2021.2649
A_s, B_s, C_s	3677.4737, 3667.6410, 2015.4032
Charge, Multiplicity	0, 1
Predicted log column density	12.098±4.103
Electronic energy	-271.42391

geom1120



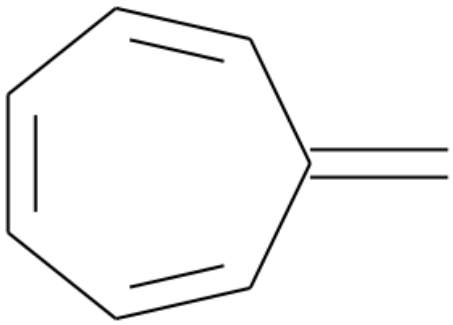
SMILES: [C+]1=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.46)

Is DFT optimized?: True

Property	Value
Formula	C6H5+
Molecular weight	77.106
IUPAC name	cyclohexatriene
$\mu_{a,b,c}$	0.0, 1.3, 0.0
A, B, C	6820.2105, 5416.8542, 3019.0317
A_s, B_s, C_s	6800.4319, 5401.1454, 3010.2765
Charge, Multiplicity	1, 1
Predicted log column density	12.491±2.195
Electronic energy	-231.17664

geom1121



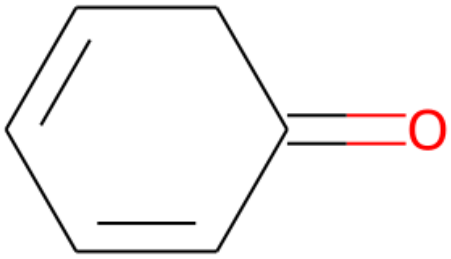
SMILES: C=C1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (6.97)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	7-methylidenecyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	3684.3587, 2001.6905, 1297.0336
A_s, B_s, C_s	3673.6740, 1995.8856, 1293.2722
Charge, Multiplicity	0, 1
Predicted log column density	12.219±3.285
Electronic energy	-309.49899

geom1122



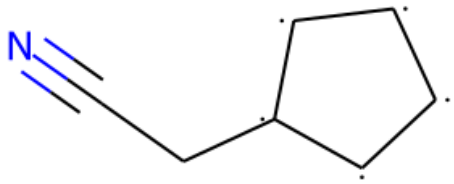
SMILES: O=C1C=CC=CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (5.56)

Is DFT optimized?: True

Property	Value
Formula	C6H6O
Molecular weight	94.113
IUPAC name	cyclohexa-2,4-dien-1-one
$\mu_{a,b,c}$	3.9, 0.5, 0.0
A, B, C	5189.4737, 2692.8929, 1792.1012
A_s, B_s, C_s	5174.4242, 2685.0836, 1786.9041
Charge, Multiplicity	0, 1
Predicted log column density	12.352±2.985
Electronic energy	-307.34794

geom1123



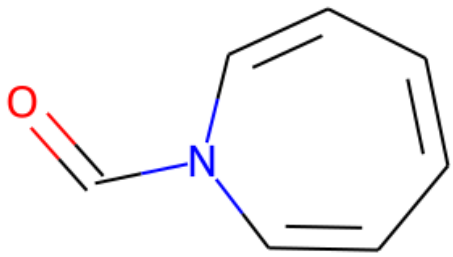
SMILES: N#CC[C]1[CH][CH][CH][CH]1

Nearest TMC-1 molecule (distance): C1C=CC=C1C#N (6.89)

Is DFT optimized?: True

Property	Value
Formula	C7H6N
Molecular weight	104.132
IUPAC name	2-cyclopentylacetonitrile
$\mu_{a,b,c}$	0.1, 1.9, 2.0
A, B, C	4557.0640, 1498.6774, 1449.5843
A_s, B_s, C_s	4543.8485, 1494.3313, 1445.3805
Charge, Multiplicity	0, 6
Predicted log column density	13.013±4.977
Electronic energy	-324.60988

geom1124



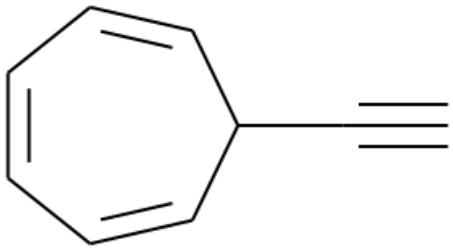
SMILES: O=CN1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.05)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	azepine-1-carbaldehyde
$\mu_{a,b,c}$	2.9, 1.7, 0.1
A, B, C	3628.8464, 1255.5304, 933.0467
A_s, B_s, C_s	3618.3227, 1251.8893, 930.3408
Charge, Multiplicity	0, 1
Predicted log column density	12.446±4.314
Electronic energy	-400.75459

geom1125



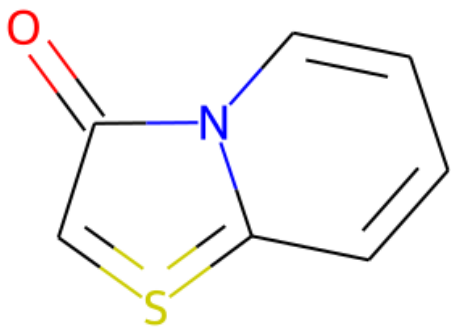
SMILES: C#CC1C=CC=CC=1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.06)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	7-ethynylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.5, 0.0, 0.4
A, B, C	2265.6826, 1621.6086, 1483.1171
A_s, B_s, C_s	2259.1121, 1616.9059, 1478.8160
Charge, Multiplicity	0, 1
Predicted log column density	11.256±4.068
Electronic energy	-347.53021

geom1126



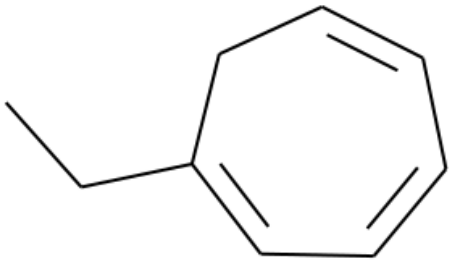
SMILES: O=C1C=S=C2C=CC=CN12

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.89)

Is DFT optimized?: False

Property	Value
Formula	C7H5NOS
Molecular weight	151.190
IUPAC name	[1,3]thiazolo[3,2-a]pyridin-3-one
$\mu_{a,b,c}$	0.0, 3.2, 5.5
A, B, C	2033.4887, 1282.7622, 786.5757
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.137±5.085
Electronic energy	-797.72934

geom1127



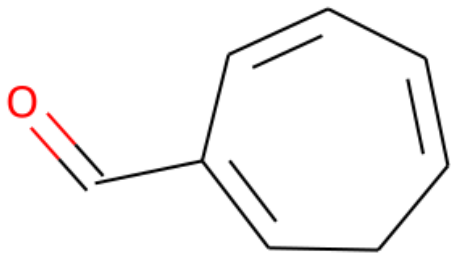
SMILES: CCC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (6.53)

Is DFT optimized?: True

Property	Value
Formula	C9H12
Molecular weight	120.195
IUPAC name	1-ethylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.7, 0.3, 0.2
A, B, C	3318.4188, 1150.4004, 935.8075
A_s, B_s, C_s	3308.7954, 1147.0642, 933.0937
Charge, Multiplicity	0, 1
Predicted log column density	11.015±4.011
Electronic energy	-350.03643

geom1128



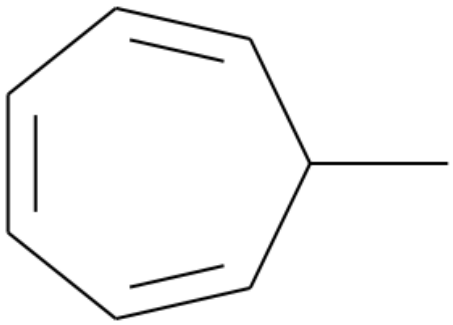
SMILES: O=CC1=CCC=CC=C1

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (7.00)

Is DFT optimized?: True

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	cyclohepta-1,4,6-triene-1-carbaldehyde
$\mu_{a,b,c}$	3.4, 2.3, 0.0
A, B, C	3333.5628, 1200.8506, 887.6182
A_s, B_s, C_s	3323.8955, 1197.3681, 885.0441
Charge, Multiplicity	0, 1
Predicted log column density	10.901±2.904
Electronic energy	-384.70845

geom1129



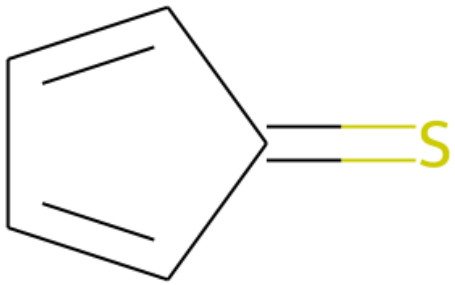
SMILES: CC1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.14)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	7-methylcyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.3, 0.0, 0.1
A, B, C	2804.7601, 2295.5045, 1704.5038
A_s, B_s, C_s	2796.6263, 2288.8476, 1699.5608
Charge, Multiplicity	0, 1
Predicted log column density	11.128±4.404
Electronic energy	-310.72745

geom1130



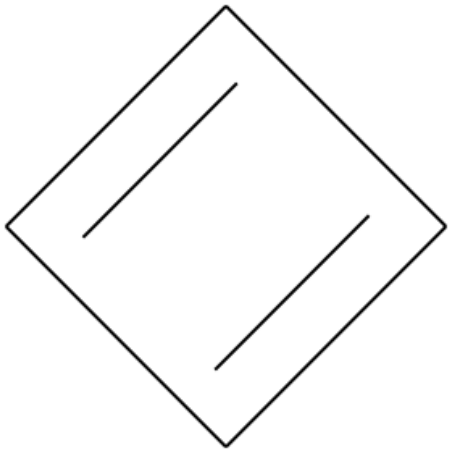
SMILES: S=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (6.08)

Is DFT optimized?: False

Property	Value
Formula	C5H4S
Molecular weight	96.154
IUPAC name	cyclopenta-2,4-diene-1-thione
$\mu_{a,b,c}$	0.0, 0.0, 2.7
A, B, C	8445.4833, 2224.6629, 1760.8337
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.910±2.874
Electronic energy	-590.97770

geom1131



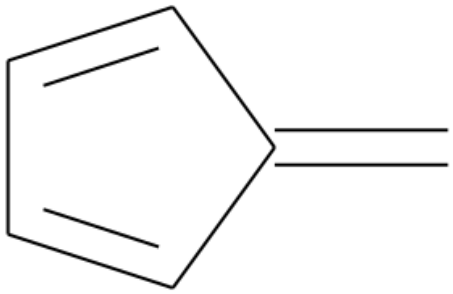
SMILES: C1=CC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.69)

Is DFT optimized?: True

Property	Value
Formula	C4H4
Molecular weight	52.076
IUPAC name	cyclobutadiene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	13779.8857, 13778.3081, 13776.8410
A_s, B_s, C_s	13739.9240, 13738.3510, 13736.8882
Charge, Multiplicity	0, 1
Predicted log column density	12.609±2.533
Electronic energy	-154.59085

geom1132



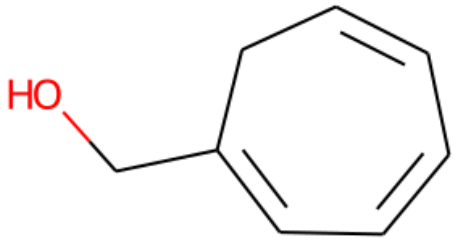
SMILES: C=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (6.15)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	fulvene
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	8210.7574, 3813.4632, 2604.0292
A_s, B_s, C_s	8186.9462, 3802.4042, 2596.4775
Charge, Multiplicity	0, 1
Predicted log column density	12.177±2.680
Electronic energy	-232.11406

geom1133



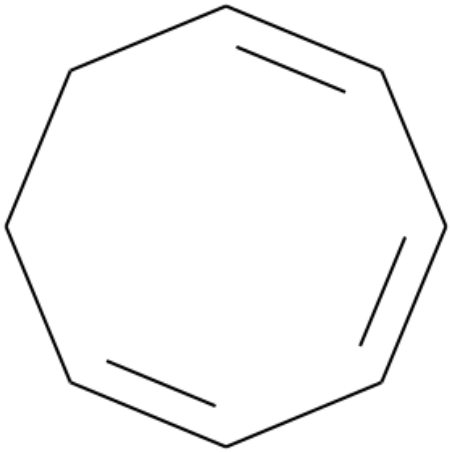
SMILES: OCC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (6.86)

Is DFT optimized?: True

Property	Value
Formula	C8H10O
Molecular weight	122.167
IUPAC name	cyclohepta-1,3,5-trien-1-ylmethanol
$\mu_{a,b,c}$	1.0, 0.3, 1.8
A, B, C	2534.0867, 1476.7124, 1202.3925
A_s, B_s, C_s	2526.7379, 1472.4299, 1198.9055
Charge, Multiplicity	0, 1
Predicted log column density	9.902±3.520
Electronic energy	-385.85483

geom1134



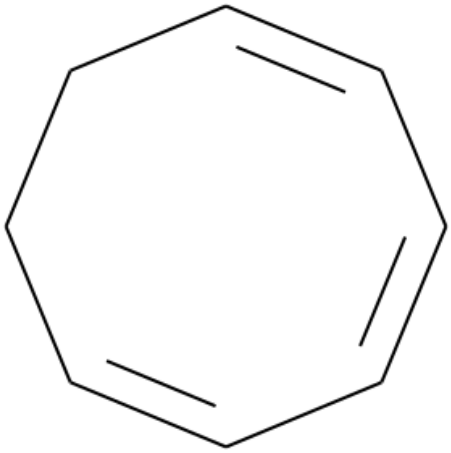
SMILES: C1=CC=CCCC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.30)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	cycloocta-1,3,5-triene
$\mu_{a,b,c}$	0.4, 2.0, 0.3
A, B, C	2777.5314, 2473.8544, 1462.1307
A_s, B_s, C_s	2769.4766, 2466.6802, 1457.8905
Charge, Multiplicity	0, 1
Predicted log column density	12.484±4.695
Electronic energy	-310.59724

geom1135



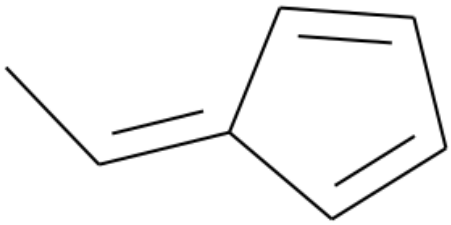
SMILES: C1=C\C=C/CC\C=C/1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.30)

Is DFT optimized?: True

Property	Value
Formula	C8H10
Molecular weight	106.168
IUPAC name	(5Z)-cycloocta-1,3,5-triene
$\mu_{a,b,c}$	0.4, 2.0, 0.3
A, B, C	2778.6530, 2473.4081, 1462.3468
A_s, B_s, C_s	2770.5949, 2466.2352, 1458.1060
Charge, Multiplicity	0, 1
Predicted log column density	12.484±4.695
Electronic energy	-310.59723

geom1136



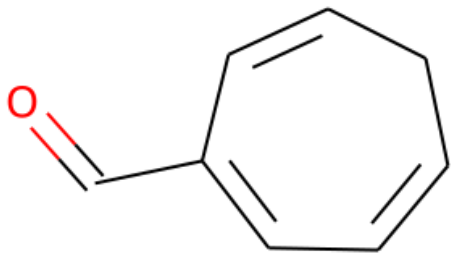
SMILES: CC=C1C=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.31)

Is DFT optimized?: True

Property	Value
Formula	C7H8
Molecular weight	92.141
IUPAC name	5-ethylidenecyclopenta-1,3-diene
$\mu_{a,b,c}$	1.5, 0.1, 0.0
A, B, C	7119.6962, 1929.3572, 1532.3768
A_s, B_s, C_s	7099.0491, 1923.7621, 1527.9329
Charge, Multiplicity	0, 1
Predicted log column density	14.580±3.682
Electronic energy	-271.42356

geom1137



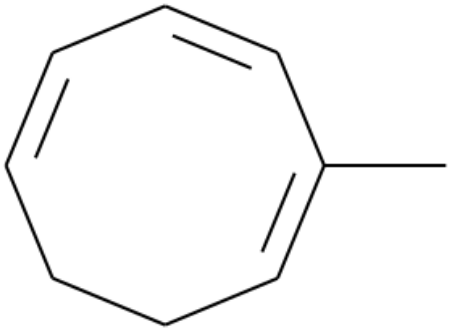
SMILES: O=CC1=CC=CCC=C1

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (7.06)

Is DFT optimized?: True

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	cyclohepta-1,3,6-triene-1-carbaldehyde
$\mu_{a,b,c}$	4.1, 1.4, 0.1
A, B, C	3394.0097, 1186.6918, 884.3591
A_s, B_s, C_s	3384.1671, 1183.2504, 881.7945
Charge, Multiplicity	0, 1
Predicted log column density	10.796±2.801
Electronic energy	-384.70992

geom1138



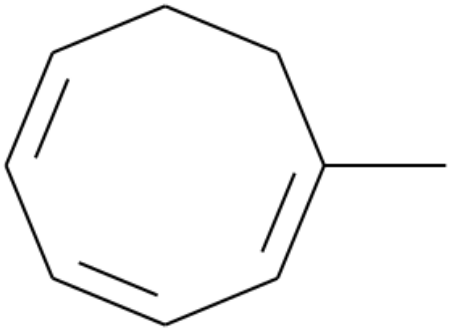
SMILES: CC1=CCC/C=C\C=C/1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.62)

Is DFT optimized?: False

Property	Value
Formula	C9H12
Molecular weight	120.195
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.8, 0.8
A, B, C	2566.5948, 1436.2227, 974.4878
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.519±4.123
Electronic energy	-349.95475

geom1139



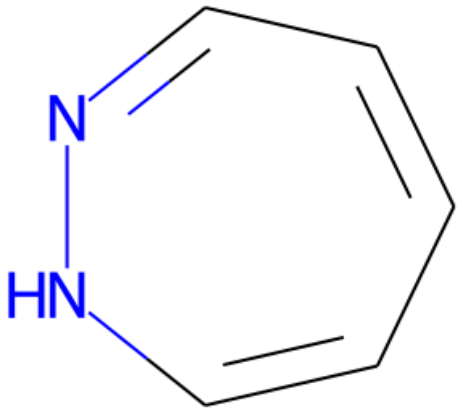
SMILES: C/C1=C/C=C\C=C/CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.71)

Is DFT optimized?: False

Property	Value
Formula	C9H12
Molecular weight	120.195
IUPAC name	(1Z,3Z,5Z)-1-methylcycloocta-1,3,5-triene
$\mu_{a,b,c}$	1.6, 1.1, 0.4
A, B, C	2508.4113, 1510.7291, 1037.4059
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.539±4.073
Electronic energy	-349.88393

geom1140



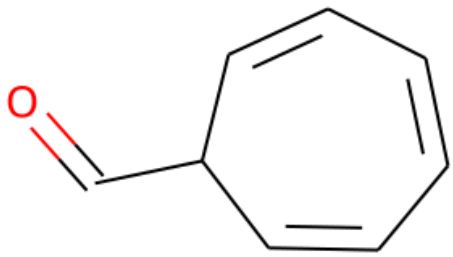
SMILES: C1=CC=NNC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.35)

Is DFT optimized?: True

Property	Value
Formula	C5H6N2
Molecular weight	94.117
IUPAC name	1H-diazepine
$\mu_{a,b,c}$	1.4, 0.5, 0.3
A, B, C	4004.9724, 3804.8870, 2090.2691
A_s, B_s, C_s	3993.3580, 3793.8529, 2084.2073
Charge, Multiplicity	0, 1
Predicted log column density	11.689±4.944
Electronic energy	-303.46312

geom1141



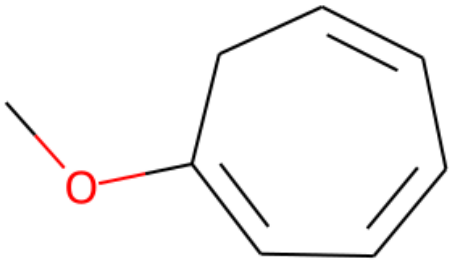
SMILES: O=CC1C=CC=CC=C1

Nearest TMC-1 molecule (distance): C1=CC=C(C=C1)C#N (7.36)

Is DFT optimized?: True

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	cyclohepta-2,4,6-triene-1-carbaldehyde
$\mu_{a,b,c}$	2.6, 0.0, 1.8
A, B, C	3280.0808, 1200.5787, 982.9918
A_s, B_s, C_s	3270.5686, 1197.0971, 980.1412
Charge, Multiplicity	0, 1
Predicted log column density	9.587±4.247
Electronic energy	-384.70618

geom1142



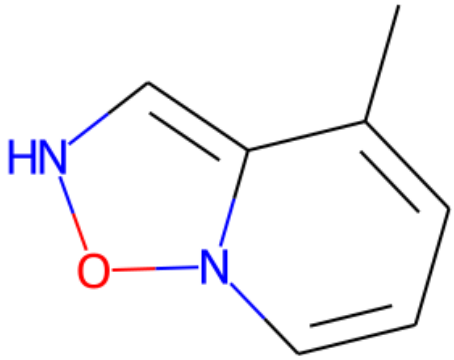
SMILES: COC1=CC=CC=CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.97)

Is DFT optimized?: False

Property	Value
Formula	C8H10O
Molecular weight	122.167
IUPAC name	1-methoxycyclohepta-1,3,5-triene
$\mu_{a,b,c}$	0.4, 1.3, 1.5
A, B, C	3315.7951, 1188.6048, 897.4241
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	15.230±4.694
Electronic energy	-385.90187

geom1143



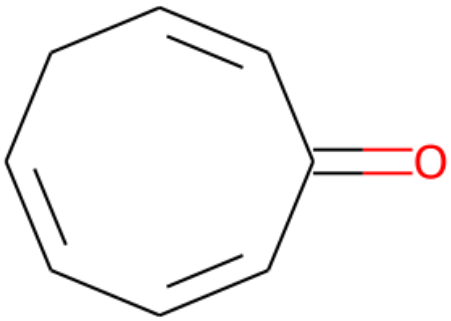
SMILES: CC1=CC=CN2ONC=C12

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (7.24)

Is DFT optimized?: True

Property	Value
Formula	C7H8N2O
Molecular weight	136.154
IUPAC name	4-methyl-2H-[1,2,5]oxadiazolo[2,3-a]pyridine
$\mu_{a,b,c}$	2.4, 0.0, 1.3
A, B, C	2186.4700, 1455.4272, 887.6337
A_s, B_s, C_s	2180.1292, 1451.2064, 885.0596
Charge, Multiplicity	0, 1
Predicted log column density	13.376±5.350
Electronic energy	-455.98562

geom1144



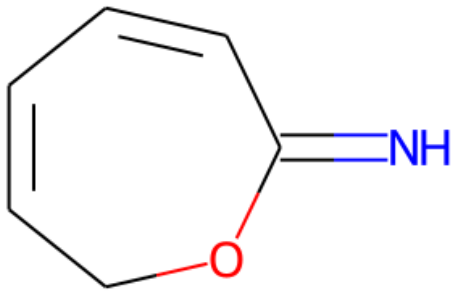
SMILES: O=C1/C=C\C=C/C/C=C\1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (7.19)

Is DFT optimized?: True

Property	Value
Formula	C8H8O
Molecular weight	120.151
IUPAC name	
$\mu_{a,b,c}$	3.1, 1.3, 1.5
A, B, C	2324.4967, 1847.5081, 1162.5105
A_s, B_s, C_s	2317.7557, 1842.1504, 1159.1392
Charge, Multiplicity	0, 1
Predicted log column density	11.188±4.124
Electronic energy	-384.67696

geom1145



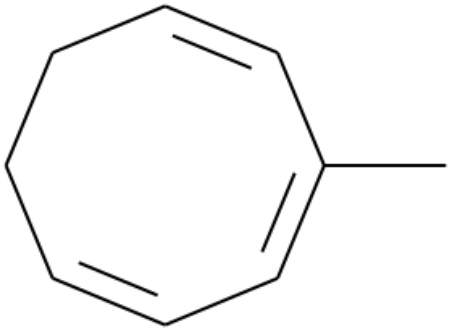
SMILES: N=C1C=CC=CCO1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.85)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	3.7, 2.2, 1.4
A, B, C	3760.7901, 2056.7234, 1424.5651
A_s, B_s, C_s	3749.8839, 2050.7589, 1420.4338
Charge, Multiplicity	0, 1
Predicted log column density	16.105±4.661
Electronic energy	-362.65562

geom1146



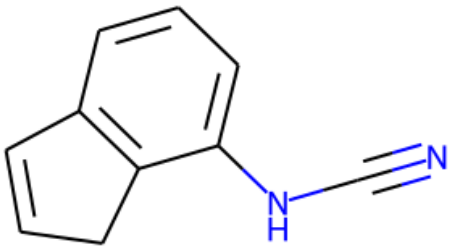
SMILES: CC1=C/C=C\CC/C=C\1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.55)

Is DFT optimized?: True

Property	Value
Formula	C9H12
Molecular weight	120.195
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.8, 0.4
A, B, C	2948.8194, 1352.7155, 1010.2448
A_s, B_s, C_s	2940.2678, 1348.7926, 1007.3151
Charge, Multiplicity	0, 1
Predicted log column density	12.419±3.755
Electronic energy	-349.99031

geom1147



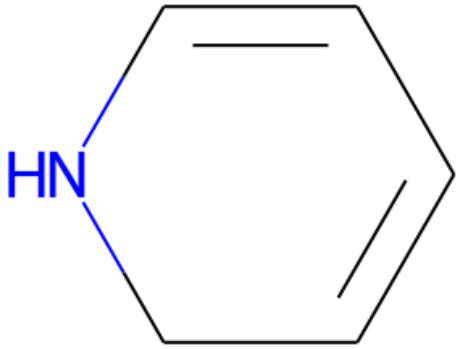
SMILES: N#CNc1cccc2c1CC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.24)

Is DFT optimized?: True

Property	Value
Formula	C10H8N2
Molecular weight	156.188
IUPAC name	
$\mu_{a,b,c}$	4.6, 1.8, 0.0
A, B, C	1902.1243, 699.1669, 512.8836
A_s, B_s, C_s	1896.6081, 697.1393, 511.3963
Charge, Multiplicity	0, 1
Predicted log column density	12.585±4.153
Electronic energy	-495.19219

geom1148



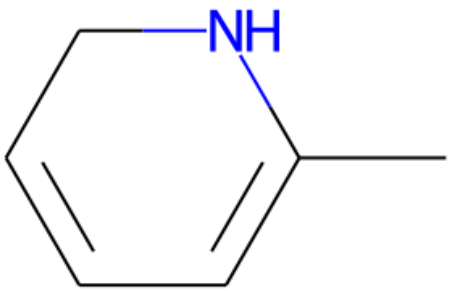
SMILES: C1=CCNC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (6.50)

Is DFT optimized?: True

Property	Value
Formula	C5H7N
Molecular weight	81.118
IUPAC name	1,2-dihydropyridine
$\mu_{a,b,c}$	1.6, 0.4, 0.4
A, B, C	5385.8775, 5302.7910, 2786.0311
A_s, B_s, C_s	5370.2585, 5287.4130, 2777.9516
Charge, Multiplicity	0, 1
Predicted log column density	11.708±5.422
Electronic energy	-249.37795

geom1149



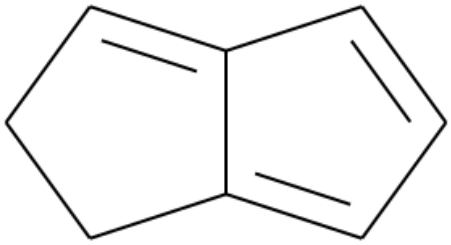
SMILES: CC1=CC=CCN1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (5.74)

Is DFT optimized?: True

Property	Value
Formula	C6H9N
Molecular weight	95.145
IUPAC name	6-methyl-1,2-dihydropyridine
$\mu_{a,b,c}$	1.0, 1.4, 0.4
A, B, C	5166.7429, 2484.2667, 1741.2426
A_s, B_s, C_s	5151.7593, 2477.0623, 1736.1930
Charge, Multiplicity	0, 1
Predicted log column density	11.249±4.317
Electronic energy	-288.68891

geom1150



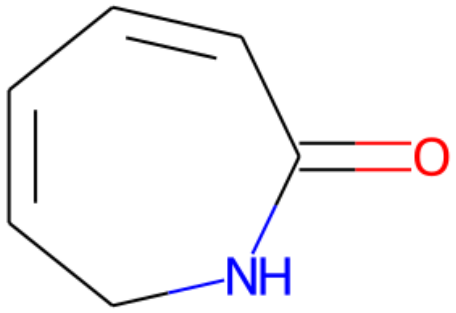
SMILES: C1=CC2=CCCC2=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (5.91)

Is DFT optimized?: True

Property	Value
Formula	C8H8
Molecular weight	104.152
IUPAC name	1,2-dihydropentalene
$\mu_{a,b,c}$	1.6, 0.1, 0.0
A, B, C	4771.9165, 2048.2945, 1458.9060
A_s, B_s, C_s	4758.0779, 2042.3544, 1454.6752
Charge, Multiplicity	0, 1
Predicted log column density	12.105±4.064
Electronic energy	-309.51523

geom1151



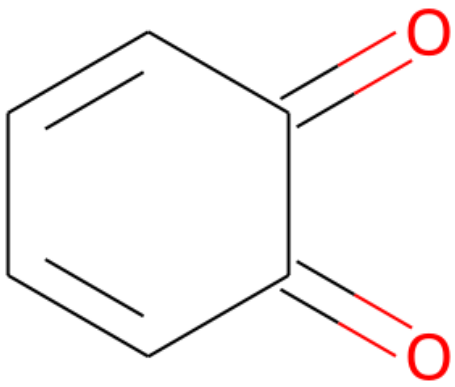
SMILES: O=C1C=CC=CCN1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.64)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	1,2-dihydroazepin-7-one
$\mu_{a,b,c}$	4.4, 1.2, 0.9
A, B, C	3629.3907, 2028.2218, 1409.6859
A_s, B_s, C_s	3618.8654, 2022.3399, 1405.5978
Charge, Multiplicity	0, 1
Predicted log column density	11.612±5.063
Electronic energy	-362.69360

geom1152



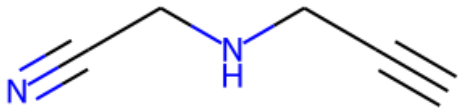
SMILES: O=C1C=CC=CC1=O

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (6.29)

Is DFT optimized?: True

Property	Value
Formula	C6H4O2
Molecular weight	108.096
IUPAC name	cyclohexa-3,5-diene-1,2-dione
$\mu_{a,b,c}$	5.8, 0.0, 0.0
A, B, C	3246.8902, 2441.9994, 1393.7535
A_s, B_s, C_s	3237.4742, 2434.9176, 1389.7116
Charge, Multiplicity	0, 1
Predicted log column density	12.024±4.440
Electronic energy	-381.32311

geom1153



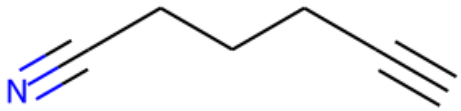
SMILES: C#CCNCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (3.81)

Is DFT optimized?: True

Property	Value
Formula	C5H6N2
Molecular weight	94.117
IUPAC name	2-(prop-2-ynylamino)acetonitrile
$\mu_{a,b,c}$	3.2, 2.7, 1.1
A, B, C	11810.7710, 1013.1425, 946.0589
A_s, B_s, C_s	11776.5198, 1010.2044, 943.3153
Charge, Multiplicity	0, 1
Predicted log column density	12.733±4.360
Electronic energy	-303.43777

geom1154



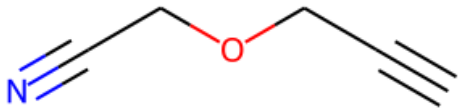
SMILES: C#CCCCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.11)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	hex-5-ynenitrile
$\mu_{a,b,c}$	3.1, 2.3, 0.0
A, B, C	11894.2153, 953.0510, 897.0499
A_s, B_s, C_s	11859.7220, 950.2872, 894.4485
Charge, Multiplicity	0, 1
Predicted log column density	10.166±3.413
Electronic energy	-287.42663

geom1155



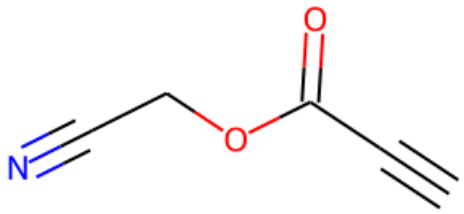
SMILES: C#CCOCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.37)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	2-prop-2-ynoxyacetonitrile
$\mu_{a,b,c}$	3.2, 3.7, 0.0
A, B, C	11705.0698, 1061.5708, 985.4233
A_s, B_s, C_s	11671.1251, 1058.4922, 982.5656
Charge, Multiplicity	0, 1
Predicted log column density	12.819±4.433
Electronic energy	-323.28895

geom1156



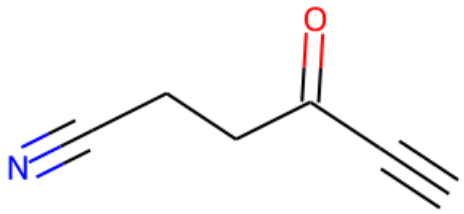
SMILES: C#CC(=O)OCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.47)

Is DFT optimized?: False

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	cyanomethyl prop-2-ynoate
$\mu_{a,b,c}$	3.8, 1.4, 2.0
A, B, C	4832.1441, 1122.4395, 1104.5198
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.432±4.476
Electronic energy	-397.28145

geom1157



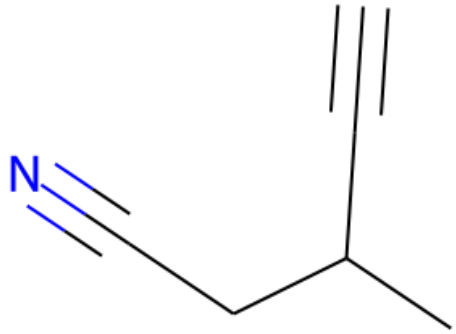
SMILES: C#CC(=O)CCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.55)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	3.7, 1.3, 0.0
A, B, C	5787.5296, 919.7321, 801.4155
A_s, B_s, C_s	5770.7458, 917.0649, 799.0914
Charge, Multiplicity	0, 1
Predicted log column density	8.548±4.047
Electronic energy	-361.41072

geom1158



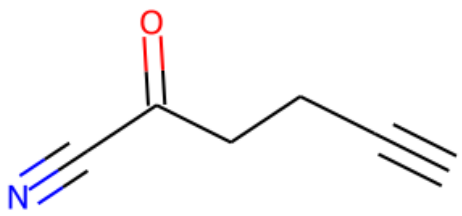
SMILES: C#CC(C)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.62)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	3-methylpent-4-ynenitrile
$\mu_{a,b,c}$	3.5, 0.4, 0.6
A, B, C	6709.9173, 1438.6383, 1239.8197
A_s, B_s, C_s	6690.4585, 1434.4662, 1236.2243
Charge, Multiplicity	0, 1
Predicted log column density	11.272±4.354
Electronic energy	-287.42753

geom1159



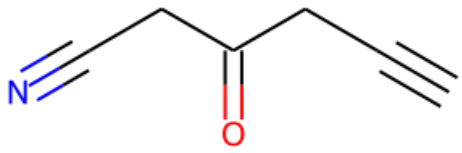
SMILES: C#CCCC(=O)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.70)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	3.1, 0.6, 0.0
A, B, C	5730.4168, 916.7575, 798.0359
A_s, B_s, C_s	5713.7986, 914.0989, 795.7216
Charge, Multiplicity	0, 1
Predicted log column density	9.334±3.960
Electronic energy	-361.40131

geom1160



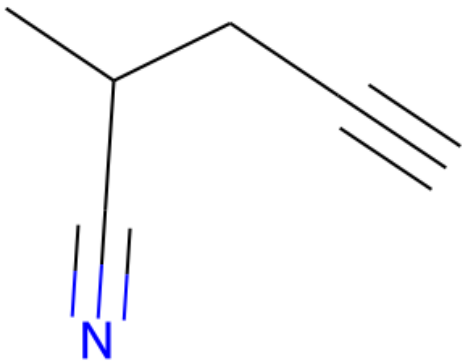
SMILES: C#CCC(=O)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.77)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.4, 0.8, 1.2
A, B, C	4196.1321, 1187.5559, 944.7299
A_s, B_s, C_s	4183.9633, 1184.1119, 941.9902
Charge, Multiplicity	0, 1
Predicted log column density	12.083±4.495
Electronic energy	-361.40838

geom1161



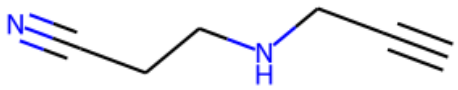
SMILES: C#CCC(C)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.78)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	2-methylpent-4-ynenitrile
$\mu_{a,b,c}$	3.5, 1.4, 0.4
A, B, C	6672.2772, 1435.9411, 1238.6741
A_s, B_s, C_s	6652.9276, 1431.7769, 1235.0820
Charge, Multiplicity	0, 1
Predicted log column density	12.495±4.268
Electronic energy	-287.42733

geom1162



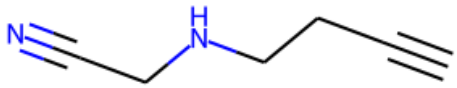
SMILES: C#CCNCCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.86)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	3-(prop-2-ynylamino)propanenitrile
$\mu_{a,b,c}$	3.6, 0.7, 0.7
A, B, C	13969.0386, 633.5377, 614.6197
A_s, B_s, C_s	13928.5284, 631.7004, 612.8373
Charge, Multiplicity	0, 1
Predicted log column density	11.699±4.624
Electronic energy	-342.74783

geom1163



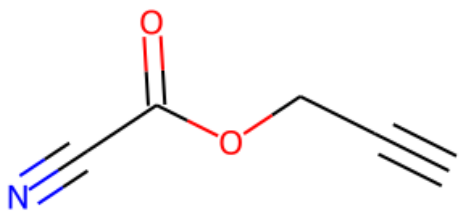
SMILES: C#CCCNCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.86)

Is DFT optimized?: True

Property	Value
Formula	C6H8N2
Molecular weight	108.144
IUPAC name	2-(but-3-ynylamino)acetonitrile
$\mu_{a,b,c}$	3.3, 1.9, 0.9
A, B, C	14117.2626, 632.6879, 613.5323
A_s, B_s, C_s	14076.3225, 630.8531, 611.7531
Charge, Multiplicity	0, 1
Predicted log column density	11.699±4.624
Electronic energy	-342.74636

geom1164



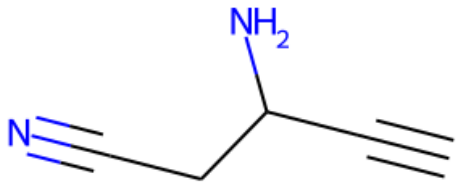
SMILES: C#CCOC(=O)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (4.90)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	prop-2-ynyl cyanoformate
$\mu_{a,b,c}$	3.9, 0.9, 1.2
A, B, C	5101.3410, 1115.7875, 1101.3289
A_s, B_s, C_s	5086.5471, 1112.5517, 1098.1351
Charge, Multiplicity	0, 1
Predicted log column density	11.210±4.817
Electronic energy	-397.29929

geom1165



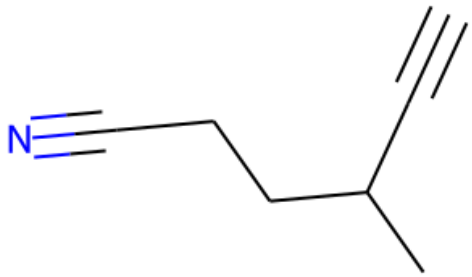
SMILES: C#CC(N)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.07)

Is DFT optimized?: True

Property	Value
Formula	C5H6N2
Molecular weight	94.117
IUPAC name	
$\mu_{a,b,c}$	4.1, 0.9, 0.9
A, B, C	3745.9635, 2018.1224, 1387.3737
A_s, B_s, C_s	3735.1002, 2012.2699, 1383.3503
Charge, Multiplicity	0, 1
Predicted log column density	8.730±4.428
Electronic energy	-303.45292

geom1166



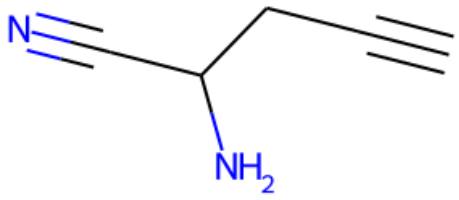
SMILES: C#CC(C)CCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.19)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	4-methylhex-5-ynenitrile
$\mu_{a,b,c}$	4.1, 0.2, 1.2
A, B, C	3746.1251, 1029.6823, 850.0447
A_s, B_s, C_s	3735.2613, 1026.6962, 847.5796
Charge, Multiplicity	0, 1
Predicted log column density	9.328±4.722
Electronic energy	-326.73286

geom1167



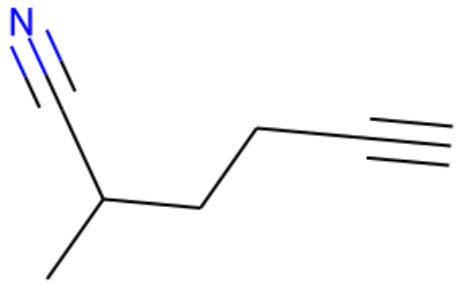
SMILES: C#CCC(N)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.23)

Is DFT optimized?: True

Property	Value
Formula	C5H6N2
Molecular weight	94.117
IUPAC name	
$\mu_{a,b,c}$	4.4, 0.4, 0.3
A, B, C	7001.5707, 1455.2360, 1256.4773
A_s, B_s, C_s	6981.2661, 1451.0158, 1252.8336
Charge, Multiplicity	0, 1
Predicted log column density	9.945±4.447
Electronic energy	-303.45155

geom1168



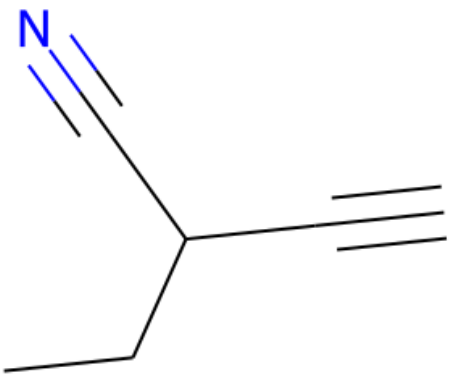
SMILES: C#CCCC(C)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.24)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	2-methylhex-5-ynenitrile
$\mu_{a,b,c}$	3.7, 1.6, 0.8
A, B, C	3890.0101, 1057.9933, 1043.7445
A_s, B_s, C_s	3878.7290, 1054.9252, 1040.7177
Charge, Multiplicity	0, 1
Predicted log column density	10.552±4.473
Electronic energy	-326.73263

geom1169



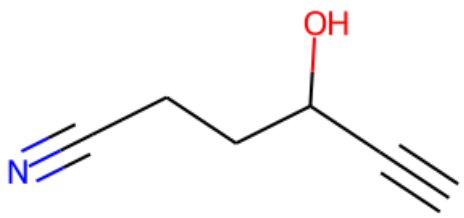
SMILES: C#CC(C#N)CC

Nearest TMC-1 molecule (distance): C#CCC#N (5.25)

Is DFT optimized?: True

Property	Value
Formula	C6H7N
Molecular weight	93.129
IUPAC name	2-ethylbut-3-ynenitrile
$\mu_{a,b,c}$	0.7, 3.9, 0.7
A, B, C	3403.6579, 2129.8351, 1382.6170
A_s, B_s, C_s	3393.7873, 2123.6586, 1378.6074
Charge, Multiplicity	0, 1
Predicted log column density	9.050±5.097
Electronic energy	-287.42041

geom1170



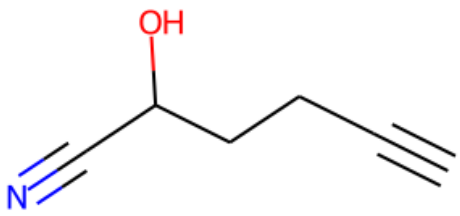
SMILES: C#CC(O)CCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.29)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	4-hydroxyhex-5-ynenitrile
$\mu_{a,b,c}$	3.3, 1.6, 0.2
A, B, C	3845.9721, 1028.0848, 852.2917
A_s, B_s, C_s	3834.8187, 1025.1034, 849.8200
Charge, Multiplicity	0, 1
Predicted log column density	8.386±4.912
Electronic energy	-362.61698

geom1171



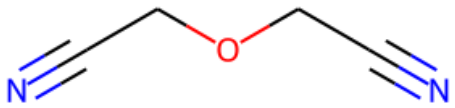
SMILES: C#CCCC(O)C#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.30)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	2-hydroxyhex-5-ynenitrile
$\mu_{a,b,c}$	2.7, 0.9, 0.1
A, B, C	5037.6785, 905.4995, 801.4240
A_s, B_s, C_s	5023.0692, 902.8736, 799.0999
Charge, Multiplicity	0, 1
Predicted log column density	9.604±4.634
Electronic energy	-362.61407

geom1172



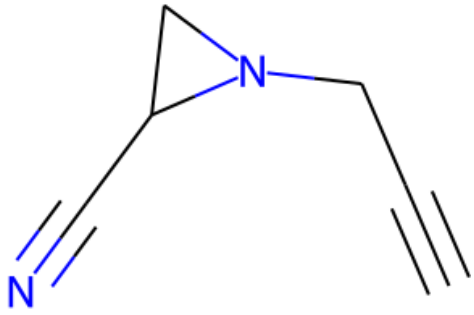
SMILES: N#CCOCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.35)

Is DFT optimized?: True

Property	Value
Formula	C4H4N2O
Molecular weight	96.089
IUPAC name	2-(cyanomethoxy)acetonitrile
$\mu_{a,b,c}$	0.0, 5.7, 0.0
A, B, C	11931.7850, 1063.9284, 989.0827
A_s, B_s, C_s	11897.1828, 1060.8430, 986.2144
Charge, Multiplicity	0, 1
Predicted log column density	11.535±4.164
Electronic energy	-339.37950

geom1173



SMILES: C#CCN1CC1C#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.42)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	1-prop-2-ynylaziridine-2-carbonitrile
$\mu_{a,b,c}$	3.7, 1.3, 2.9
A, B, C	8116.8290, 939.8428, 913.4773
A_s, B_s, C_s	8093.2902, 937.1173, 910.8283
Charge, Multiplicity	0, 1
Predicted log column density	11.522±5.507
Electronic energy	-341.49703

geom1174

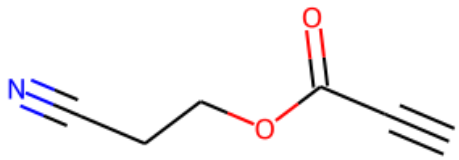
SMILES: C#CC1CN1CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.43)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	
$\mu_{a,b,c}$	1.9, 4.1, 1.3
A, B, C	3515.4019, 1356.1676, 1027.1153
A_s, B_s, C_s	3505.2072, 1352.2347, 1024.1366
Charge, Multiplicity	0, 1
Predicted log column density	10.742±5.249
Electronic energy	-341.49706

geom1175



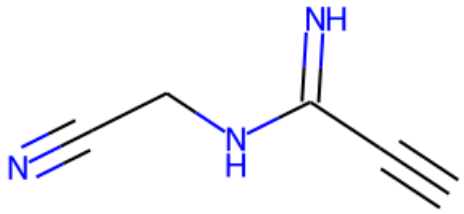
SMILES: C#CC(=O)OCCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.45)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	2-cyanoethyl prop-2-ynoate
$\mu_{a,b,c}$	4.1, 2.2, 0.8
A, B, C	6657.0857, 674.1419, 647.1451
A_s, B_s, C_s	6637.7801, 672.1869, 645.2683
Charge, Multiplicity	0, 1
Predicted log column density	9.445±5.304
Electronic energy	-436.61987

geom1176



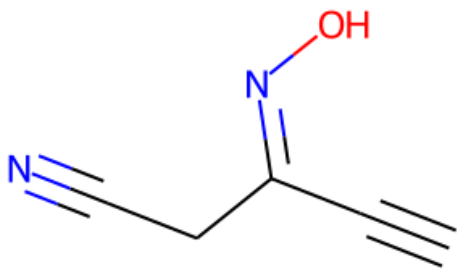
SMILES: C#CC(=N)NCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.46)

Is DFT optimized?: True

Property	Value
Formula	C5H5N3
Molecular weight	107.116
IUPAC name	
$\mu_{a,b,c}$	3.9, 0.6, 0.6
A, B, C	5395.8323, 998.1699, 847.2062
A_s, B_s, C_s	5380.1843, 995.2752, 844.7493
Charge, Multiplicity	0, 1
Predicted log column density	12.954±4.898
Electronic energy	-357.57286

geom1177



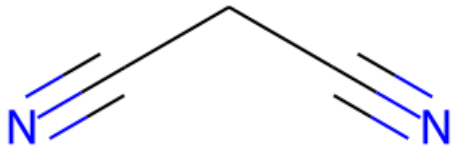
SMILES: C#CC(CC#N)=NO

Nearest TMC-1 molecule (distance): C#CCC#N (5.47)

Is DFT optimized?: True

Property	Value
Formula	C5H4N2O
Molecular weight	108.100
IUPAC name	
$\mu_{a,b,c}$	2.6, 1.7, 2.3
A, B, C	2453.8900, 1771.4844, 1140.5469
A_s, B_s, C_s	2446.7737, 1766.3471, 1137.2393
Charge, Multiplicity	0, 1
Predicted log column density	8.110±5.421
Electronic energy	-377.38628

geom1178



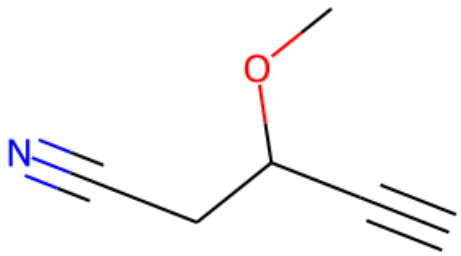
SMILES: N#CCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.48)

Is DFT optimized?: True

Property	Value
Formula	C3H2N2
Molecular weight	66.063
IUPAC name	propanedinitrile
$\mu_{a,b,c}$	0.0, 4.0, 0.0
A, B, C	20860.4649, 2929.7359, 2610.7612
A_s, B_s, C_s	20799.9696, 2921.2396, 2603.1900
Charge, Multiplicity	0, 1
Predicted log column density	10.370±2.375
Electronic energy	-224.90038

geom1179



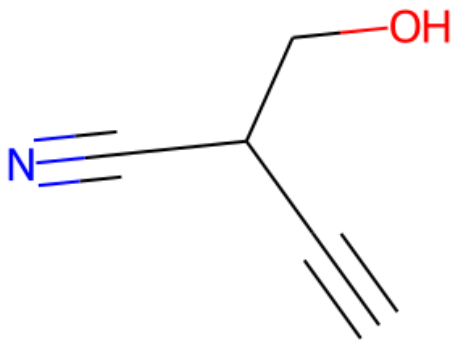
SMILES: C#CC(CC#N)OC

Nearest TMC-1 molecule (distance): C#CCC#N (5.49)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	4.6, 1.1, 0.4
A, B, C	3268.7194, 1368.5369, 1007.6640
A_s, B_s, C_s	3259.2401, 1364.5681, 1004.7418
Charge, Multiplicity	0, 1
Predicted log column density	10.394±4.913
Electronic energy	-362.60452

geom1180



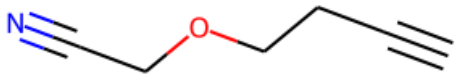
SMILES: C#CC(C#N)CO

Nearest TMC-1 molecule (distance): C#CCC#N (5.51)

Is DFT optimized?: True

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	
$\mu_{a,b,c}$	3.1, 1.4, 0.1
A, B, C	3357.0329, 2214.0049, 1400.5929
A_s, B_s, C_s	3347.2975, 2207.5842, 1396.5312
Charge, Multiplicity	0, 1
Predicted log column density	8.597±4.650
Electronic energy	-323.30633

geom1181



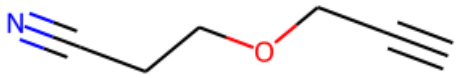
SMILES: C#CCCOCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.52)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	2-but-3-ynoxyacetonitrile
$\mu_{a,b,c}$	3.3, 2.8, 0.0
A, B, C	14471.9667, 658.0548, 636.9969
A_s, B_s, C_s	14429.9980, 656.1465, 635.1497
Charge, Multiplicity	0, 1
Predicted log column density	11.855±4.960
Electronic energy	-362.60103

geom1182



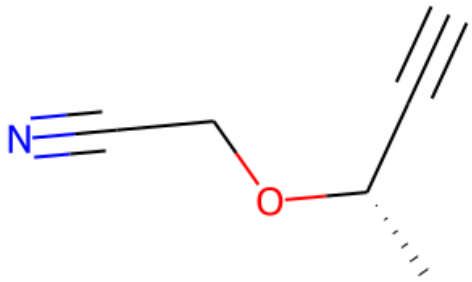
SMILES: C#CCOCCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.52)

Is DFT optimized?: False

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	3-prop-2-ynoxypropanenitrile
$\mu_{a,b,c}$	1.3, 0.5, 3.2
A, B, C	14203.5935, 636.5548, 616.3177
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.855±4.960
Electronic energy	-362.58045

geom1183



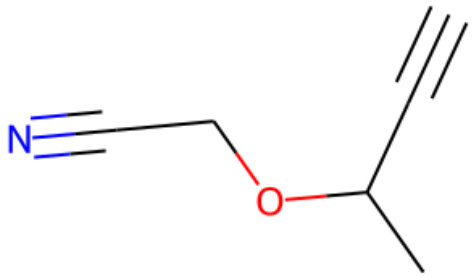
SMILES: C#C[C@H](C)OCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	3.6, 3.3, 1.5
A, B, C	4481.3398, 1013.4125, 859.1389
A_s, B_s, C_s	4468.3439, 1010.4736, 856.6474
Charge, Multiplicity	0, 1
Predicted log column density	10.452±5.203
Electronic energy	-362.59658

geom1184



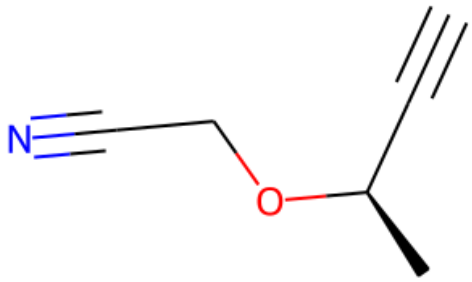
SMILES: C#CC(C)OCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	4.4, 1.0, 1.9
A, B, C	3920.6941, 1113.0340, 910.7856
A_s, B_s, C_s	3909.3241, 1109.8062, 908.1444
Charge, Multiplicity	0, 1
Predicted log column density	10.452±5.203
Electronic energy	-362.60168

geom1185



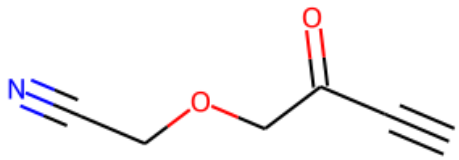
SMILES: C#C[C@@H](C)OCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.53)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	4.4, 1.0, 1.9
A, B, C	3914.2377, 1113.5524, 911.2823
A_s, B_s, C_s	3902.8864, 1110.3231, 908.6396
Charge, Multiplicity	0, 1
Predicted log column density	10.452±5.203
Electronic energy	-362.60168

geom1186



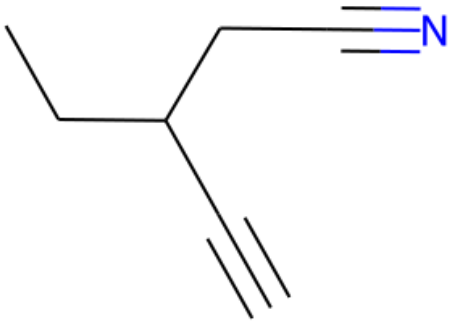
SMILES: C#CC(=O)COCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.60)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.1, 1.8, 0.6
A, B, C	3240.1744, 831.5741, 668.2397
A_s, B_s, C_s	3230.7779, 829.1626, 666.3018
Charge, Multiplicity	0, 1
Predicted log column density	11.130±5.578
Electronic energy	-436.57716

geom1187



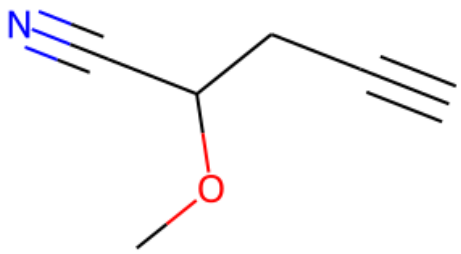
SMILES: C#CC(CC)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.61)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	
$\mu_{a,b,c}$	3.4, 1.0, 0.6
A, B, C	2990.3465, 1325.6184, 961.6664
A_s, B_s, C_s	2981.6745, 1321.7742, 958.8776
Charge, Multiplicity	0, 1
Predicted log column density	8.888±5.320
Electronic energy	-326.73169

geom1188



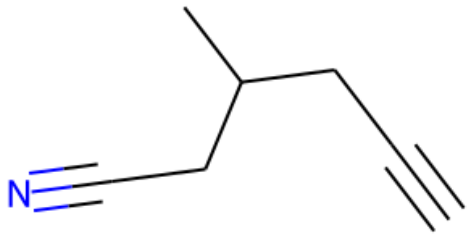
SMILES: C#CCC(C#N)OC

Nearest TMC-1 molecule (distance): C#CCC#N (5.62)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	
$\mu_{a,b,c}$	0.5, 2.9, 1.4
A, B, C	3461.8873, 1344.2531, 1033.4030
A_s, B_s, C_s	3451.8479, 1340.3548, 1030.4061
Charge, Multiplicity	0, 1
Predicted log column density	11.611±4.959
Electronic energy	-362.60284

geom1189



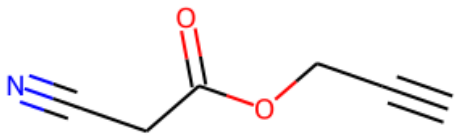
SMILES: C#CCC(C)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.65)

Is DFT optimized?: True

Property	Value
Formula	C7H9N
Molecular weight	107.156
IUPAC name	
$\mu_{a,b,c}$	3.2, 1.6, 1.2
A, B, C	6089.0899, 911.4023, 851.6564
A_s, B_s, C_s	6071.4315, 908.7592, 849.1866
Charge, Multiplicity	0, 1
Predicted log column density	10.539±4.887
Electronic energy	-326.73291

geom1190



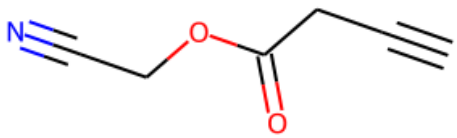
SMILES: C#CCOC(=O)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.71)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	prop-2-ynyl 2-cyanoacetate
$\mu_{a,b,c}$	4.1, 3.0, 1.9
A, B, C	4647.8832, 763.4031, 733.4668
A_s, B_s, C_s	4634.4043, 761.1892, 731.3397
Charge, Multiplicity	0, 1
Predicted log column density	11.133±4.791
Electronic energy	-436.61882

geom1191



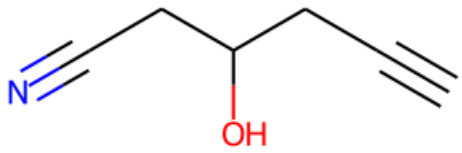
SMILES: C#CCC(=O)OCC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.71)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	cyanomethyl but-3-ynoate
$\mu_{a,b,c}$	3.1, 2.0, 1.4
A, B, C	3895.2689, 857.7251, 781.3249
A_s, B_s, C_s	3883.9727, 855.2377, 779.0591
Charge, Multiplicity	0, 1
Predicted log column density	11.133±4.791
Electronic energy	-436.61703

geom1192



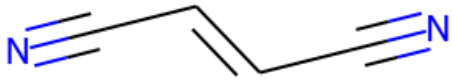
SMILES: C#CCC(O)CC#N

Nearest TMC-1 molecule (distance): C#CCC#N (5.71)

Is DFT optimized?: True

Property	Value
Formula	C6H7NO
Molecular weight	109.128
IUPAC name	3-hydroxyhex-5-ynenitrile
$\mu_{a,b,c}$	3.0, 0.6, 1.1
A, B, C	2834.8160, 1450.7547, 1142.5217
A_s, B_s, C_s	2826.5950, 1446.5475, 1139.2084
Charge, Multiplicity	0, 1
Predicted log column density	12.847±5.450
Electronic energy	-362.62420

geom1193



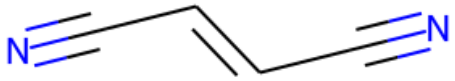
SMILES: N#CC=CC#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (5.04)

Is DFT optimized?: True

Property	Value
Formula	C4H2N2
Molecular weight	78.074
IUPAC name	but-2-enedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	46293.1656, 1484.1477, 1438.0444
A_s, B_s, C_s	46158.9154, 1479.8437, 1433.8740
Charge, Multiplicity	0, 1
Predicted log column density	11.098±1.942
Electronic energy	-262.97519

geom1194



SMILES: N#C/C=C/C#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (5.04)

Is DFT optimized?: True

Property	Value
Formula	C4H2N2
Molecular weight	78.074
IUPAC name	(E)-but-2-enedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	46293.7501, 1484.1481, 1438.0453
A_s, B_s, C_s	46159.4982, 1479.8441, 1433.8750
Charge, Multiplicity	0, 1
Predicted log column density	11.098±1.942
Electronic energy	-262.97519

geom1195

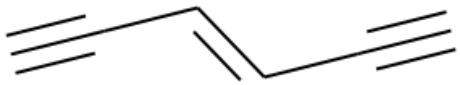
SMILES: C#CC=CC#C

Nearest TMC-1 molecule (distance): C#C / C=C / C#N (5.04)

Is DFT optimized?: True

Property	Value
Formula	C6H4
Molecular weight	76.098
IUPAC name	hex-3-en-1,5-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	46819.2456, 1451.9659, 1408.2917
A_s, B_s, C_s	46683.4698, 1447.7551, 1404.2076
Charge, Multiplicity	0, 1
Predicted log column density	11.066±2.038
Electronic energy	-230.79617

geom1196



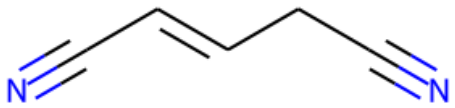
SMILES: C#C/C=C/C#C

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (5.04)

Is DFT optimized?: True

Property	Value
Formula	C6H4
Molecular weight	76.098
IUPAC name	(E)-hex-3-en-1,5-diyne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	46657.3100, 1452.2907, 1408.4503
A_s, B_s, C_s	46522.0038, 1448.0791, 1404.3658
Charge, Multiplicity	0, 1
Predicted log column density	11.066±2.038
Electronic energy	-230.79617

geom1197



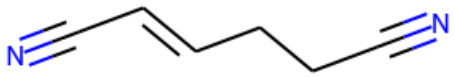
SMILES: N#CC=CCC#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (5.06)

Is DFT optimized?: True

Property	Value
Formula	C5H4N2
Molecular weight	92.101
IUPAC name	pent-2-enedinitrile
$\mu_{a,b,c}$	1.0, 4.1, 0.1
A, B, C	11377.0872, 1026.4609, 973.2088
A_s, B_s, C_s	11344.0936, 1023.4841, 970.3865
Charge, Multiplicity	0, 1
Predicted log column density	9.517±2.597
Electronic energy	-302.28148

geom1198



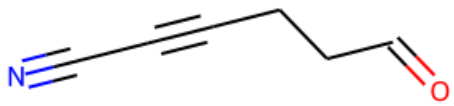
SMILES: N#CC=CCCC#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (5.76)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	hex-2-enedinitrile
$\mu_{a,b,c}$	0.5, 0.0, 0.3
A, B, C	14936.8795, 627.5223, 619.6706
A_s, B_s, C_s	14893.5625, 625.7025, 617.8736
Charge, Multiplicity	0, 1
Predicted log column density	8.356±3.430
Electronic energy	-341.58984

geom1199



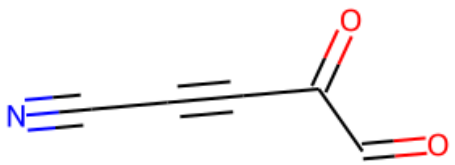
SMILES: N#CC#CCCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (5.41)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	6-oxohex-2-ynenitrile
$\mu_{a,b,c}$	3.8, 1.7, 0.0
A, B, C	15188.9200, 621.6433, 601.5939
A_s, B_s, C_s	15144.8721, 619.8405, 599.8493
Charge, Multiplicity	0, 1
Predicted log column density	6.923±3.571
Electronic energy	-361.41218

geom1200



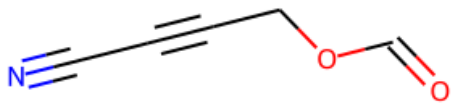
SMILES: N#CC#CC(=O)C=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (5.56)

Is DFT optimized?: True

Property	Value
Formula	C5HNO2
Molecular weight	107.068
IUPAC name	
$\mu_{a,b,c}$	2.8, 0.3, 0.0
A, B, C	4654.3492, 1004.8846, 826.4518
A_s, B_s, C_s	4640.8516, 1001.9704, 824.0551
Charge, Multiplicity	0, 1
Predicted log column density	8.983±2.940
Electronic energy	-396.07051

geom1201



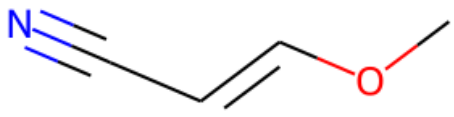
SMILES: N#CC#CCOC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (5.63)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	
$\mu_{a,b,c}$	4.1, 2.8, 0.2
A, B, C	5521.7951, 895.9045, 819.0460
A_s, B_s, C_s	5505.7819, 893.3064, 816.6708
Charge, Multiplicity	0, 1
Predicted log column density	10.579±3.839
Electronic energy	-397.31401

geom1202



SMILES: COC=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (5.80)

Is DFT optimized?: True

Property	Value
Formula	C4H5NO
Molecular weight	83.090
IUPAC name	3-methoxyprop-2-enenitrile
$\mu_{a,b,c}$	5.8, 0.4, 0.0
A, B, C	22690.6011, 1459.6643, 1383.6484
A_s, B_s, C_s	22624.7984, 1455.4313, 1379.6358
Charge, Multiplicity	0, 1
Predicted log column density	13.891±4.052
Electronic energy	-285.26688

geom1203

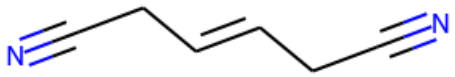
SMILES: N#CC/C=C\CC#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (6.53)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	(Z)-hex-3-enedinitrile
$\mu_{a,b,c}$	0.0, 1.4, 0.0
A, B, C	14168.2861, 676.6259, 650.9713
A_s, B_s, C_s	14127.1981, 674.6637, 649.0835
Charge, Multiplicity	0, 1
Predicted log column density	7.902±4.135
Electronic energy	-341.58117

geom1204



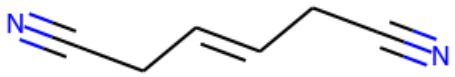
SMILES: N#CCC=CCC#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (6.53)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	hex-3-enedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	10515.9314, 675.6341, 651.5585
A_s, B_s, C_s	10485.4352, 673.6748, 649.6690
Charge, Multiplicity	0, 1
Predicted log column density	7.902±4.135
Electronic energy	-341.58585

geom1205



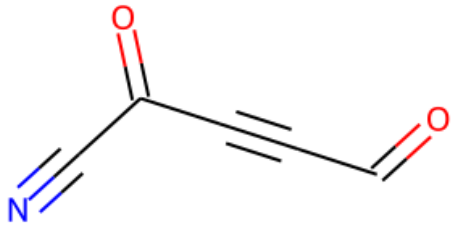
SMILES: N#CC/C=C/CC#N

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (6.53)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2
Molecular weight	106.128
IUPAC name	(E)-hex-3-enedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	10521.2938, 675.6097, 651.5280
A_s, B_s, C_s	10490.7820, 673.6505, 649.6386
Charge, Multiplicity	0, 1
Predicted log column density	7.902±4.135
Electronic energy	-341.58584

geom1206



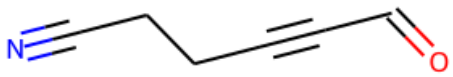
SMILES: N#CC(=O)C#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (5.85)

Is DFT optimized?: True

Property	Value
Formula	C5HNO2
Molecular weight	107.068
IUPAC name	
$\mu_{a,b,c}$	1.7, 0.6, 2.2
A, B, C	4908.8865, 909.3662, 790.5866
A_s, B_s, C_s	4894.6508, 906.7290, 788.2939
Charge, Multiplicity	0, 1
Predicted log column density	8.254±3.521
Electronic energy	-396.06160

geom1207



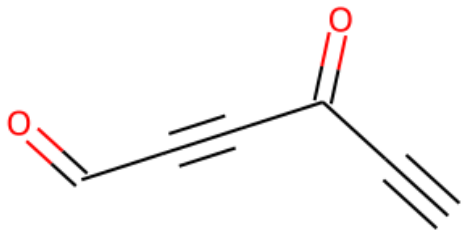
SMILES: N#CCCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#N (5.77)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.3, 2.2, 0.1
A, B, C	18985.5387, 583.6152, 570.2214
A_s, B_s, C_s	18930.4806, 581.9227, 568.5678
Charge, Multiplicity	0, 1
Predicted log column density	8.137±3.658
Electronic energy	-361.40750

geom1208



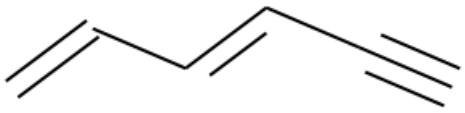
SMILES: C#CC(=O)C#CC=O

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (5.69)

Is DFT optimized?: True

Property	Value
Formula	C6H2O2
Molecular weight	106.080
IUPAC name	
$\mu_{a,b,c}$	1.2, 2.6, 2.1
A, B, C	4768.3636, 915.4244, 790.5665
A_s, B_s, C_s	4754.5353, 912.7696, 788.2738
Charge, Multiplicity	0, 1
Predicted log column density	8.788±3.928
Electronic energy	-379.97941

geom1209



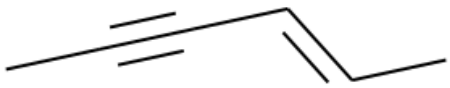
SMILES: C#CC=CC=C

Nearest TMC-1 molecule (distance): C=CC#C (5.66)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	hexa-1,3-dien-5-yne
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	27045.4865, 1418.2912, 1347.6212
A_s, B_s, C_s	26967.0545, 1414.1781, 1343.7131
Charge, Multiplicity	0, 1
Predicted log column density	11.694±3.292
Electronic energy	-232.05727

geom1210



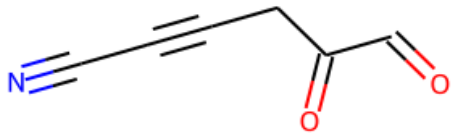
SMILES: CC#CC=CC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (6.48)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	hex-2-en-4-yne
$\mu_{a,b,c}$	0.0, 0.3, 0.0
A, B, C	27829.9324, 1194.9328, 1162.3233
A_s, B_s, C_s	27749.2256, 1191.4675, 1158.9526
Charge, Multiplicity	0, 1
Predicted log column density	13.001±2.334
Electronic energy	-233.30033

geom1211



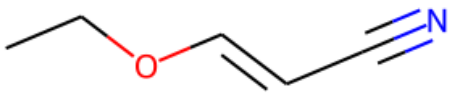
SMILES: N#CC#CCC(=O)C=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.32)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	4.5, 1.2, 0.0
A, B, C	6703.6711, 602.1719, 554.3955
A_s, B_s, C_s	6684.2304, 600.4256, 552.7877
Charge, Multiplicity	0, 1
Predicted log column density	9.551±3.640
Electronic energy	-435.38665

geom1212



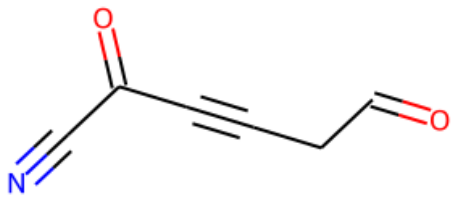
SMILES: CCOC=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (6.43)

Is DFT optimized?: True

Property	Value
Formula	C5H7NO
Molecular weight	97.117
IUPAC name	3-ethoxyprop-2-enenitrile
$\mu_{a,b,c}$	6.1, 0.4, 0.0
A, B, C	19301.4340, 911.6891, 880.2580
A_s, B_s, C_s	19245.4598, 909.0452, 877.7052
Charge, Multiplicity	0, 1
Predicted log column density	14.648±5.530
Electronic energy	-324.57574

geom1213



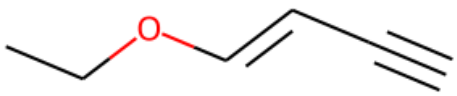
SMILES: N#CC(=O)C#CCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.28)

Is DFT optimized?: False

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	4.1, 0.9, 5.4
A, B, C	3082.3033, 753.1987, 613.1212
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	5.769±4.440
Electronic energy	-435.35410

geom1214



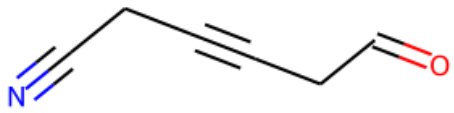
SMILES: C#CC=COCC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.82)

Is DFT optimized?: True

Property	Value
Formula	C6H8O
Molecular weight	96.129
IUPAC name	1-ethoxybut-1-en-3-yne
$\mu_{a,b,c}$	2.3, 1.5, 0.0
A, B, C	19438.9553, 905.1928, 874.7935
A_s, B_s, C_s	19382.5823, 902.5677, 872.2566
Charge, Multiplicity	0, 1
Predicted log column density	14.635±5.683
Electronic energy	-308.47954

geom1215



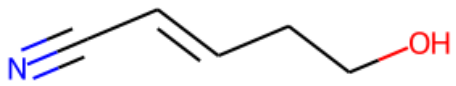
SMILES: N#CCC#CCC=O

Nearest TMC-1 molecule (distance): CC#CC#N (5.99)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.2, 2.3, 0.4
A, B, C	9199.7173, 635.5592, 621.3588
A_s, B_s, C_s	9173.0382, 633.7161, 619.5569
Charge, Multiplicity	0, 1
Predicted log column density	6.092±4.156
Electronic energy	-361.40497

geom1216



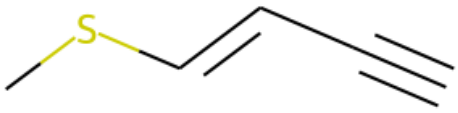
SMILES: N#CC=CCCO

Nearest TMC-1 molecule (distance): C=CC#N (6.43)

Is DFT optimized?: False

Property	Value
Formula	C5H7NO
Molecular weight	97.117
IUPAC name	5-hydroxypent-2-enenitrile
$\mu_{a,b,c}$	0.9, 1.6, 3.8
A, B, C	7051.8205, 1068.5474, 990.8471
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.060±3.683
Electronic energy	-324.55119

geom1217



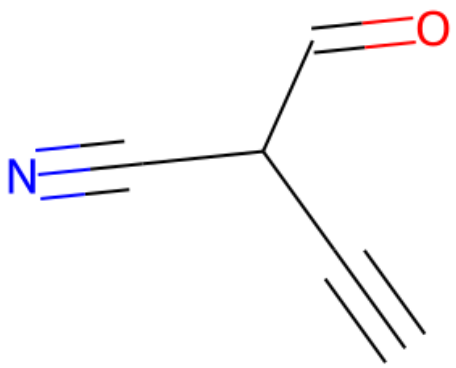
SMILES: C#CC=CSC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (6.00)

Is DFT optimized?: True

Property	Value
Formula	C5H6S
Molecular weight	98.170
IUPAC name	1-methylsulfanylbut-1-en-3-yne
$\mu_{a,b,c}$	1.3, 1.6, 0.0
A, B, C	12583.8046, 1127.1430, 1041.3998
A_s, B_s, C_s	12547.3115, 1123.8742, 1038.3797
Charge, Multiplicity	0, 1
Predicted log column density	13.917±5.739
Electronic energy	-592.15323

geom1218



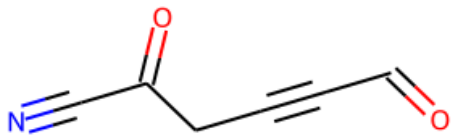
SMILES: C#CC(C#N)C=O

Nearest TMC-1 molecule (distance): [C]#CC#N (5.83)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO
Molecular weight	93.085
IUPAC name	
$\mu_{a,b,c}$	0.3, 3.1, 0.2
A, B, C	2781.3097, 2689.5242, 1445.4516
A_s, B_s, C_s	2773.2439, 2681.7246, 1441.2598
Charge, Multiplicity	0, 1
Predicted log column density	8.253±4.120
Electronic energy	-322.08601

geom1219



SMILES: N#CC(=O)CC#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.24)

Is DFT optimized?: False

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	3.8, 1.1, 0.2
A, B, C	5324.6610, 600.7318, 587.5643
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	8.987±3.818
Electronic energy	-435.37173

geom1220

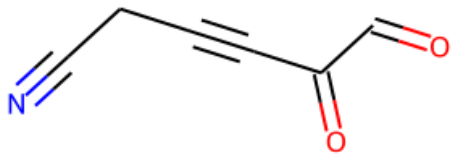
SMILES: O=CC#CCC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (6.06)

Is DFT optimized?: True

Property	Value
Formula	C5H4O2
Molecular weight	96.085
IUPAC name	pent-2-ynedial
$\mu_{a,b,c}$	3.7, 2.0, 0.6
A, B, C	9522.5203, 1051.3157, 955.3325
A_s, B_s, C_s	9494.9050, 1048.2669, 952.5620
Charge, Multiplicity	0, 1
Predicted log column density	6.616±3.735
Electronic energy	-343.17782

geom1221



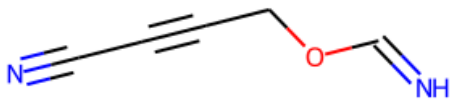
SMILES: N#CCC#CC(=O)C=O

Nearest TMC-1 molecule (distance): CC#CC#N (6.31)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	0.9, 1.6, 2.8
A, B, C	3497.3354, 688.8064, 623.3655
A_s, B_s, C_s	3487.1931, 686.8089, 621.5578
Charge, Multiplicity	0, 1
Predicted log column density	7.007±3.598
Electronic energy	-435.37814

geom1222



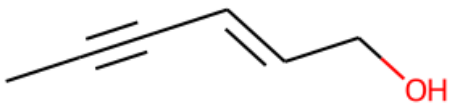
SMILES: N#CC#CCOC=N

Nearest TMC-1 molecule (distance): C=CC#CC#N (5.87)

Is DFT optimized?: True

Property	Value
Formula	C5H4N2O
Molecular weight	108.100
IUPAC name	
$\mu_{a,b,c}$	1.8, 2.9, 0.0
A, B, C	12639.3518, 638.0604, 609.7421
A_s, B_s, C_s	12602.6977, 636.2100, 607.9739
Charge, Multiplicity	0, 1
Predicted log column density	13.374±4.726
Electronic energy	-377.42075

geom1223



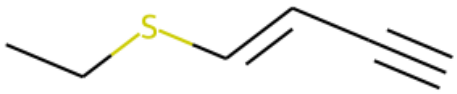
SMILES: CC#CC=CCO

Nearest TMC-1 molecule (distance): [C]#C[C]=O (6.92)

Is DFT optimized?: True

Property	Value
Formula	C6H8O
Molecular weight	96.129
IUPAC name	hex-2-en-4-yn-1-ol
$\mu_{a,b,c}$	2.2, 0.4, 0.7
A, B, C	14477.2051, 797.8004, 781.0114
A_s, B_s, C_s	14435.2212, 795.4867, 778.7465
Charge, Multiplicity	0, 1
Predicted log column density	9.709±3.239
Electronic energy	-308.48958

geom1224



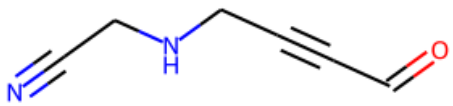
SMILES: C#CC=CSCC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (6.51)

Is DFT optimized?: True

Property	Value
Formula	C6H8S
Molecular weight	112.197
IUPAC name	1-ethylsulfanylbut-1-en-3-yne
$\mu_{a,b,c}$	1.5, 1.6, 0.1
A, B, C	11013.6097, 754.3859, 715.2610
A_s, B_s, C_s	10981.6702, 752.1982, 713.1868
Charge, Multiplicity	0, 1
Predicted log column density	11.968±5.476
Electronic energy	-631.45749

geom1225



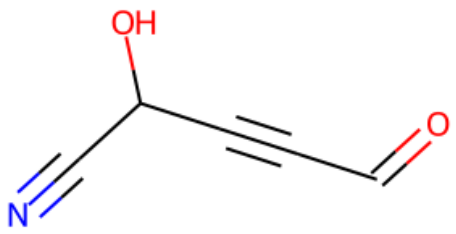
SMILES: N#CCNCC#CC=O

Nearest TMC-1 molecule (distance): CC#CC#N (6.19)

Is DFT optimized?: False

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	0.9, 2.9, 2.6
A, B, C	5876.6432, 441.9621, 420.4558
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.652±4.866
Electronic energy	-416.68263

geom1226



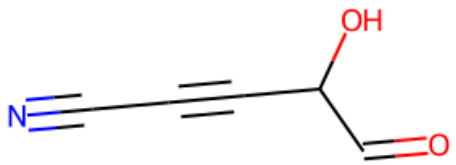
SMILES: N#CC(O)C#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (5.98)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	
$\mu_{a,b,c}$	0.2, 3.2, 1.3
A, B, C	4376.8015, 914.1590, 784.4361
A_s, B_s, C_s	4364.1088, 911.5080, 782.1612
Charge, Multiplicity	0, 1
Predicted log column density	8.515±4.419
Electronic energy	-397.27781

geom1227



SMILES: N#CC#CC(O)C=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.18)

Is DFT optimized?: True

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	
$\mu_{a,b,c}$	3.0, 0.8, 2.2
A, B, C	5968.9464, 857.0330, 787.9023
A_s, B_s, C_s	5951.6365, 854.5476, 785.6174
Charge, Multiplicity	0, 1
Predicted log column density	8.555±4.511
Electronic energy	-397.29065

geom1228

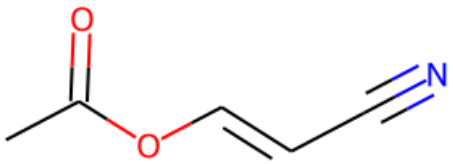
SMILES: O=CC#CC=O

Nearest TMC-1 molecule (distance): [C]#C[C]=O (5.97)

Is DFT optimized?: True

Property	Value
Formula	C4H2O2
Molecular weight	82.058
IUPAC name	but-2-ynedial
$\mu_{a,b,c}$	0.0, 2.8, 0.0
A, B, C	27297.5498, 1326.2976, 1318.6095
A_s, B_s, C_s	27218.3870, 1322.4514, 1314.7856
Charge, Multiplicity	0, 1
Predicted log column density	9.093±3.075
Electronic energy	-303.86682

geom1229



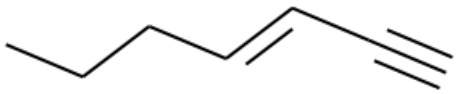
SMILES: CC(=O)OC=CC#N

Nearest TMC-1 molecule (distance): C=C=CC#N (7.00)

Is DFT optimized?: False

Property	Value
Formula	C5H5NO2
Molecular weight	111.100
IUPAC name	2-cyanoethenyl acetate
$\mu_{a,b,c}$	0.3, 0.8, 5.7
A, B, C	7928.0150, 797.6577, 728.1426
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.935±4.971
Electronic energy	-398.56259

geom1230



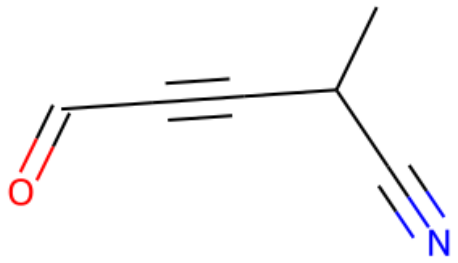
SMILES: C#CC=CCCC

Nearest TMC-1 molecule (distance): [C]#C[C]=O (6.08)

Is DFT optimized?: True

Property	Value
Formula	C7H10
Molecular weight	94.157
IUPAC name	hept-3-en-1-yne
$\mu_{a,b,c}$	1.2, 0.0, 0.1
A, B, C	14278.7711, 854.5737, 842.1535
A_s, B_s, C_s	14237.3627, 852.0954, 839.7113
Charge, Multiplicity	0, 1
Predicted log column density	9.047±3.843
Electronic energy	-272.59424

geom1231



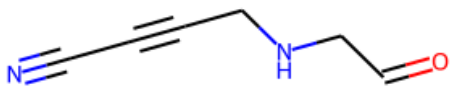
SMILES: CC(C#N)C#CC=O

Nearest TMC-1 molecule (distance): CC#CC#N (6.05)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.7, 1.8, 0.8
A, B, C	4783.8460, 881.4960, 766.5797
A_s, B_s, C_s	4769.9728, 878.9397, 764.3567
Charge, Multiplicity	0, 1
Predicted log column density	8.414±4.350
Electronic energy	-361.40103

geom1232



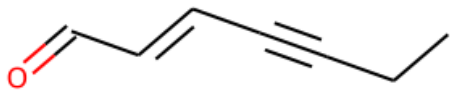
SMILES: N#CC#CCNCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.01)

Is DFT optimized?: True

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	2.0, 2.6, 0.1
A, B, C	8590.4722, 435.2538, 418.2789
A_s, B_s, C_s	8565.5599, 433.9916, 417.0659
Charge, Multiplicity	0, 1
Predicted log column density	9.436±5.160
Electronic energy	-416.72827

geom1233



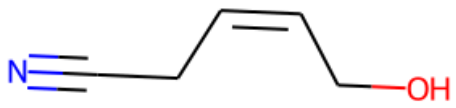
SMILES: CCC#CC=CC=O

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (7.14)

Is DFT optimized?: True

Property	Value
Formula	C7H8O
Molecular weight	108.140
IUPAC name	hept-2-en-4-ynal
$\mu_{a,b,c}$	4.8, 1.1, 0.2
A, B, C	15250.9766, 552.3202, 537.5473
A_s, B_s, C_s	15206.7488, 550.7184, 535.9884
Charge, Multiplicity	0, 1
Predicted log column density	8.792±3.844
Electronic energy	-346.58830

geom1234



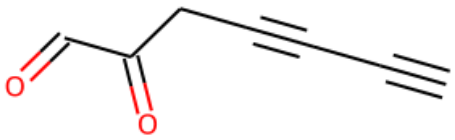
SMILES: N#CC/C=C\CO

Nearest TMC-1 molecule (distance): C=CC#N (6.95)

Is DFT optimized?: True

Property	Value
Formula	C5H7NO
Molecular weight	97.117
IUPAC name	(Z)-5-hydroxypent-3-enenitrile
$\mu_{a,b,c}$	4.4, 1.3, 1.9
A, B, C	6181.4652, 1293.9990, 1179.9770
A_s, B_s, C_s	6163.5389, 1290.2464, 1176.5551
Charge, Multiplicity	0, 1
Predicted log column density	8.234±3.896
Electronic energy	-324.56815

geom1235



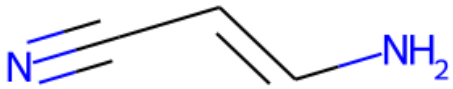
SMILES: C#CC#CCC(=O)C=O

Nearest TMC-1 molecule (distance): CC#CC#C (6.37)

Is DFT optimized?: True

Property	Value
Formula	C7H4O2
Molecular weight	120.107
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.6, 0.0
A, B, C	6687.3624, 601.4997, 553.7084
A_s, B_s, C_s	6667.9690, 599.7553, 552.1026
Charge, Multiplicity	0, 1
Predicted log column density	9.679±3.623
Electronic energy	-419.29970

geom1236



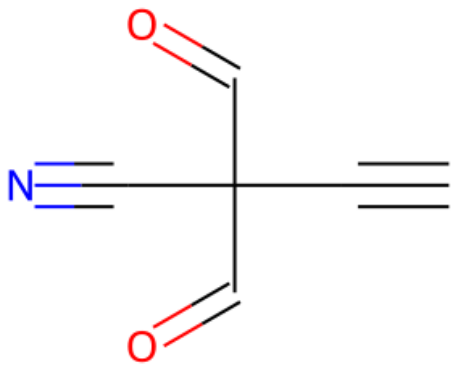
SMILES: N#CC=CN

Nearest TMC-1 molecule (distance): C=C=CC#N (5.66)

Is DFT optimized?: True

Property	Value
Formula	C3H4N2
Molecular weight	68.079
IUPAC name	3-aminoprop-2-enenitrile
$\mu_{a,b,c}$	6.9, 0.4, 0.0
A, B, C	42123.2795, 2371.9571, 2245.5126
A_s, B_s, C_s	42001.1219, 2365.0784, 2239.0006
Charge, Multiplicity	0, 1
Predicted log column density	13.155±4.164
Electronic energy	-226.12188

geom1237



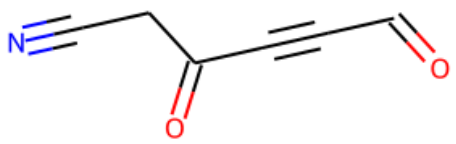
SMILES: C#CC(C#N)(C=O)C=O

Nearest TMC-1 molecule (distance): C#C/C=C/C#N (7.16)

Is DFT optimized?: False

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	1.6, 0.4, 2.4
A, B, C	1717.1690, 1466.2356, 1295.9075
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.423±6.116
Electronic energy	-435.33356

geom1238



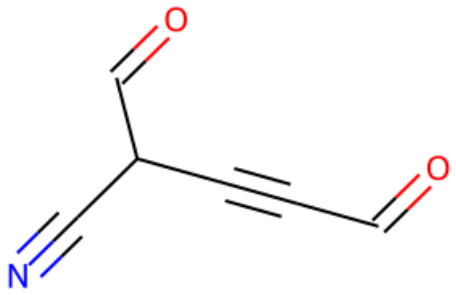
SMILES: N#CCC(=O)C#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.47)

Is DFT optimized?: True

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	1.4, 0.7, 0.2
A, B, C	2345.3428, 914.6311, 690.8210
A_s, B_s, C_s	2338.5413, 911.9787, 688.8176
Charge, Multiplicity	0, 1
Predicted log column density	8.649±4.132
Electronic energy	-435.38241

geom1239



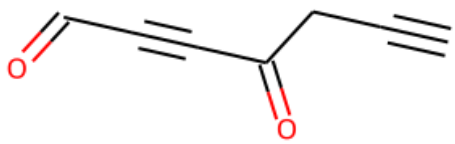
SMILES: N#CC(C#CC=O)C=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (7.12)

Is DFT optimized?: False

Property	Value
Formula	C6H3NO2
Molecular weight	121.095
IUPAC name	
$\mu_{a,b,c}$	1.7, 2.3, 1.7
A, B, C	2389.9143, 826.5680, 642.9898
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	6.127±4.582
Electronic energy	-435.32551

geom1240



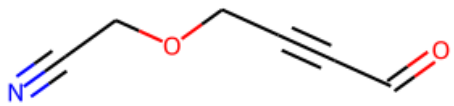
SMILES: C#CCC(=O)C#CC=O

Nearest TMC-1 molecule (distance): CC#CC#C (6.41)

Is DFT optimized?: True

Property	Value
Formula	C7H4O2
Molecular weight	120.107
IUPAC name	
$\mu_{a,b,c}$	1.5, 2.2, 0.9
A, B, C	2324.1242, 899.6869, 685.5699
A_s, B_s, C_s	2317.3842, 897.0778, 683.5818
Charge, Multiplicity	0, 1
Predicted log column density	9.964±3.805
Electronic energy	-419.29064

geom1241



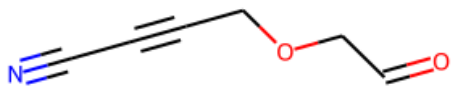
SMILES: N#CCOCC#CC=O

Nearest TMC-1 molecule (distance): C#CC#CC#N (6.88)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.3, 7.2, 0.0
A, B, C	4817.9126, 508.4670, 462.6179
A_s, B_s, C_s	4803.9407, 506.9924, 461.2763
Charge, Multiplicity	0, 1
Predicted log column density	9.768±4.645
Electronic energy	-436.57379

geom1242



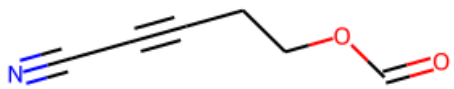
SMILES: N#CC#CCOCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.22)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	2.0, 3.2, 0.0
A, B, C	8723.3193, 449.7862, 430.0553
A_s, B_s, C_s	8698.0217, 448.4818, 428.8081
Charge, Multiplicity	0, 1
Predicted log column density	8.746±4.880
Electronic energy	-436.58196

geom1243



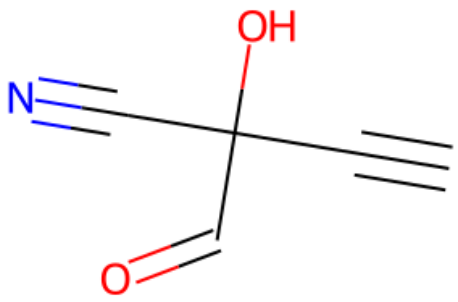
SMILES: N#CC#CCCOC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.31)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	3.6, 2.1, 1.0
A, B, C	4266.6010, 642.3115, 609.2277
A_s, B_s, C_s	4254.2279, 640.4488, 607.4609
Charge, Multiplicity	0, 1
Predicted log column density	9.620±4.499
Electronic energy	-436.62704

geom1244



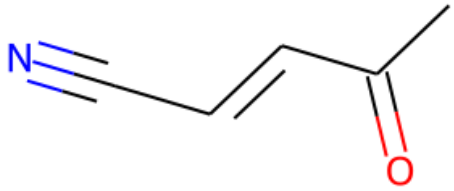
SMILES: C#CC(O)(C#N)C=O

Nearest TMC-1 molecule (distance): [C]#CC#N (6.93)

Is DFT optimized?: False

Property	Value
Formula	C5H3NO2
Molecular weight	109.084
IUPAC name	
$\mu_{a,b,c}$	2.3, 1.3, 1.5
A, B, C	2249.9852, 1877.8683, 1514.4769
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	13.156±5.747
Electronic energy	-397.24658

geom1245



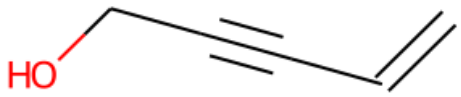
SMILES: CC(=O)C=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (6.61)

Is DFT optimized?: False

Property	Value
Formula	C5H5NO
Molecular weight	95.101
IUPAC name	4-oxopent-2-enenitrile
$\mu_{a,b,c}$	0.1, 0.6, 3.6
A, B, C	9180.4753, 1220.0112, 1084.4022
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.283±3.943
Electronic energy	-323.37259

geom1246



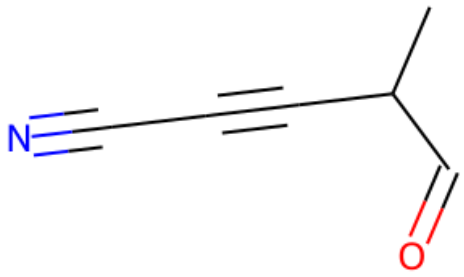
SMILES: C=CC#CCO

Nearest TMC-1 molecule (distance): C=CC#C (5.41)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	pent-4-en-2-yn-1-ol
$\mu_{a,b,c}$	1.4, 0.3, 1.2
A, B, C	13808.8612, 1394.5855, 1282.4009
A_s, B_s, C_s	13768.8155, 1390.5412, 1278.6820
Charge, Multiplicity	0, 1
Predicted log column density	10.092±3.510
Electronic energy	-269.17671

geom1247



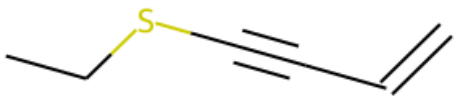
SMILES: CC(C#CC#N)C=O

Nearest TMC-1 molecule (distance): CC#CC#N (6.02)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	2.8, 1.3, 1.8
A, B, C	5788.4104, 837.5854, 761.9822
A_s, B_s, C_s	5771.6240, 835.1564, 759.7724
Charge, Multiplicity	0, 1
Predicted log column density	8.442±4.038
Electronic energy	-361.40817

geom1248



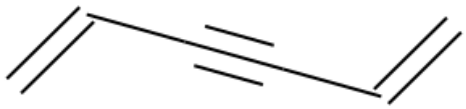
SMILES: C=CC#CSCC

Nearest TMC-1 molecule (distance): C=C=CC#N (6.09)

Is DFT optimized?: False

Property	Value
Formula	C6H8S
Molecular weight	112.197
IUPAC name	4-ethylsulfanylbut-1-en-3-yne
$\mu_{a,b,c}$	1.6, 0.1, 0.4
A, B, C	8988.7488, 708.9492, 683.4743
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.212±5.282
Electronic energy	-631.44040

geom1249



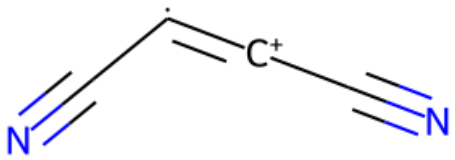
SMILES: C=CC#CC=C

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.22)

Is DFT optimized?: True

Property	Value
Formula	C6H6
Molecular weight	78.114
IUPAC name	hexa-1,5-dien-3-yne
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	26483.4293, 1356.1388, 1290.4320
A_s, B_s, C_s	26406.6274, 1352.2060, 1286.6898
Charge, Multiplicity	0, 1
Predicted log column density	10.695±2.259
Electronic energy	-232.05823

geom1250



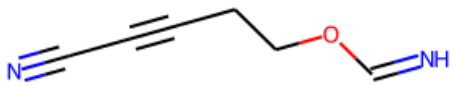
SMILES: N#C[C]=[C+]C#N

Nearest TMC-1 molecule (distance): N#CC#[NH+] (5.10)

Is DFT optimized?: True

Property	Value
Formula	C4N2+
Molecular weight	76.058
IUPAC name	but-2-enedinitrile
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	39761652381212.7734, 1336.5666, 1336.5666
A_s, B_s, C_s	39646343589307.2578, 1332.6906, 1332.6906
Charge, Multiplicity	1, 2
Predicted log column density	11.973±1.777
Electronic energy	-261.28423

geom1251



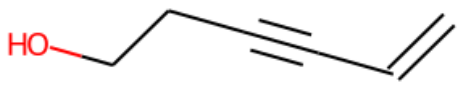
SMILES: N#CC#CCCOC=N

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.47)

Is DFT optimized?: False

Property	Value
Formula	C6H6N2O
Molecular weight	122.127
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.7, 1.4
A, B, C	11718.7615, 419.9924, 407.5184
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.427±5.279
Electronic energy	-416.71488

geom1252



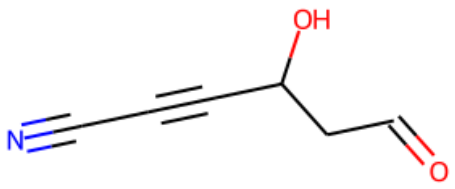
SMILES: C=CC#CCCO

Nearest TMC-1 molecule (distance): C=CC#C (6.15)

Is DFT optimized?: True

Property	Value
Formula	C6H8O
Molecular weight	96.129
IUPAC name	hex-5-en-3-yn-1-ol
$\mu_{a,b,c}$	1.3, 1.0, 0.7
A, B, C	7850.6868, 1033.2992, 949.6256
A_s, B_s, C_s	7827.9198, 1030.3026, 946.8717
Charge, Multiplicity	0, 1
Predicted log column density	9.629±4.127
Electronic energy	-308.48639

geom1253



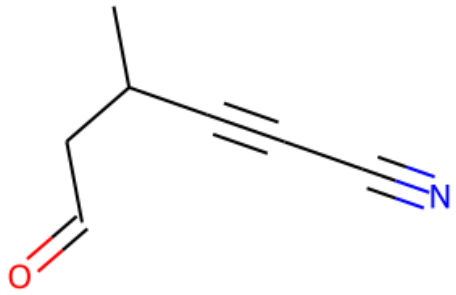
SMILES: N#CC#CC(O)CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.50)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	4.9, 0.1, 3.5
A, B, C	3027.0126, 829.4200, 750.8237
A_s, B_s, C_s	3018.2342, 827.0147, 748.6463
Charge, Multiplicity	0, 1
Predicted log column density	6.734±5.205
Electronic energy	-436.60158

geom1254



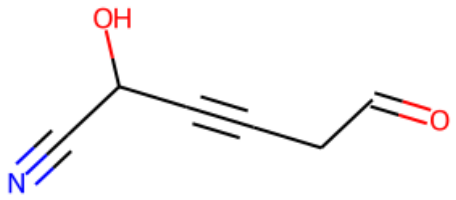
SMILES: CC(C#CC#N)CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.54)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	2.4, 3.8, 0.3
A, B, C	2359.2939, 788.0834, 608.0939
A_s, B_s, C_s	2352.4520, 785.7979, 606.3305
Charge, Multiplicity	0, 1
Predicted log column density	7.686±4.930
Electronic energy	-400.71369

geom1255



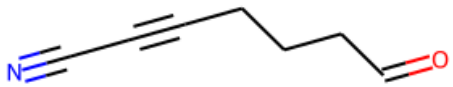
SMILES: N#CC(O)C#CCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.60)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.5, 2.6, 0.8
A, B, C	3564.4076, 623.1209, 545.6761
A_s, B_s, C_s	3554.0708, 621.3138, 544.0936
Charge, Multiplicity	0, 1
Predicted log column density	6.029±5.383
Electronic energy	-436.58909

geom1256



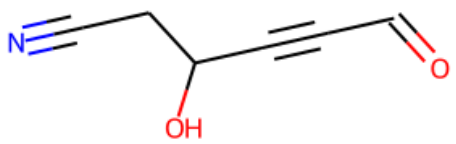
SMILES: N#CC#CCCCC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.61)

Is DFT optimized?: True

Property	Value
Formula	C7H7NO
Molecular weight	121.139
IUPAC name	
$\mu_{a,b,c}$	5.0, 4.7, 0.0
A, B, C	5294.0589, 482.8807, 446.1524
A_s, B_s, C_s	5278.7061, 481.4804, 444.8585
Charge, Multiplicity	0, 1
Predicted log column density	5.870±4.258
Electronic energy	-400.71551

geom1257



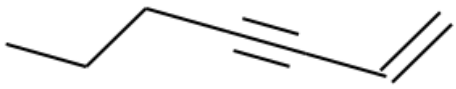
SMILES: N#CCC(O)C#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.62)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	1.5, 2.1, 1.0
A, B, C	2672.4606, 814.9488, 705.6412
A_s, B_s, C_s	2664.7104, 812.5854, 703.5948
Charge, Multiplicity	0, 1
Predicted log column density	8.227±4.892
Electronic energy	-436.59709

geom1258



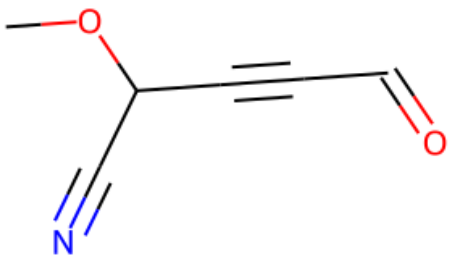
SMILES: C=CC#CCCC

Nearest TMC-1 molecule (distance): C=CC#C (5.89)

Is DFT optimized?: True

Property	Value
Formula	C7H10
Molecular weight	94.157
IUPAC name	hept-1-en-3-yne
$\mu_{a,b,c}$	0.7, 0.1, 0.0
A, B, C	10432.4499, 868.6906, 814.0481
A_s, B_s, C_s	10402.1958, 866.1714, 811.6874
Charge, Multiplicity	0, 1
Predicted log column density	9.663±3.728
Electronic energy	-272.59854

geom1259



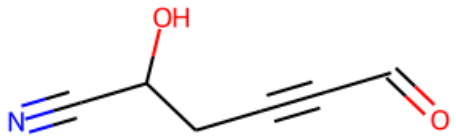
SMILES: COC(C#N)C#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.65)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	1.9, 0.8, 2.3
A, B, C	3190.0112, 735.4214, 613.1677
A_s, B_s, C_s	3180.7602, 733.2887, 611.3895
Charge, Multiplicity	0, 1
Predicted log column density	9.201±4.888
Electronic energy	-436.57025

geom1260



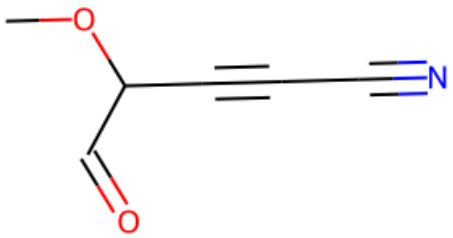
SMILES: N#CC(O)CC#CC=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.65)

Is DFT optimized?: False

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	0.5, 2.6, 0.1
A, B, C	6261.2030, 553.1119, 523.0022
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	8.433±5.000
Electronic energy	-436.55219

geom1261



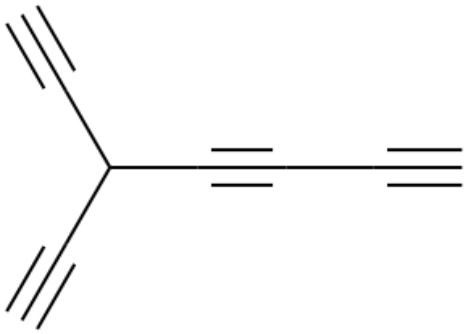
SMILES: COC(C#CC#N)C=O

Nearest TMC-1 molecule (distance): C=CC#CC#N (6.66)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO2
Molecular weight	123.111
IUPAC name	
$\mu_{a,b,c}$	3.6, 3.1, 0.5
A, B, C	2221.7335, 907.3030, 664.6009
A_s, B_s, C_s	2215.2905, 904.6719, 662.6736
Charge, Multiplicity	0, 1
Predicted log column density	10.012±4.668
Electronic energy	-436.58079

geom1262



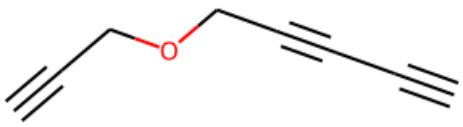
SMILES: C#CC#CC(C#C)C#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (7.14)

Is DFT optimized?: True

Property	Value
Formula	C9H4
Molecular weight	112.131
IUPAC name	
$\mu_{a,b,c}$	0.2, 0.0, 0.2
A, B, C	2676.5552, 846.9863, 667.6583
A_s, B_s, C_s	2668.7932, 844.5300, 665.7221
Charge, Multiplicity	0, 1
Predicted log column density	9.142±4.490
Electronic energy	-344.93847

geom1263



SMILES: C#CC#CCOCC#C

Nearest TMC-1 molecule (distance): [C]#CC#CC#C (6.40)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	
$\mu_{a,b,c}$	0.6, 1.8, 0.0
A, B, C	6481.8173, 495.7702, 463.2333
A_s, B_s, C_s	6463.0200, 494.3325, 461.8899
Charge, Multiplicity	0, 1
Predicted log column density	12.530±4.943
Electronic energy	-383.31916

geom1264

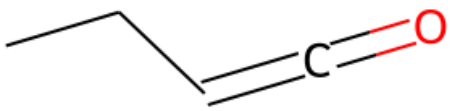
SMILES: C=C=C=C=[C+]C#CC

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (5.23)

Is DFT optimized?: True

Property	Value
Formula	C8H5+
Molecular weight	101.128
IUPAC name	
$\mu_{a,b,c}$	2.2, 0.1, 0.1
A, B, C	101766.3809, 519.7138, 518.7524
A_s, B_s, C_s	101471.2584, 518.2067, 517.2480
Charge, Multiplicity	1, 1
Predicted log column density	11.396±1.968
Electronic energy	-307.25500

geom1265



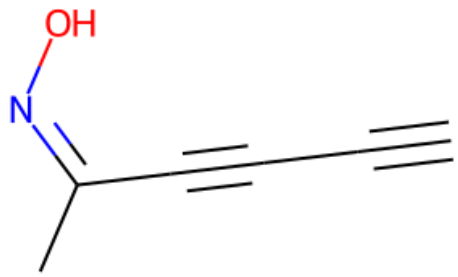
SMILES: CCC=C=O

Nearest TMC-1 molecule (distance): C=C=O (4.00)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	
$\mu_{a,b,c}$	2.0, 0.6, 0.1
A, B, C	19111.1750, 2322.0903, 2292.3986
A_s, B_s, C_s	19055.7525, 2315.3562, 2285.7506
Charge, Multiplicity	0, 1
Predicted log column density	10.127±3.185
Electronic energy	-231.15640

geom1266



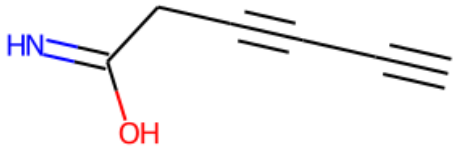
SMILES: C#CC#CC(C)=NO

Nearest TMC-1 molecule (distance): [C]#CC#[C]=O (5.80)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	0.5, 0.7, 0.0
A, B, C	7963.7401, 792.7000, 724.1745
A_s, B_s, C_s	7940.6453, 790.4011, 722.0744
Charge, Multiplicity	0, 1
Predicted log column density	6.936±5.006
Electronic energy	-361.31004

geom1267



SMILES: C#CC#CCC(=N)O

Nearest TMC-1 molecule (distance): C#CC#C[C+]=O (5.96)

Is DFT optimized?: True

Property	Value
Formula	C6H5NO
Molecular weight	107.112
IUPAC name	
$\mu_{a,b,c}$	3.4, 2.6, 0.9
A, B, C	7448.8852, 825.2573, 761.9696
A_s, B_s, C_s	7427.2834, 822.8641, 759.7599
Charge, Multiplicity	0, 1
Predicted log column density	12.214±4.236
Electronic energy	-361.35411

geom1268

SMILES: N=[SiH+]

Nearest TMC-1 molecule (distance): C=[N] (1.67)

Is DFT optimized?: True

Property	Value
Formula	H2NSi+
Molecular weight	44.109
IUPAC name	iminosilanylium
$\mu_{a,b,c}$	2.8, 0.0, 0.0
A, B, C	9815841355.7780, 17402.1748, 17402.1439
A_s, B_s, C_s	9787375415.8462, 17351.7085, 17351.6777
Charge, Multiplicity	1, 1
Predicted log column density	13.527±1.815
Electronic energy	-345.01549

geom1269

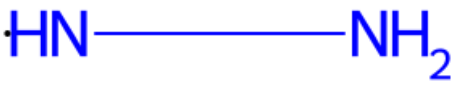
SMILES: C[NH]

Nearest TMC-1 molecule (distance): C=[N] (1.88)

Is DFT optimized?: True

Property	Value
Formula	CH4N
Molecular weight	30.050
IUPAC name	methanamine
$\mu_{a,b,c}$	1.5, 1.8, 0.0
A, B, C	124324.6983, 25438.3846, 24305.0461
A_s, B_s, C_s	123964.1566, 25364.6132, 24234.5614
Charge, Multiplicity	0, 2
Predicted log column density	13.812±1.896
Electronic energy	-95.16033

geom1270



SMILES: [NH]N

Nearest TMC-1 molecule (distance): C=[N] (2.08)

Is DFT optimized?: True

Property	Value
Formula	H3N2
Molecular weight	31.038
IUPAC name	hydrazine
$\mu_{a,b,c}$	2.2, 1.7, 0.8
A, B, C	203596.5253, 30731.8031, 27138.6384
A_s, B_s, C_s	203006.0954, 30642.6808, 27059.9364
Charge, Multiplicity	0, 2
Predicted log column density	13.555±2.050
Electronic energy	-111.19333

geom1271

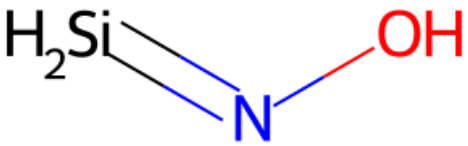
SMILES: N=N

Nearest TMC-1 molecule (distance): C=[N] (2.19)

Is DFT optimized?: True

Property	Value
Formula	H2N2
Molecular weight	30.030
IUPAC name	diazene
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	304076.5988, 39624.6938, 35056.4368
A_s, B_s, C_s	303194.7766, 39509.7822, 34954.7731
Charge, Multiplicity	0, 1
Predicted log column density	14.406±2.630
Electronic energy	-110.60529

geom1272



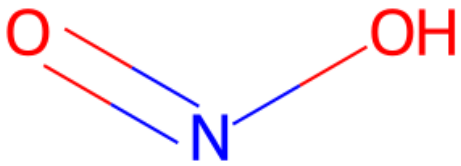
SMILES: ON=[SiH2]

Nearest TMC-1 molecule (distance): C#N[O] (1.80)

Is DFT optimized?: True

Property	Value
Formula	H3NOSi
Molecular weight	61.116
IUPAC name	hydroxyiminosilane
$\mu_{a,b,c}$	1.1, 0.4, 0.0
A, B, C	55491.3196, 6009.0515, 5421.9257
A_s, B_s, C_s	55330.3947, 5991.6252, 5406.2022
Charge, Multiplicity	0, 1
Predicted log column density	9.909±2.569
Electronic energy	-421.09527

geom1273



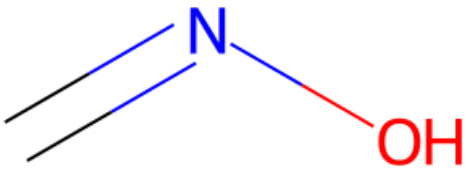
SMILES: O=NO

Nearest TMC-1 molecule (distance): C#N[O] (2.98)

Is DFT optimized?: True

Property	Value
Formula	HNO2
Molecular weight	47.013
IUPAC name	nitrous acid
$\mu_{a,b,c}$	0.0, 2.0, 1.4
A, B, C	95466.3839, 12868.0116, 11339.5430
A_s, B_s, C_s	95189.5314, 12830.6943, 11306.6583
Charge, Multiplicity	0, 1
Predicted log column density	10.705±3.314
Electronic energy	-205.64040

geom1274



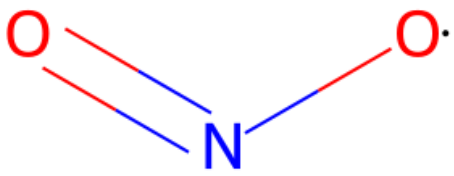
SMILES: C=NO

Nearest TMC-1 molecule (distance): C#N[O] (3.07)

Is DFT optimized?: True

Property	Value
Formula	CH3NO
Molecular weight	45.041
IUPAC name	N-methylidenehydroxylamine
$\mu_{a,b,c}$	0.3, 0.1, 0.0
A, B, C	69796.2580, 11939.6930, 10195.5857
A_s, B_s, C_s	69593.8488, 11905.0679, 10166.0185
Charge, Multiplicity	0, 1
Predicted log column density	9.388±3.078
Electronic energy	-169.76048

geom1275



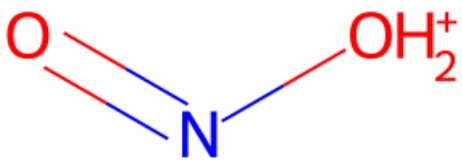
SMILES: [O]N=O

Nearest TMC-1 molecule (distance): S=O (2.54)

Is DFT optimized?: True

Property	Value
Formula	NO2
Molecular weight	46.005
IUPAC name	nitrous acid
$\mu_{a,b,c}$	0.0, 0.0, 0.4
A, B, C	239194.4725, 13075.4599, 12397.7428
A_s, B_s, C_s	238500.8085, 13037.5411, 12361.7894
Charge, Multiplicity	0, 2
Predicted log column density	11.307±2.181
Electronic energy	-205.01240

geom1276



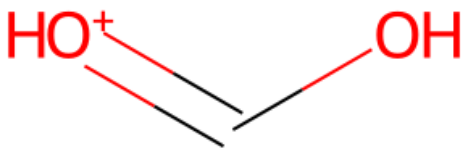
SMILES: O=N[OH2+]

Nearest TMC-1 molecule (distance): N (3.35)

Is DFT optimized?: True

Property	Value
Formula	H2NO2+
Molecular weight	48.021
IUPAC name	nitrosooxidanium
$\mu_{a,b,c}$	0.5, 0.0, 0.0
A, B, C	72066.3312, 7273.3809, 6606.6017
A_s, B_s, C_s	71857.3388, 7252.2881, 6587.4426
Charge, Multiplicity	1, 1
Predicted log column density	11.210±2.524
Electronic energy	-205.93467

geom1277



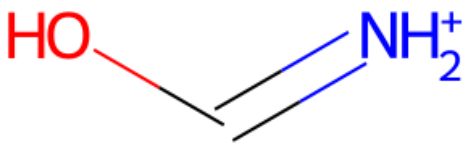
SMILES: OC=[OH+]

Nearest TMC-1 molecule (distance): C(=O)O (2.92)

Is DFT optimized?: True

Property	Value
Formula	CH3O2+
Molecular weight	47.033
IUPAC name	hydroxymethylideneoxidanium
$\mu_{a,b,c}$	0.0, 4.3, 0.0
A, B, C	76519.3203, 11477.7035, 9980.6338
A_s, B_s, C_s	76297.4142, 11444.4181, 9951.6900
Charge, Multiplicity	1, 1
Predicted log column density	11.707±2.429
Electronic energy	-189.99328

geom1278



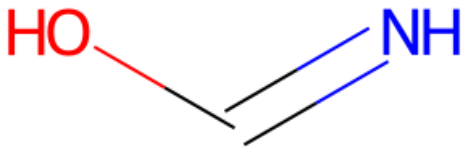
SMILES: [NH2+]=CO

Nearest TMC-1 molecule (distance): C(=O)O (2.95)

Is DFT optimized?: True

Property	Value
Formula	CH4NO+
Molecular weight	46.049
IUPAC name	formylazanium
$\mu_{a,b,c}$	0.0, 2.8, 1.2
A, B, C	63098.1709, 10764.7750, 9195.9183
A_s, B_s, C_s	62915.1863, 10733.5572, 9169.2501
Charge, Multiplicity	1, 1
Predicted log column density	13.410±2.492
Electronic energy	-170.16518

geom1279



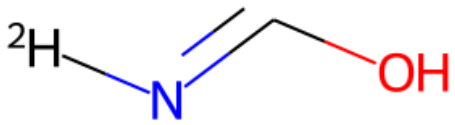
SMILES: N=CO

Nearest TMC-1 molecule (distance): C (=O) O (3.02)

Is DFT optimized?: True

Property	Value
Formula	CH3NO
Molecular weight	45.041
IUPAC name	formamide
$\mu_{a,b,c}$	0.3, 1.2, 0.0
A, B, C	71153.2403, 11520.5011, 9915.1311
A_s, B_s, C_s	70946.8959, 11487.0917, 9886.3772
Charge, Multiplicity	0, 1
Predicted log column density	13.280±2.736
Electronic energy	-169.82092

geom1280



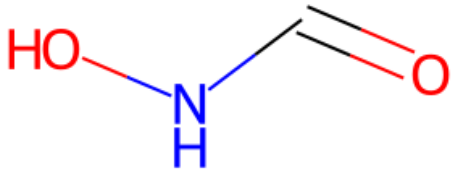
SMILES: [2H]N=CO

Nearest TMC-1 molecule (distance): C(=O)O (3.22)

Is DFT optimized?: True

Property	Value
Formula	CH3NO
Molecular weight	46.047
IUPAC name	N-deuteriomethanimidic acid
$\mu_{a,b,c}$	1.5, 1.8, 0.0
A, B, C	67193.2999, 11309.9166, 9680.5029
A_s, B_s, C_s	66998.4393, 11277.1178, 9652.4295
Charge, Multiplicity	0, 1
Predicted log column density	10.914±3.135
Electronic energy	-169.81404

geom1281



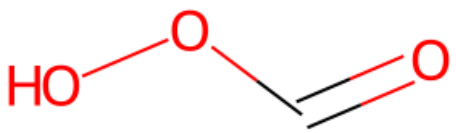
SMILES: O=CNO

Nearest TMC-1 molecule (distance): C (=O) O (3.28)

Is DFT optimized?: True

Property	Value
Formula	CH3NO2
Molecular weight	61.040
IUPAC name	N-hydroxyformamide
$\mu_{a,b,c}$	1.2, 3.1, 0.0
A, B, C	20827.5991, 7068.4127, 5277.4024
A_s, B_s, C_s	20767.1991, 7047.9143, 5262.0980
Charge, Multiplicity	0, 1
Predicted log column density	10.037±3.777
Electronic energy	-244.97887

geom1282



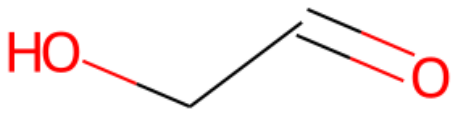
SMILES: O=COO

Nearest TMC-1 molecule (distance): C (=O) O (3.51)

Is DFT optimized?: True

Property	Value
Formula	CH2O3
Molecular weight	62.024
IUPAC name	peroxyformic acid
$\mu_{a,b,c}$	2.2, 2.5, 0.0
A, B, C	22127.9581, 6997.9693, 5316.6220
A_s, B_s, C_s	22063.7870, 6977.6752, 5301.2038
Charge, Multiplicity	0, 1
Predicted log column density	8.201±3.387
Electronic energy	-264.80109

geom1283



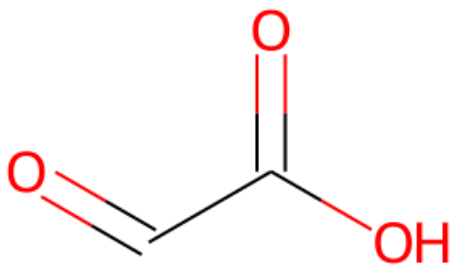
SMILES: O=CCO

Nearest TMC-1 molecule (distance): C (=O) O (3.56)

Is DFT optimized?: False

Property	Value
Formula	C2H4O2
Molecular weight	60.052
IUPAC name	2-hydroxyacetaldehyde
$\mu_{a,b,c}$	0.9, 1.3, 2.3
A, B, C	18367.6854, 6268.4166, 4841.4780
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	8.769±3.489
Electronic energy	-228.97275

geom1284



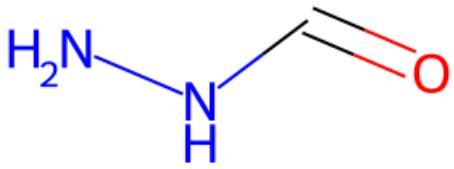
SMILES: O=CC(=O)O

Nearest TMC-1 molecule (distance): C(=O)O (3.87)

Is DFT optimized?: True

Property	Value
Formula	C2H2O3
Molecular weight	74.035
IUPAC name	oxaldehydic acid
$\mu_{a,b,c}$	2.1, 0.2, 0.0
A, B, C	11001.9048, 4596.1479, 3241.8394
A_s, B_s, C_s	10969.9992, 4582.8191, 3232.4381
Charge, Multiplicity	0, 1
Predicted log column density	10.316±3.162
Electronic energy	-302.98532

geom1285



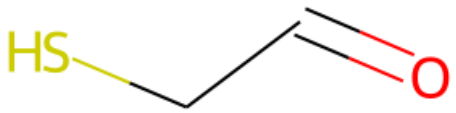
SMILES: NNC=O

Nearest TMC-1 molecule (distance): C (=O) O (3.98)

Is DFT optimized?: True

Property	Value
Formula	CH4N2O
Molecular weight	60.056
IUPAC name	formohydrazide
$\mu_{a,b,c}$	4.7, 1.1, 0.0
A, B, C	50405.7459, 4476.5909, 4206.6084
A_s, B_s, C_s	50259.5693, 4463.6088, 4194.4093
Charge, Multiplicity	0, 1
Predicted log column density	11.507±3.702
Electronic energy	-225.14492

geom1286



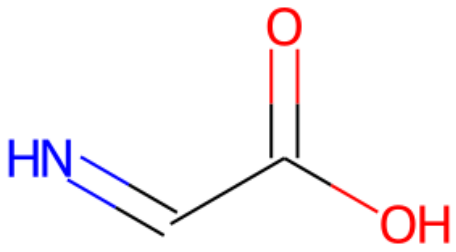
SMILES: O=CCS

Nearest TMC-1 molecule (distance): CC=O (3.93)

Is DFT optimized?: True

Property	Value
Formula	C2H4OS
Molecular weight	76.120
IUPAC name	2-sulfanylacetaldehyde
$\mu_{a,b,c}$	1.2, 1.0, 0.4
A, B, C	21125.7768, 2915.6444, 2784.6737
A_s, B_s, C_s	21064.5120, 2907.1890, 2776.5981
Charge, Multiplicity	0, 1
Predicted log column density	10.253±4.282
Electronic energy	-551.94968

geom1287



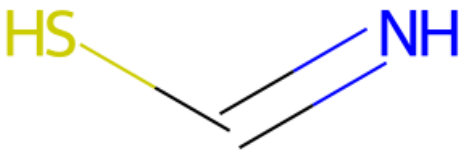
SMILES: N=CC(=O)O

Nearest TMC-1 molecule (distance): C(=O)O (4.01)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO2
Molecular weight	73.051
IUPAC name	2-iminoacetic acid
$\mu_{a,b,c}$	4.4, 1.0, 0.0
A, B, C	10986.6112, 4570.5074, 3227.7435
A_s, B_s, C_s	10954.7500, 4557.2530, 3218.3830
Charge, Multiplicity	0, 1
Predicted log column density	12.937±3.586
Electronic energy	-283.12004

geom1288



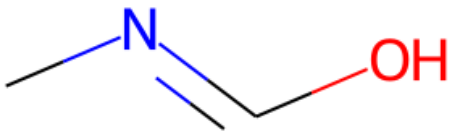
SMILES: N=CS

Nearest TMC-1 molecule (distance): C=[N] (3.38)

Is DFT optimized?: True

Property	Value
Formula	CH3NS
Molecular weight	61.109
IUPAC name	methanethioamide
$\mu_{a,b,c}$	0.5, 1.4, 0.0
A, B, C	57791.8960, 6056.5846, 5482.0648
A_s, B_s, C_s	57624.2995, 6039.0205, 5466.1669
Charge, Multiplicity	0, 1
Predicted log column density	14.956±3.143
Electronic energy	-492.77684

geom1289



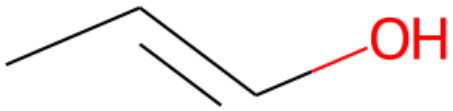
SMILES: CN=CO

Nearest TMC-1 molecule (distance): C (=O) O (4.18)

Is DFT optimized?: True

Property	Value
Formula	C2H5NO
Molecular weight	59.068
IUPAC name	N-methylformamide
$\mu_{a,b,c}$	0.8, 0.6, 0.0
A, B, C	46691.0632, 4369.4029, 4097.2299
A_s, B_s, C_s	46555.6591, 4356.7317, 4085.3479
Charge, Multiplicity	0, 1
Predicted log column density	10.611±4.067
Electronic energy	-209.11817

geom1290



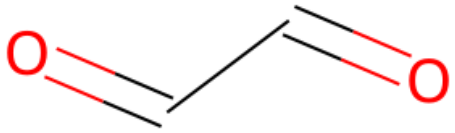
SMILES: CC=CO

Nearest TMC-1 molecule (distance): C (=O) O (4.24)

Is DFT optimized?: True

Property	Value
Formula	C3H6O
Molecular weight	58.080
IUPAC name	prop-1-en-1-ol
$\mu_{a,b,c}$	0.9, 1.0, 0.0
A, B, C	40695.7000, 3908.7583, 3647.4772
A_s, B_s, C_s	40577.6824, 3897.4229, 3636.8995
Charge, Multiplicity	0, 1
Predicted log column density	13.022±3.074
Electronic energy	-193.06448

geom1291



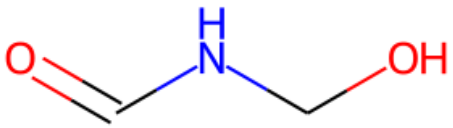
SMILES: O=CC=O

Nearest TMC-1 molecule (distance): CC=O (4.24)

Is DFT optimized?: True

Property	Value
Formula	C2H2O2
Molecular weight	58.036
IUPAC name	oxaldehyde
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	55519.6786, 4784.2370, 4404.6979
A_s, B_s, C_s	55358.6715, 4770.3627, 4391.9243
Charge, Multiplicity	0, 1
Predicted log column density	10.129±3.272
Electronic energy	-227.75300

geom1292



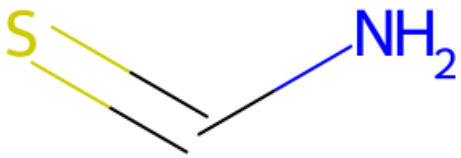
SMILES: O=CNCO

Nearest TMC-1 molecule (distance): C (=O) O (4.31)

Is DFT optimized?: True

Property	Value
Formula	C2H5NO2
Molecular weight	75.067
IUPAC name	N-(hydroxymethyl)formamide
$\mu_{a,b,c}$	2.4, 0.7, 1.2
A, B, C	20438.5916, 2425.8262, 2370.9877
A_s, B_s, C_s	20379.3197, 2418.7913, 2364.1119
Charge, Multiplicity	0, 1
Predicted log column density	12.289±4.655
Electronic energy	-284.33893

geom1293



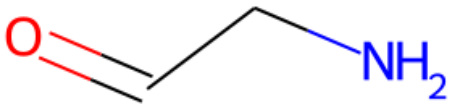
SMILES: NC=S

Nearest TMC-1 molecule (distance): CC=O (4.08)

Is DFT optimized?: True

Property	Value
Formula	CH3NS
Molecular weight	61.109
IUPAC name	methanethioamide
$\mu_{a,b,c}$	4.7, 0.3, 0.0
A, B, C	62438.3751, 6056.9613, 5521.3518
A_s, B_s, C_s	62257.3038, 6039.3961, 5505.3399
Charge, Multiplicity	0, 1
Predicted log column density	15.112±3.407
Electronic energy	-492.79885

geom1294



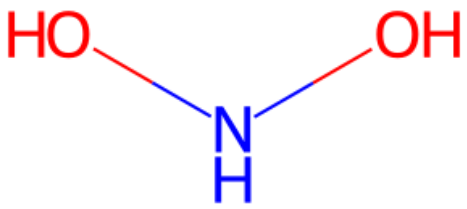
SMILES: NCC=O

Nearest TMC-1 molecule (distance): CC=O (4.13)

Is DFT optimized?: True

Property	Value
Formula	C2H5NO
Molecular weight	59.068
IUPAC name	2-aminoacetaldehyde
$\mu_{a,b,c}$	3.2, 0.7, 0.2
A, B, C	33688.1229, 4278.9643, 4039.3994
A_s, B_s, C_s	33590.4273, 4266.5553, 4027.6852
Charge, Multiplicity	0, 1
Predicted log column density	7.709±3.790
Electronic energy	-209.11353

geom1295



SMILES: ONO

Nearest TMC-1 molecule (distance): CO (3.35)

Is DFT optimized?: True

Property	Value
Formula	H3NO2
Molecular weight	49.029
IUPAC name	azonous acid
$\mu_{a,b,c}$	0.0, 0.5, 1.9
A, B, C	49782.3003, 10448.2869, 9361.8062
A_s, B_s, C_s	49637.9316, 10417.9869, 9334.6569
Charge, Multiplicity	0, 1
Predicted log column density	9.436±3.884
Electronic energy	-206.83253

geom1296

SMILES: OC=CO

Nearest TMC-1 molecule (distance): C (=O) O (4.38)

Is DFT optimized?: True

Property	Value
Formula	C2H4O2
Molecular weight	60.052
IUPAC name	ethene-1,2-diol
$\mu_{a,b,c}$	1.1, 3.0, 0.0
A, B, C	51615.1250, 4108.2857, 3805.3967
A_s, B_s, C_s	51465.4412, 4096.3717, 3794.3610
Charge, Multiplicity	0, 1
Predicted log column density	10.785±3.956
Electronic energy	-228.94803

geom1297

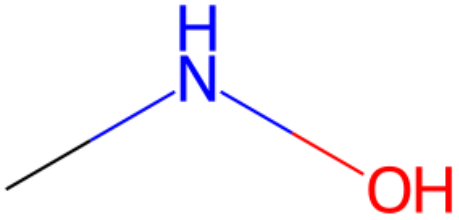
SMILES: [NH3+]O

Nearest TMC-1 molecule (distance): CO (2.23)

Is DFT optimized?: True

Property	Value
Formula	H4NO+
Molecular weight	34.038
IUPAC name	hydroxyazanium
$\mu_{a,b,c}$	3.7, 1.8, 0.0
A, B, C	139304.3251, 24849.7514, 23981.7026
A_s, B_s, C_s	138900.3425, 24777.6871, 23912.1557
Charge, Multiplicity	1, 1
Predicted log column density	9.607±2.594
Electronic energy	-131.99837

geom1298



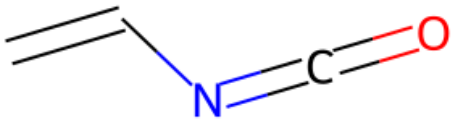
SMILES: CNO

Nearest TMC-1 molecule (distance): CO (2.48)

Is DFT optimized?: True

Property	Value
Formula	CH5NO
Molecular weight	47.057
IUPAC name	N-methylhydroxylamine
$\mu_{a,b,c}$	0.6, 0.4, 0.1
A, B, C	39752.4606, 9992.2299, 8781.2275
A_s, B_s, C_s	39637.1784, 9963.2524, 8755.7620
Charge, Multiplicity	0, 1
Predicted log column density	11.901±3.220
Electronic energy	-170.97553

geom1299



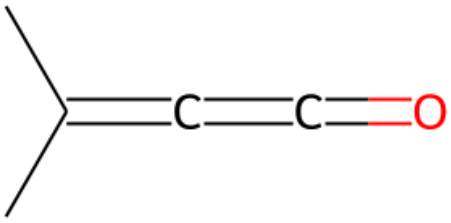
SMILES: C=CN=C=O

Nearest TMC-1 molecule (distance): C=C=C=O (4.62)

Is DFT optimized?: True

Property	Value
Formula	C3H3NO
Molecular weight	69.063
IUPAC name	isocyanatoethene
$\mu_{a,b,c}$	2.2, 0.9, 0.0
A, B, C	64943.8700, 2406.9279, 2320.9111
A_s, B_s, C_s	64755.5328, 2399.9478, 2314.1804
Charge, Multiplicity	0, 1
Predicted log column density	9.030±2.606
Electronic energy	-245.99277

geom1300



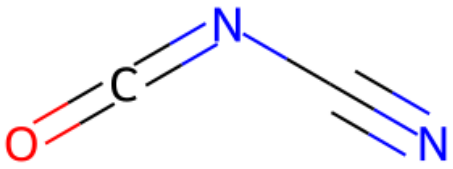
SMILES: CC(C)=C=C=O

Nearest TMC-1 molecule (distance): C=C=C=O (5.15)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	
$\mu_{a,b,c}$	4.3, 0.0, 0.0
A, B, C	8328.0091, 1856.5233, 1547.1081
A_s, B_s, C_s	8303.8579, 1851.1394, 1542.6215
Charge, Multiplicity	0, 1
Predicted log column density	9.729±4.385
Electronic energy	-269.20881

geom1301



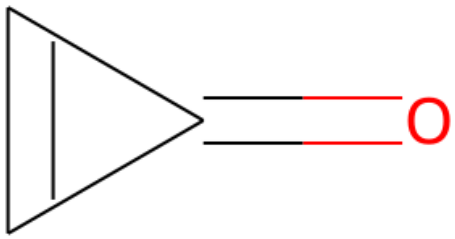
SMILES: N#CN=C=O

Nearest TMC-1 molecule (distance): C=C=C=O (5.17)

Is DFT optimized?: True

Property	Value
Formula	C2N2O
Molecular weight	68.035
IUPAC name	carbononitridic isocyanate
$\mu_{a,b,c}$	2.5, 0.4, 0.0
A, B, C	94805.5805, 2610.6862, 2540.7216
A_s, B_s, C_s	94530.6443, 2603.1152, 2533.3536
Charge, Multiplicity	0, 1
Predicted log column density	9.475±2.151
Electronic energy	-260.81184

geom1302



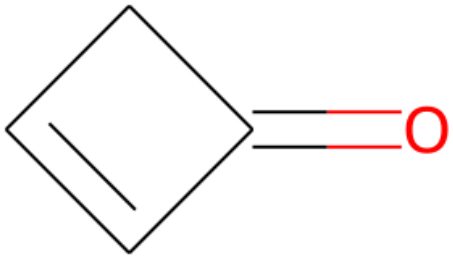
SMILES: O=c1cc1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (3.38)

Is DFT optimized?: True

Property	Value
Formula	C3H2O
Molecular weight	54.048
IUPAC name	cyclopropanone
$\mu_{a,b,c}$	4.5, 0.0, 0.0
A, B, C	32190.9707, 7813.8765, 6287.6467
A_s, B_s, C_s	32097.6168, 7791.2162, 6269.4125
Charge, Multiplicity	0, 1
Predicted log column density	13.484±2.502
Electronic energy	-190.58178

geom1303



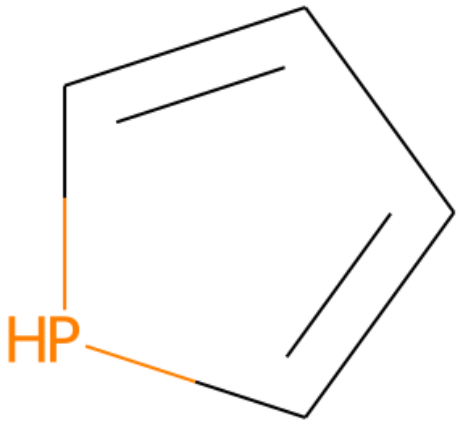
SMILES: O=C1C=CC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (3.47)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	cyclobut-2-en-1-one
$\mu_{a,b,c}$	3.7, 0.1, 0.0
A, B, C	12615.9384, 5320.1217, 3833.7882
A_s, B_s, C_s	12579.3522, 5304.6933, 3822.6702
Charge, Multiplicity	0, 1
Predicted log column density	12.324±2.655
Electronic energy	-229.92278

geom1304



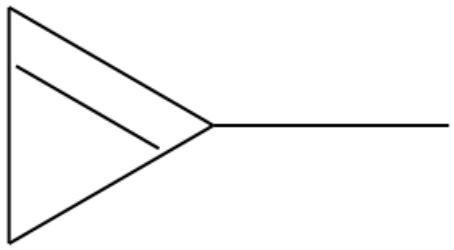
SMILES: `c1cc[pH]c1`

Nearest TMC-1 molecule (distance): `C1=C(=O)=C1` (3.59)

Is DFT optimized?: True

Property	Value
Formula	C4H5P
Molecular weight	84.058
IUPAC name	1H-phosphole
$\mu_{a,b,c}$	1.6, 0.1, 0.4
A, B, C	5790.5203, 4106.8263, 2692.2898
A_s, B_s, C_s	5773.7278, 4094.9165, 2684.4822
Charge, Multiplicity	0, 1
Predicted log column density	12.716±2.308
Electronic energy	-499.13276

geom1305



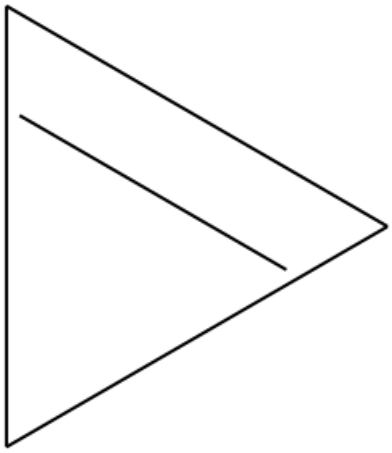
SMILES: CC1=CC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (3.62)

Is DFT optimized?: True

Property	Value
Formula	C4H6
Molecular weight	54.092
IUPAC name	1-methylcyclopropene
$\mu_{a,b,c}$	0.9, 0.3, 0.0
A, B, C	20625.6649, 6355.3321, 5182.6112
A_s, B_s, C_s	20565.8504, 6336.9016, 5167.5817
Charge, Multiplicity	0, 1
Predicted log column density	12.487±3.212
Electronic energy	-155.89318

geom1306



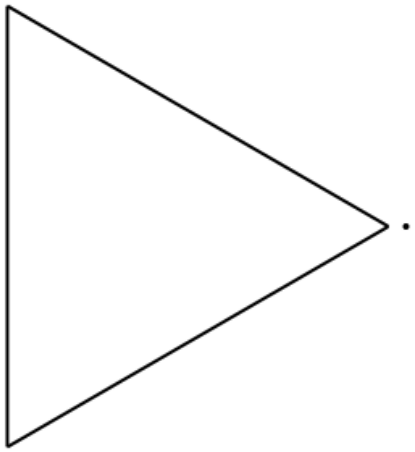
SMILES: C1=CC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.05)

Is DFT optimized?: True

Property	Value
Formula	C3H4
Molecular weight	40.065
IUPAC name	cyclopropene
$\mu_{a,b,c}$	0.5, 0.0, 0.0
A, B, C	30177.0110, 21852.4841, 13845.1062
A_s, B_s, C_s	30089.4976, 21789.1119, 13804.9554
Charge, Multiplicity	0, 1
Predicted log column density	12.023±2.633
Electronic energy	-116.57982

geom1307



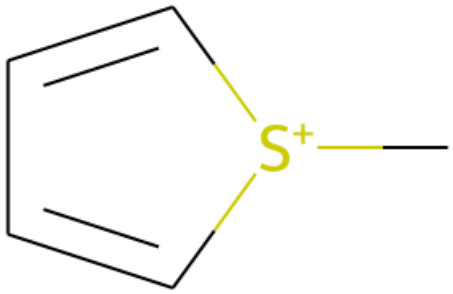
SMILES: [CH]1CC1

Nearest TMC-1 molecule (distance): S=O (3.73)

Is DFT optimized?: True

Property	Value
Formula	C3H5
Molecular weight	41.073
IUPAC name	cyclopropane
$\mu_{a,b,c}$	0.0, 0.4, 0.6
A, B, C	23712.5819, 20742.8978, 13216.0006
A_s, B_s, C_s	23643.8154, 20682.7434, 13177.6742
Charge, Multiplicity	0, 2
Predicted log column density	12.278±2.725
Electronic energy	-117.17667

geom1308



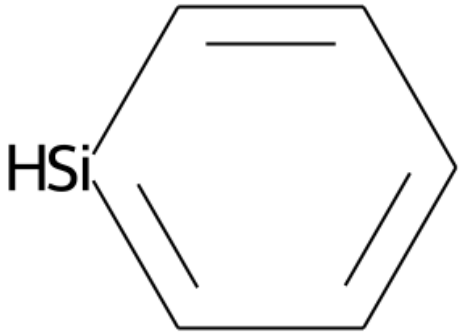
SMILES: C[s+]1cccc1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.14)

Is DFT optimized?: True

Property	Value
Formula	C5H7S+
Molecular weight	99.178
IUPAC name	1-methylthiophen-1-ium
$\mu_{a,b,c}$	0.8, 0.1, 0.9
A, B, C	4462.1704, 2512.1030, 2086.3091
A_s, B_s, C_s	4449.2301, 2504.8179, 2080.2588
Charge, Multiplicity	1, 1
Predicted log column density	11.756±3.341
Electronic energy	-595.02660

geom1309



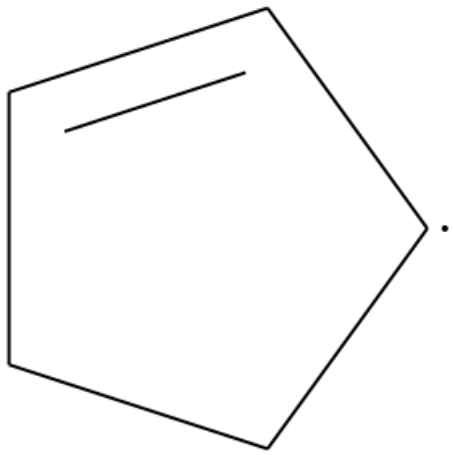
SMILES: `c1cc[siH]cc1`

Nearest TMC-1 molecule (distance): `C1=C(=O)=C1` (4.31)

Is DFT optimized?: True

Property	Value
Formula	C5H6Si
Molecular weight	94.189
IUPAC name	siline
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	4655.6031, 3682.3816, 2056.0973
A_s, B_s, C_s	4642.1019, 3671.7027, 2050.1346
Charge, Multiplicity	0, 1
Predicted log column density	12.365±2.597
Electronic energy	-483.50695

geom1310



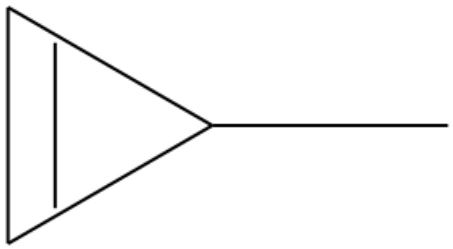
SMILES: [CH]1C=CCC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.44)

Is DFT optimized?: True

Property	Value
Formula	C5H7
Molecular weight	67.111
IUPAC name	cyclopentene
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	7876.0477, 7541.9847, 4044.3816
A_s, B_s, C_s	7853.2072, 7520.1130, 4032.6529
Charge, Multiplicity	0, 2
Predicted log column density	12.240±3.238
Electronic energy	-194.62553

geom1311



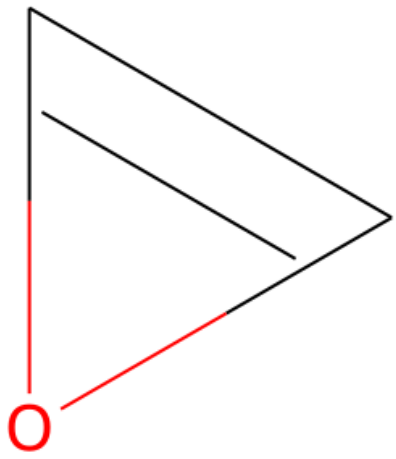
SMILES: CC1C=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.45)

Is DFT optimized?: True

Property	Value
Formula	C4H6
Molecular weight	54.092
IUPAC name	3-methylcyclopropene
$\mu_{a,b,c}$	0.3, 0.0, 0.2
A, B, C	20261.3227, 6461.0984, 5834.9736
A_s, B_s, C_s	20202.5649, 6442.3613, 5818.0522
Charge, Multiplicity	0, 1
Predicted log column density	11.031±3.986
Electronic energy	-155.88644

geom1312



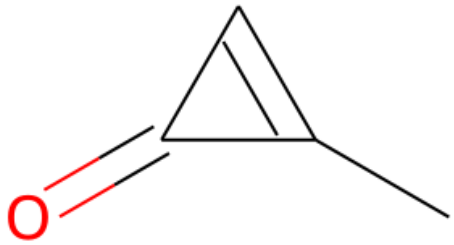
SMILES: C1=CO1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.54)

Is DFT optimized?: True

Property	Value
Formula	C2H2O
Molecular weight	42.037
IUPAC name	oxirene
$\mu_{a,b,c}$	2.7, 0.0, 0.0
A, B, C	33391.0694, 26810.2813, 14870.5006
A_s, B_s, C_s	33294.2353, 26732.5315, 14827.3762
Charge, Multiplicity	0, 1
Predicted log column density	15.123±4.721
Electronic energy	-152.42221

geom1313



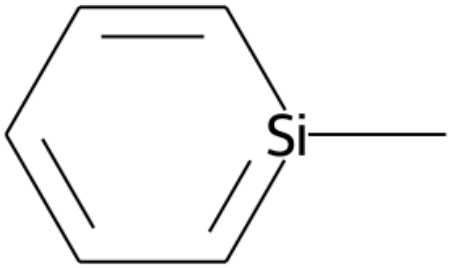
SMILES: Cc1cc1=O

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.54)

Is DFT optimized?: True

Property	Value
Formula	C4H4O
Molecular weight	68.075
IUPAC name	2-methylcyclopropan-1-one
$\mu_{a,b,c}$	4.6, 1.8, 0.0
A, B, C	13350.8107, 3858.6982, 3049.9774
A_s, B_s, C_s	13312.0934, 3847.5079, 3041.1324
Charge, Multiplicity	0, 1
Predicted log column density	13.261±3.631
Electronic energy	-229.89805

geom1314



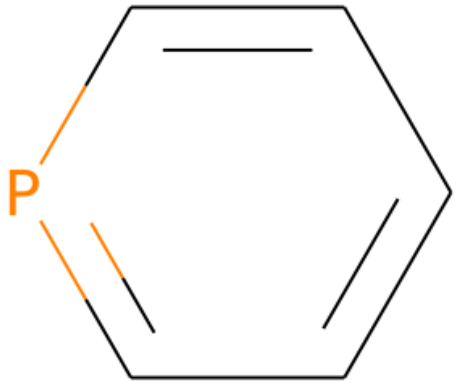
SMILES: C[si]1ccccc1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.55)

Is DFT optimized?: True

Property	Value
Formula	C6H8Si
Molecular weight	108.216
IUPAC name	1-methylsiline
$\mu_{a,b,c}$	1.6, 0.0, 0.0
A, B, C	4543.1048, 1820.9816, 1310.5941
A_s, B_s, C_s	4529.9298, 1815.7007, 1306.7934
Charge, Multiplicity	0, 1
Predicted log column density	12.545±2.617
Electronic energy	-522.82567

geom1315



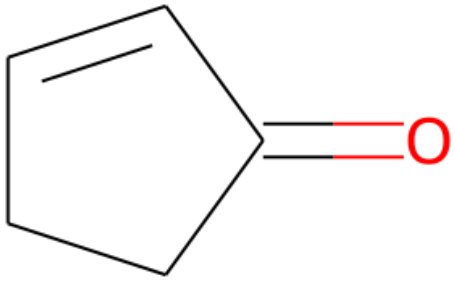
SMILES: `c1ccpcc1`

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.56)

Is DFT optimized?: True

Property	Value
Formula	C5H5P
Molecular weight	96.069
IUPAC name	phosphinine
$\mu_{a,b,c}$	0.0, 1.9, 0.0
A, B, C	5120.1664, 3500.6238, 2079.1338
A_s, B_s, C_s	5105.3180, 3490.4720, 2073.1043
Charge, Multiplicity	0, 1
Predicted log column density	12.263±2.938
Electronic energy	-534.79119

geom1316



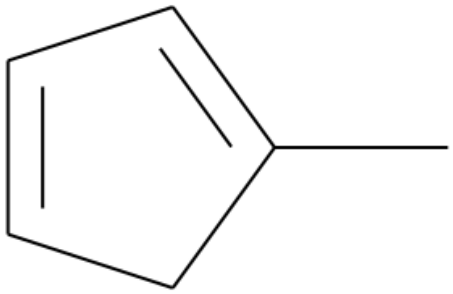
SMILES: O=C1C=CCC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.68)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	cyclopent-2-en-1-one
$\mu_{a,b,c}$	4.1, 0.2, 0.0
A, B, C	7431.2032, 3589.7855, 2494.9966
A_s, B_s, C_s	7409.6527, 3579.3751, 2487.7611
Charge, Multiplicity	0, 1
Predicted log column density	11.333±3.610
Electronic energy	-269.27090

geom1317



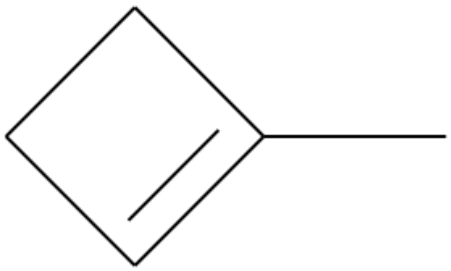
SMILES: CC1=CC=CC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.71)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	1-methylcyclopenta-1,3-diene
$\mu_{a,b,c}$	0.6, 0.5, 0.0
A, B, C	8054.6403, 3238.8222, 2378.0014
A_s, B_s, C_s	8031.2818, 3229.4296, 2371.1052
Charge, Multiplicity	0, 1
Predicted log column density	12.457±2.845
Electronic energy	-233.34914

geom1318



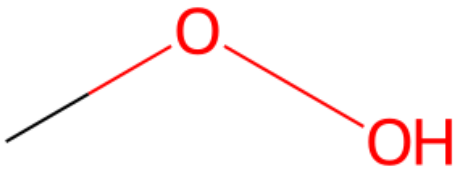
SMILES: CC1=CCC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.73)

Is DFT optimized?: True

Property	Value
Formula	C5H8
Molecular weight	68.119
IUPAC name	1-methylcyclobutene
$\mu_{a,b,c}$	0.3, 0.2, 0.0
A, B, C	11751.6312, 4227.0563, 3302.7304
A_s, B_s, C_s	11717.5514, 4214.7978, 3293.1525
Charge, Multiplicity	0, 1
Predicted log column density	11.514±3.928
Electronic energy	-195.23767

geom1319



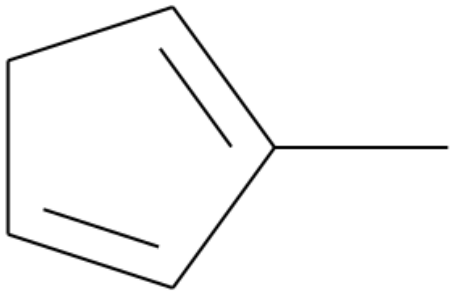
SMILES: COO

Nearest TMC-1 molecule (distance): CO (2.54)

Is DFT optimized?: True

Property	Value
Formula	CH4O2
Molecular weight	48.041
IUPAC name	hydroperoxymethane
$\mu_{a,b,c}$	0.3, 0.2, 0.0
A, B, C	44687.0600, 10706.8604, 9146.6872
A_s, B_s, C_s	44557.4675, 10675.8105, 9120.1618
Charge, Multiplicity	0, 1
Predicted log column density	11.764±2.933
Electronic energy	-190.79484

geom1320



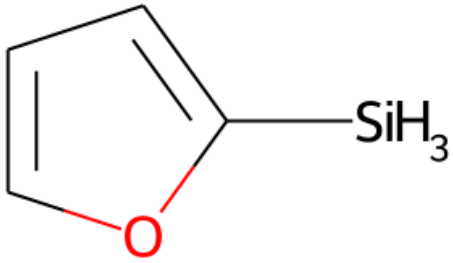
SMILES: CC1=CCC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.77)

Is DFT optimized?: False

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	2-methylcyclopenta-1,3-diene
$\mu_{a,b,c}$	0.0, 0.1, 0.1
A, B, C	8011.1524, 3311.6734, 2414.8616
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.095±2.669
Electronic energy	-233.34812

geom1321



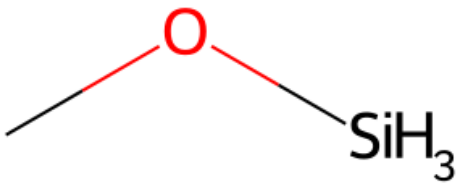
SMILES: [SiH3]c1ccco1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.77)

Is DFT optimized?: True

Property	Value
Formula	C4H6OSi
Molecular weight	98.177
IUPAC name	furan-2-ylsilane
$\mu_{a,b,c}$	0.8, 0.6, 0.0
A, B, C	8441.2142, 1982.0801, 1635.6015
A_s, B_s, C_s	8416.7347, 1976.3320, 1630.8582
Charge, Multiplicity	0, 1
Predicted log column density	13.771±3.664
Electronic energy	-520.62757

geom1322



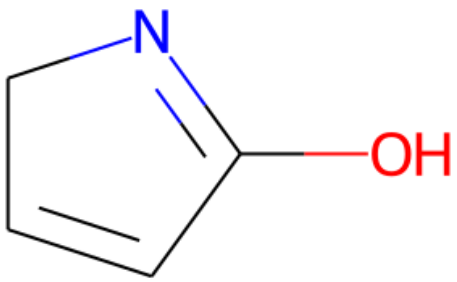
SMILES: CO[SiH3]

Nearest TMC-1 molecule (distance): CO (2.92)

Is DFT optimized?: True

Property	Value
Formula	CH6OSi
Molecular weight	62.144
IUPAC name	methoxysilane
$\mu_{a,b,c}$	0.5, 1.2, 0.0
A, B, C	33143.3224, 5612.2025, 5252.0799
A_s, B_s, C_s	33047.2067, 5595.9271, 5236.8489
Charge, Multiplicity	0, 1
Predicted log column density	12.851±2.611
Electronic energy	-406.39018

geom1323



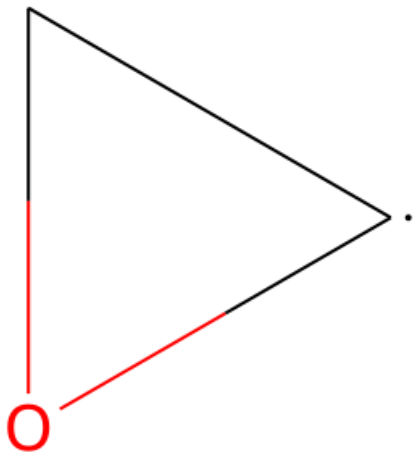
SMILES: OC1=NCC=C1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.81)

Is DFT optimized?: False

Property	Value
Formula	C4H5NO
Molecular weight	83.090
IUPAC name	1,2-dihydropyrrol-5-one
$\mu_{a,b,c}$	0.0, 1.1, 1.4
A, B, C	8191.0831, 3860.4026, 2668.4566
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.911±4.227
Electronic energy	-285.29190

geom1324



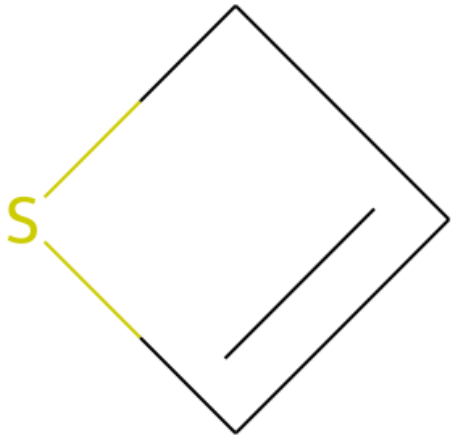
SMILES: [CH]1CO1

Nearest TMC-1 molecule (distance): S=O (4.20)

Is DFT optimized?: True

Property	Value
Formula	C2H3O
Molecular weight	43.045
IUPAC name	oxirane
$\mu_{a,b,c}$	1.3, 1.2, 0.7
A, B, C	30134.5638, 23867.9401, 15059.8497
A_s, B_s, C_s	30047.1736, 23798.7231, 15016.1762
Charge, Multiplicity	0, 2
Predicted log column density	13.004±3.886
Electronic energy	-153.06848

geom1325



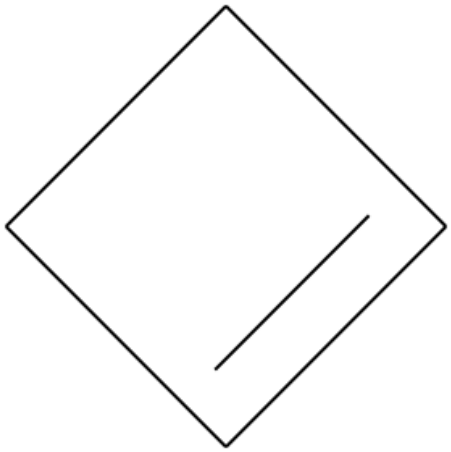
SMILES: C1=CSC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.82)

Is DFT optimized?: True

Property	Value
Formula	C3H4S
Molecular weight	72.132
IUPAC name	2H-thiete
$\mu_{a,b,c}$	1.5, 0.4, 0.0
A, B, C	12389.7290, 7432.6607, 4788.7644
A_s, B_s, C_s	12353.7988, 7411.1060, 4774.8769
Charge, Multiplicity	0, 1
Predicted log column density	12.211±5.049
Electronic energy	-514.80329

geom1326



SMILES: C1=CCC1

Nearest TMC-1 molecule (distance): C1=C(=O)=C1 (4.83)

Is DFT optimized?: True

Property	Value
Formula	C4H6
Molecular weight	54.092
IUPAC name	cyclobutene
$\mu_{a,b,c}$	0.2, 0.0, 0.0
A, B, C	12977.6850, 12275.5082, 6856.2800
A_s, B_s, C_s	12940.0497, 12239.9092, 6836.3968
Charge, Multiplicity	0, 1
Predicted log column density	12.375±3.329
Electronic energy	-155.92568

geom1327

SMILES: [NH]

Nearest TMC-1 molecule (distance): [CH] (0.00)

Is DFT optimized?: True

Property	Value
Formula	HN
Molecular weight	15.015
IUPAC name	azane
$\mu_{a,b,c}$	1.8, 0.0, 0.0
A, B, C	∞, 495176.4334, 495176.4334
A_s, B_s, C_s	∞, 493740.4218, 493740.4218
Charge, Multiplicity	0, 3
Predicted log column density	12.584±1.455
Electronic energy	-55.20122

geom1328

SMILES: [SiH+]

Nearest TMC-1 molecule (distance): [CH] (0.00)

Is DFT optimized?: True

Property	Value
Formula	HSi+
Molecular weight	29.094
IUPAC name	silicon(1+) monohydride
$\mu_{a,b,c}$	0.4, 0.0, 0.0
A, B, C	∞, 220758.5395, 220758.5395
A_s, B_s, C_s	∞, 220118.3398, 220118.3398
Charge, Multiplicity	1, 3
Predicted log column density	12.583±1.455
Electronic energy	-289.58441

geom1329

SMILES: [SiH5+]

Nearest TMC-1 molecule (distance): [CH] (0.00)

Is DFT optimized?: True

Property	Value
Formula	H5Si+
Molecular weight	33.126
IUPAC name	
$\mu_{a,b,c}$	1.6, 0.1, 0.0
A, B, C	75026.6582, 52359.3784, 50994.6855
A_s, B_s, C_s	74809.0809, 52207.5362, 50846.8009
Charge, Multiplicity	1, 1
Predicted log column density	12.582±1.455
Electronic energy	-292.10072

geom1330

SMILES: [SiH2+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2Si+
Molecular weight	30.102
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.2
A, B, C	476339.1102, 152573.2938, 115559.2203
A_s, B_s, C_s	474957.7268, 152130.8313, 115224.0985
Charge, Multiplicity	1, 2
Predicted log column density	12.582±1.455
Electronic energy	-290.25356

geom1331

SMILES: [OH+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	HO+
Molecular weight	17.007
IUPAC name	oxidanium
$\mu_{a,b,c}$	2.4, 0.0, 0.0
A, B, C	∞, 497687.0227, 497687.0227
A_s, B_s, C_s	∞, 496243.7303, 496243.7303
Charge, Multiplicity	1, 3
Predicted log column density	12.583±1.456
Electronic energy	-75.22569

geom1332

SMILES: [CH5+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	CH5+
Molecular weight	17.051
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 1.4
A, B, C	122282.9557, 122282.8783, 119730.8482
A_s, B_s, C_s	121928.3351, 121928.2580, 119383.6288
Charge, Multiplicity	1, 1
Predicted log column density	12.584±1.455
Electronic energy	-40.70898

geom1333

SMILES: [PH]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	HP
Molecular weight	31.982
IUPAC name	phosphane
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	∞, 253385.2544, 253385.2544
A_s, B_s, C_s	∞, 252650.4372, 252650.4372
Charge, Multiplicity	0, 3
Predicted log column density	12.580±1.456
Electronic energy	-341.85074

geom1334

SMILES: [NH2+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2N+
Molecular weight	16.023
IUPAC name	azanium
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	4615823.0249, 248344.7092, 235665.2339
A_s, B_s, C_s	4602437.1381, 247624.5095, 234981.8047
Charge, Multiplicity	1, 3
Predicted log column density	12.583±1.455
Electronic energy	-55.44467

geom1335

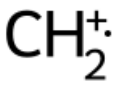
SMILES: [PH2]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2P
Molecular weight	32.990
IUPAC name	phosphane
$\mu_{a,b,c}$	0.0, 0.0, 0.9
A, B, C	274273.7572, 237930.8369, 127406.4804
A_s, B_s, C_s	273478.3633, 237240.8375, 127037.0016
Charge, Multiplicity	0, 2
Predicted log column density	12.583±1.455
Electronic energy	-342.47841

geom1336



SMILES: [CH2+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	CH2+
Molecular weight	14.027
IUPAC name	carbanylium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 209845.7379, 209845.7379
A_s, B_s, C_s	∞, 209237.1853, 209237.1853
Charge, Multiplicity	1, 2
Predicted log column density	12.584±1.455
Electronic energy	-38.75241

geom1337

SMILES: [PH+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	HP+
Molecular weight	31.982
IUPAC name	phosphanium
$\mu_{a,b,c}$	1.0, 0.0, 0.0
A, B, C	∞, 260875.4799, 260875.4799
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 4
Predicted log column density	12.584±1.455
Electronic energy	-341.41011

geom1338

SMILES: [C−]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	C-
Molecular weight	12.011
IUPAC name	carbanide
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-1, 4
Predicted log column density	12.582±1.455
Electronic energy	-37.88230

geom1339

SMILES: [CH3]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	CH3
Molecular weight	15.035
IUPAC name	methane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	285008.8334, 284818.3721, 142456.7854
A_s, B_s, C_s	284182.3077, 283992.3988, 142043.6608
Charge, Multiplicity	0, 2
Predicted log column density	12.581±1.456
Electronic energy	-39.82330

geom1340

SMILES: [SiH3-]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	H3Si-
Molecular weight	31.110
IUPAC name	silanide
$\mu_{a,b,c}$	0.8, 1.1, 0.5
A, B, C	138282.7775, 138282.3810, 86095.1611
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-1, 1
Predicted log column density	12.583±1.455
Electronic energy	-291.24038

geom1341

SMILES: [SiH2]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2Si
Molecular weight	30.102
IUPAC name	
$\mu_{a,b,c}$	0.1, 0.0, 0.0
A, B, C	459405.6108, 154194.1625, 115446.0391
A_s, B_s, C_s	458073.3345, 153746.9994, 115111.2455
Charge, Multiplicity	0, 3
Predicted log column density	12.588±1.456
Electronic energy	-290.55229

geom1342

SMILES: [SH]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	HS
Molecular weight	33.075
IUPAC name	sulfane
$\mu_{a,b,c}$	1.2, 0.0, 0.0
A, B, C	∞, 299029.3129, 299029.3129
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	12.581±1.456
Electronic energy	-398.71715

geom1343

SMILES: [SiH3]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H3Si
Molecular weight	31.110
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.1
A, B, C	140526.7482, 140510.7476, 83761.4456
A_s, B_s, C_s	140119.2206, 140103.2664, 83518.5374
Charge, Multiplicity	0, 2
Predicted log column density	12.584±1.455
Electronic energy	-291.20440

geom1344

SMILES: [CH+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	CH+
Molecular weight	13.019
IUPAC name	carbanylium
$\mu_{a,b,c}$	1.1, 0.0, 0.0
A, B, C	∞, 425403.6288, 425403.6288
A_s, B_s, C_s	∞, 424169.9583, 424169.9583
Charge, Multiplicity	1, 3
Predicted log column density	12.584±1.456
Electronic energy	-38.03684

geom1345

SMILES: [NH2]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2N
Molecular weight	16.023
IUPAC name	azane
$\mu_{a,b,c}$	2.2, 0.0, 0.0
A, B, C	713517.7696, 381565.9183, 248614.8465
A_s, B_s, C_s	711448.5681, 380459.3771, 247893.8634
Charge, Multiplicity	0, 2
Predicted log column density	12.581±1.456
Electronic energy	-55.85550

geom1346

SMILES: [PH3+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H3P+
Molecular weight	33.998
IUPAC name	phosphanium
$\mu_{a,b,c}$	0.0, 0.0, 0.6
A, B, C	161067.0681, 161012.8846, 92014.9774
A_s, B_s, C_s	160599.9736, 160545.9472, 91748.1340
Charge, Multiplicity	1, 2
Predicted log column density	12.583±1.456
Electronic energy	-342.75691

geom1347

SMILES: [O+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	O+
Molecular weight	15.999
IUPAC name	oxidanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 4
Predicted log column density	12.586±1.456
Electronic energy	-74.53330

geom1348

SMILES: [SiH4+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H4Si+
Molecular weight	32.118
IUPAC name	
$\mu_{a,b,c}$	1.4, 0.0, 0.2
A, B, C	77667.4667, 74449.4565, 74354.6350
A_s, B_s, C_s	77442.2310, 74233.5531, 74139.0065
Charge, Multiplicity	1, 2
Predicted log column density	12.587±1.456
Electronic energy	-291.42328

geom1349

SMILES: [SiH3+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H3Si+
Molecular weight	31.110
IUPAC name	silanylium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	155389.8588, 155315.7528, 77676.3985
A_s, B_s, C_s	154939.2282, 154865.3371, 77451.1369
Charge, Multiplicity	1, 1
Predicted log column density	12.582±1.455
Electronic energy	-290.90727

geom1350

SMILES: [SiH]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	HSi
Molecular weight	29.094
IUPAC name	lambda1-silane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 230987.3635, 230987.3635
A_s, B_s, C_s	∞, 230317.5001, 230317.5001
Charge, Multiplicity	0, 4
Predicted log column density	12.583±1.456
Electronic energy	-289.89201

geom1351

SMILES: [NH3+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H3N+
Molecular weight	17.031
IUPAC name	azanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	317538.7831, 317491.2287, 158757.5021
A_s, B_s, C_s	316617.9207, 316570.5042, 158297.1053
Charge, Multiplicity	1, 2
Predicted log column density	12.585±1.456
Electronic energy	-56.16583

geom1352

SMILES: [SH+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	HS+
Molecular weight	33.075
IUPAC name	sulfanium
$\mu_{a,b,c}$	1.5, 0.0, 0.0
A, B, C	∞, 278279.0784, 278279.0784
A_s, B_s, C_s	∞, 277472.0691, 277472.0691
Charge, Multiplicity	1, 3
Predicted log column density	12.579±1.455
Electronic energy	-398.33525

geom1353

SMILES: [SH2+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2S+
Molecular weight	34.083
IUPAC name	sulfanium
$\mu_{a,b,c}$	0.0, 0.0, 2.0
A, B, C	313264.3569, 253280.9960, 140048.6438
A_s, B_s, C_s	312355.8903, 252546.4811, 139642.5027
Charge, Multiplicity	1, 2
Predicted log column density	12.583±1.456
Electronic energy	-398.98248

geom1354

SMILES: [C+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	C+
Molecular weight	12.011
IUPAC name	carbanylium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 4
Predicted log column density	12.583±1.455
Electronic energy	-37.24383

geom1355

SMILES: [N+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	N+
Molecular weight	14.007
IUPAC name	azanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 5
Predicted log column density	12.584±1.455
Electronic energy	-53.83366

geom1356

SMILES: [O−]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	O-
Molecular weight	15.999
IUPAC name	hydroxide
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-1, 2
Predicted log column density	12.582±1.455
Electronic energy	-75.09563

geom1357

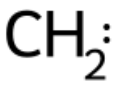
SMILES: [OH2+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2O+
Molecular weight	18.015
IUPAC name	oxidanium
$\mu_{a,b,c}$	2.6, 0.0, 0.0
A, B, C	846887.0614, 369851.8609, 257428.0726
A_s, B_s, C_s	844431.0889, 368779.2905, 256681.5312
Charge, Multiplicity	1, 2
Predicted log column density	12.581±1.455
Electronic energy	-75.93606

geom1358



SMILES: [CH2]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	CH2
Molecular weight	14.027
IUPAC name	methane
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 218080.1587, 218080.1587
A_s, B_s, C_s	∞, 217447.7263, 217447.7263
Charge, Multiplicity	0, 3
Predicted log column density	12.583±1.455
Electronic energy	-39.12812

geom1359

SMILES: [S+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	S+
Molecular weight	32.067
IUPAC name	sulfanium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	1, 4
Predicted log column density	12.584±1.455
Electronic energy	-397.69875

geom1360

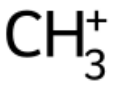
SMILES: [CH4+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	CH4+
Molecular weight	16.043
IUPAC name	
$\mu_{a,b,c}$	-, -, -
A, B, C	157637.4951, 157636.8181, 157636.6525
A_s, B_s, C_s	-, -, -
Charge, Multiplicity	1, 2
Predicted log column density	12.585±1.455
Electronic energy	-

geom1361



SMILES: [CH3+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	CH3+
Molecular weight	15.035
IUPAC name	carbanylium
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	280256.4379, 280005.6205, 140065.4865
A_s, B_s, C_s	279443.6943, 279193.6042, 139659.2966
Charge, Multiplicity	1, 1
Predicted log column density	12.583±1.455
Electronic energy	-39.46586

geom1362

SMILES: [S−]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: False

Property	Value
Formula	S-
Molecular weight	32.067
IUPAC name	sulfanide
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, ∞, ∞
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	-1, 2
Predicted log column density	12.586±1.455
Electronic energy	-398.16188

geom1363

SMILES: [PH2+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	H2P+
Molecular weight	32.990
IUPAC name	phosphanium
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	569798.8643, 164708.7816, 127773.8595
A_s, B_s, C_s	568146.4476, 164231.1262, 127403.3153
Charge, Multiplicity	1, 3
Predicted log column density	12.579±1.456
Electronic energy	-342.08971

geom1364

SMILES: [NH+]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	HN+
Molecular weight	15.015
IUPAC name	azanium
$\mu_{a,b,c}$	1.8, 0.0, 0.0
A, B, C	∞, 451054.1142, 451054.1142
A_s, B_s, C_s	∞, 449746.0572, 449746.0572
Charge, Multiplicity	1, 4
Predicted log column density	12.587±1.455
Electronic energy	-54.70142

geom1365

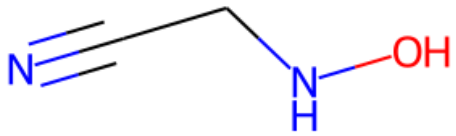
SMILES: [OH]

Nearest TMC-1 molecule (distance): [CH] (0.01)

Is DFT optimized?: True

Property	Value
Formula	HO
Molecular weight	17.007
IUPAC name	oxidane
$\mu_{a,b,c}$	1.9, 0.0, 0.0
A, B, C	∞, 557892.6128, 557892.6128
A_s, B_s, C_s	∞, 556274.7242, 556274.7242
Charge, Multiplicity	0, 2
Predicted log column density	12.585±1.455
Electronic energy	-75.70635

geom1366



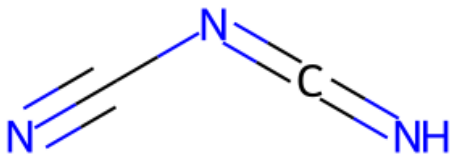
SMILES: N#CCNO

Nearest TMC-1 molecule (distance): OC#N (4.00)

Is DFT optimized?: True

Property	Value
Formula	C2H4N2O
Molecular weight	72.067
IUPAC name	2-(hydroxyamino)acetonitrile
$\mu_{a,b,c}$	3.2, 0.9, 0.2
A, B, C	30123.2059, 2402.0023, 2282.3161
A_s, B_s, C_s	30035.8486, 2395.0365, 2275.6974
Charge, Multiplicity	0, 1
Predicted log column density	10.179±4.061
Electronic energy	-263.17838

geom1367



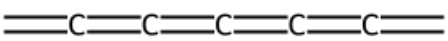
SMILES: N#CN=C=N

Nearest TMC-1 molecule (distance): [C]#NC#N (4.60)

Is DFT optimized?: True

Property	Value
Formula	C2HN3
Molecular weight	67.051
IUPAC name	
$\mu_{a,b,c}$	4.7, 0.1, 1.6
A, B, C	52598.5247, 2736.4783, 2616.4358
A_s, B_s, C_s	52445.9890, 2728.5425, 2608.8482
Charge, Multiplicity	0, 1
Predicted log column density	12.394±2.185
Electronic energy	-240.91983

geom1368



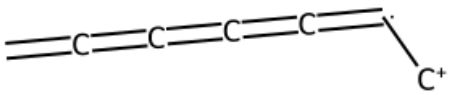
SMILES: C=C=C=C=C=C=C

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (2.58)

Is DFT optimized?: True

Property	Value
Formula	C7H4
Molecular weight	88.109
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	144852.5754, 792.5348, 792.5347
A_s, B_s, C_s	144432.5030, 790.2365, 790.2364
Charge, Multiplicity	0, 1
Predicted log column density	10.338±1.905
Electronic energy	-268.84322

geom1369



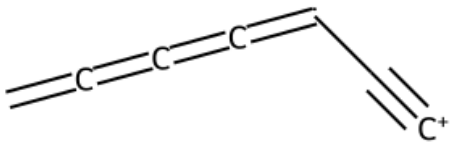
SMILES: C=C=C=C=C=[C][CH2+]

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (3.31)

Is DFT optimized?: True

Property	Value
Formula	C7H4+
Molecular weight	88.109
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	143123.1507, 794.8500, 791.7964
A_s, B_s, C_s	142708.0936, 792.5449, 789.5002
Charge, Multiplicity	1, 2
Predicted log column density	10.234±1.772
Electronic energy	-268.55182

geom1370



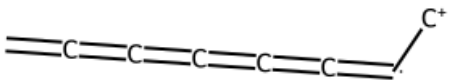
SMILES: [C+]#C[C]=C=C=C=C

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (4.49)

Is DFT optimized?: True

Property	Value
Formula	C7H2+
Molecular weight	86.093
IUPAC name	
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	286189.1771, 852.5570, 850.0248
A_s, B_s, C_s	285359.2285, 850.0846, 847.5597
Charge, Multiplicity	1, 2
Predicted log column density	10.564±1.845
Electronic energy	-267.19574

geom1371



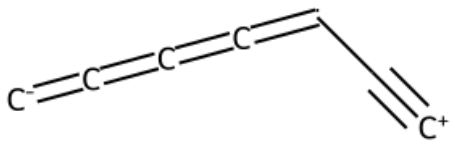
SMILES: C=C=C=C=C=C=[C][CH2+]

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (5.30)

Is DFT optimized?: True

Property	Value
Formula	C8H4+
Molecular weight	100.120
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	143406.9031, 539.3939, 537.8611
A_s, B_s, C_s	142991.0231, 537.8296, 536.3013
Charge, Multiplicity	1, 2
Predicted log column density	9.866±2.060
Electronic energy	-306.61768

geom1372



SMILES: [C+]#C[C]=C=C=C=[CH−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (6.27)

Is DFT optimized?: False

Property	Value
Formula	C7H
Molecular weight	85.085
IUPAC name	
$\mu_{a,b,c}$	6.1, 1.3, 7.6
A, B, C	144506.0965, 928.1186, 922.1956
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	10.114±2.259
Electronic energy	-266.78864

geom1373

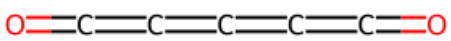
SMILES: C=C=C=C=C=[C+]C#CC

Nearest TMC-1 molecule (distance): C#CC#CC#C[C+]=O (6.84)

Is DFT optimized?: True

Property	Value
Formula	C9H5+
Molecular weight	113.139
IUPAC name	
$\mu_{a,b,c}$	1.9, 0.1, 0.0
A, B, C	101755.1294, 370.9246, 370.4529
A_s, B_s, C_s	101460.0396, 369.8489, 369.3786
Charge, Multiplicity	1, 1
Predicted log column density	10.976±2.113
Electronic energy	-345.32151

geom1374



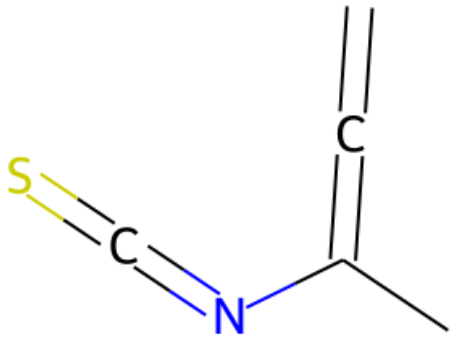
SMILES: O=C=C=C=C=C=O

Nearest TMC-1 molecule (distance): C=C=C=C=C=[C] (7.05)

Is DFT optimized?: True

Property	Value
Formula	C5O2
Molecular weight	92.053
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	∞, 791.6558, 791.6558
A_s, B_s, C_s	∞, 789.3600, 789.3600
Charge, Multiplicity	0, 1
Predicted log column density	8.723±2.361
Electronic energy	-340.73709

geom1375



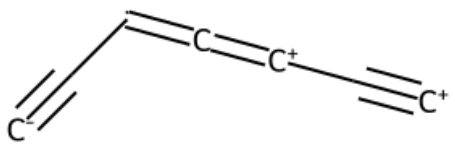
SMILES: C=C=C(C)N=C=S

Nearest TMC-1 molecule (distance): C=C=C=O (5.35)

Is DFT optimized?: True

Property	Value
Formula	C5H5NS
Molecular weight	111.169
IUPAC name	
$\mu_{a,b,c}$	3.2, 1.1, 0.0
A, B, C	6173.2784, 929.3158, 816.4123
A_s, B_s, C_s	6155.3759, 926.6208, 814.0447
Charge, Multiplicity	0, 1
Predicted log column density	12.353±3.469
Electronic energy	-646.30647

geom1376



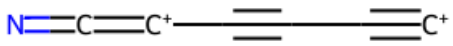
SMILES: [C+]#C[C+]=C=[C]C#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (6.90)

Is DFT optimized?: True

Property	Value
Formula	C7+
Molecular weight	84.077
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	956682207.4698, 922.2622, 922.2613
A_s, B_s, C_s	953907829.0681, 919.5876, 919.5868
Charge, Multiplicity	1, 2
Predicted log column density	10.917±2.051
Electronic energy	-265.80249

geom1377



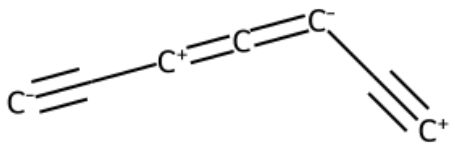
SMILES: [C+]#CC#C[C+]=C=[N−]

Nearest TMC-1 molecule (distance): C#CC#CC#[C−] (7.00)

Is DFT optimized?: True

Property	Value
Formula	C6N+
Molecular weight	86.073
IUPAC name	
$\mu_{a,b,c}$	3.5, 0.0, 0.0
A, B, C	3560231781.3602, 873.0584, 873.0582
A_s, B_s, C_s	3549907109.1943, 870.5265, 870.5263
Charge, Multiplicity	1, 1
Predicted log column density	12.476±3.383
Electronic energy	-282.63660

geom1378



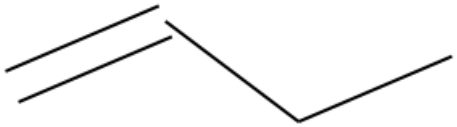
SMILES: [C+]#C[C−]=C=[C+]C#[C−]

Nearest TMC-1 molecule (distance): [CH+]=C=C=C=[C−] (6.46)

Is DFT optimized?: True

Property	Value
Formula	C7
Molecular weight	84.077
IUPAC name	
$\mu_{a,b,c}$	0.0, 0.0, 0.0
A, B, C	4533200935.9640, 915.2575, 915.2573
A_s, B_s, C_s	4520054653.2497, 912.6033, 912.6031
Charge, Multiplicity	0, 1
Predicted log column density	11.504±2.403
Electronic energy	-266.23188

geom1379



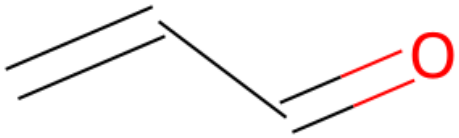
SMILES: C=CCC

Nearest TMC-1 molecule (distance): CC=C (3.24)

Is DFT optimized?: True

Property	Value
Formula	C4H8
Molecular weight	56.108
IUPAC name	but-1-ene
$\mu_{a,b,c}$	0.4, 0.1, 0.1
A, B, C	22360.0172, 4157.0937, 4068.2250
A_s, B_s, C_s	22295.1731, 4145.0381, 4056.4272
Charge, Multiplicity	0, 1
Predicted log column density	10.967±3.520
Electronic energy	-157.17167

geom1380



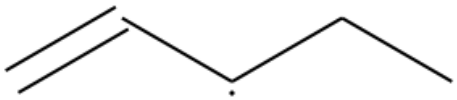
SMILES: C=CC=O

Nearest TMC-1 molecule (distance): CC=C (3.43)

Is DFT optimized?: True

Property	Value
Formula	C3H4O
Molecular weight	56.064
IUPAC name	prop-2-enal
$\mu_{a,b,c}$	3.4, 0.8, 0.0
A, B, C	47798.0384, 4648.4905, 4236.5024
A_s, B_s, C_s	47659.4240, 4635.0099, 4224.2165
Charge, Multiplicity	0, 1
Predicted log column density	11.187±2.920
Electronic energy	-191.85239

geom1381



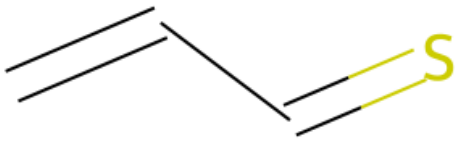
SMILES: C=C[CH]CC

Nearest TMC-1 molecule (distance): CC=C (3.52)

Is DFT optimized?: True

Property	Value
Formula	C5H9
Molecular weight	69.127
IUPAC name	pent-1-ene
$\mu_{a,b,c}$	0.5, 0.2, 0.0
A, B, C	22452.2479, 2115.1507, 1980.6416
A_s, B_s, C_s	22387.1364, 2109.0168, 1974.8977
Charge, Multiplicity	0, 2
Predicted log column density	11.257±3.550
Electronic energy	-195.82922

geom1382



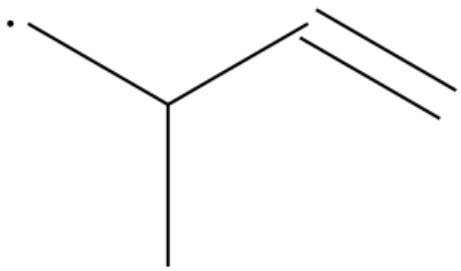
SMILES: C=CC=S

Nearest TMC-1 molecule (distance): CC=C (3.72)

Is DFT optimized?: True

Property	Value
Formula	C3H4S
Molecular weight	72.132
IUPAC name	prop-2-enethial
$\mu_{a,b,c}$	3.1, 0.5, 0.0
A, B, C	46257.8108, 2788.5746, 2630.0278
A_s, B_s, C_s	46123.6631, 2780.4877, 2622.4007
Charge, Multiplicity	0, 1
Predicted log column density	14.253±3.344
Electronic energy	-514.81101

geom1383



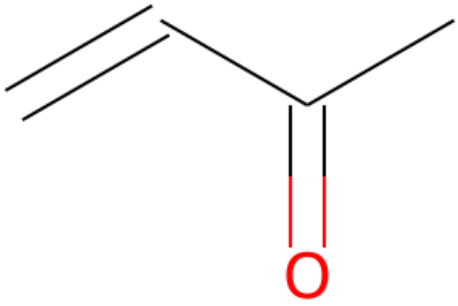
SMILES: [CH2]C(C)C=C

Nearest TMC-1 molecule (distance): CC=C (3.79)

Is DFT optimized?: True

Property	Value
Formula	C5H9
Molecular weight	69.127
IUPAC name	3-methylbut-1-ene
$\mu_{a,b,c}$	0.2, 0.2, 0.1
A, B, C	7986.1095, 3633.2492, 2808.5629
A_s, B_s, C_s	7962.9498, 3622.7128, 2800.4181
Charge, Multiplicity	0, 2
Predicted log column density	10.171±3.528
Electronic energy	-195.80229

geom1384



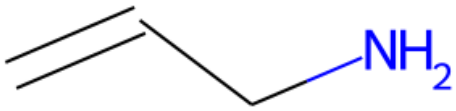
SMILES: C=CC(C)=O

Nearest TMC-1 molecule (distance): CC=C (3.89)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	but-3-en-2-one
$\mu_{a,b,c}$	2.6, 2.2, 0.0
A, B, C	8965.7836, 4194.4521, 2909.1860
A_s, B_s, C_s	8939.7829, 4182.2882, 2900.7494
Charge, Multiplicity	0, 1
Predicted log column density	11.309±3.716
Electronic energy	-231.16367

geom1385



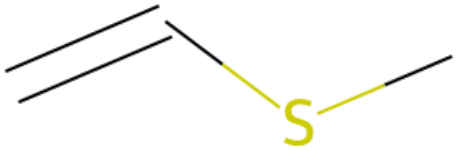
SMILES: C=CCN

Nearest TMC-1 molecule (distance): CC=C (4.08)

Is DFT optimized?: True

Property	Value
Formula	C3H7N
Molecular weight	57.096
IUPAC name	prop-2-en-1-amine
$\mu_{a,b,c}$	0.2, 1.0, 1.0
A, B, C	25374.8530, 4242.9491, 4121.4406
A_s, B_s, C_s	25301.2659, 4230.6445, 4109.4884
Charge, Multiplicity	0, 1
Predicted log column density	9.356±3.462
Electronic energy	-173.19800

geom1386



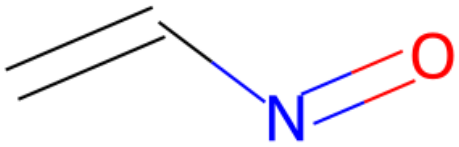
SMILES: C=CSC

Nearest TMC-1 molecule (distance): CC=C (4.12)

Is DFT optimized?: True

Property	Value
Formula	C3H6S
Molecular weight	74.148
IUPAC name	methylsulfanylethene
$\mu_{a,b,c}$	0.8, 1.6, 0.0
A, B, C	18372.0336, 3456.6508, 2964.4857
A_s, B_s, C_s	18318.7547, 3446.6265, 2955.8887
Charge, Multiplicity	0, 1
Predicted log column density	13.981±4.711
Electronic energy	-516.03452

geom1387



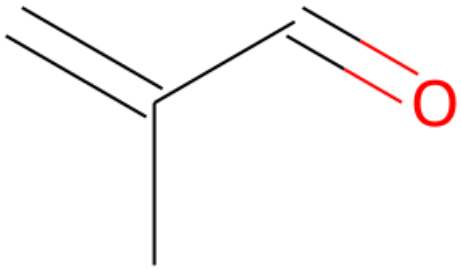
SMILES: C=CN=O

Nearest TMC-1 molecule (distance): CC=C (4.17)

Is DFT optimized?: True

Property	Value
Formula	C2H3NO
Molecular weight	57.052
IUPAC name	nitrosoethene
$\mu_{a,b,c}$	3.3, 0.8, 0.0
A, B, C	53169.8663, 5096.7716, 4650.9405
A_s, B_s, C_s	53015.6737, 5081.9910, 4637.4528
Charge, Multiplicity	0, 1
Predicted log column density	11.343±3.054
Electronic energy	-207.81501

geom1388



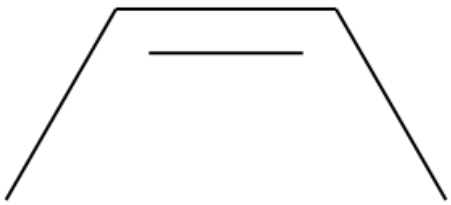
SMILES: C=C(C)C=O

Nearest TMC-1 molecule (distance): CC=C (4.32)

Is DFT optimized?: False

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	2-methylprop-2-enal
$\mu_{a,b,c}$	0.6, 0.8, 3.0
A, B, C	8701.3542, 4376.9978, 2966.5923
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.825±3.977
Electronic energy	-231.16198

geom1389



SMILES: C/C=C\C

Nearest TMC-1 molecule (distance): CC=C (4.35)

Is DFT optimized?: True

Property	Value
Formula	C4H8
Molecular weight	56.108
IUPAC name	(Z)-but-2-ene
$\mu_{a,b,c}$	0.1, 0.3, 0.0
A, B, C	15632.7038, 5301.9519, 4163.8617
A_s, B_s, C_s	15587.3690, 5286.5763, 4151.7865
Charge, Multiplicity	0, 1
Predicted log column density	15.125±3.087
Electronic energy	-157.17329

geom1390

SMILES: CC=CC

Nearest TMC-1 molecule (distance): CC=C (4.35)

Is DFT optimized?: True

Property	Value
Formula	C4H8
Molecular weight	56.108
IUPAC name	but-2-ene
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	34617.1762, 3707.5051, 3494.2975
A_s, B_s, C_s	34516.7864, 3696.7533, 3484.1640
Charge, Multiplicity	0, 1
Predicted log column density	15.125±3.087
Electronic energy	-157.17300

geom1391

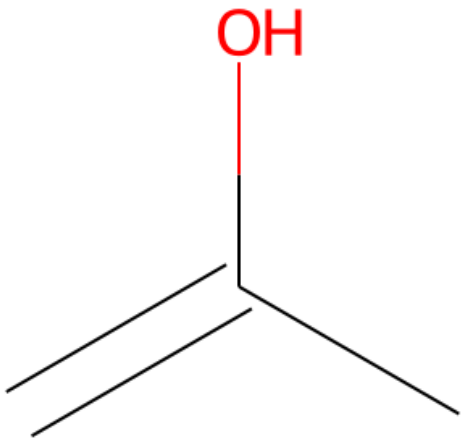
SMILES: C/C=C/C

Nearest TMC-1 molecule (distance): CC=C (4.35)

Is DFT optimized?: True

Property	Value
Formula	C4H8
Molecular weight	56.108
IUPAC name	(E)-but-2-ene
$\mu_{a,b,c}$	0.0, 0.1, 0.0
A, B, C	34617.1405, 3707.4999, 3494.2926
A_s, B_s, C_s	34516.7508, 3696.7482, 3484.1592
Charge, Multiplicity	0, 1
Predicted log column density	15.125±3.087
Electronic energy	-157.17300

geom1392



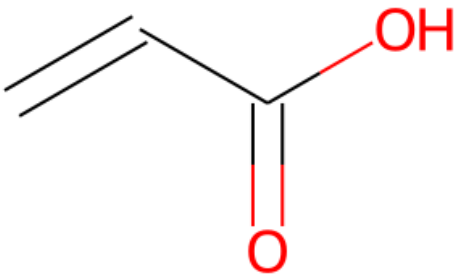
SMILES: C=C(C)O

Nearest TMC-1 molecule (distance): C=O (4.05)

Is DFT optimized?: True

Property	Value
Formula	C3H6O
Molecular weight	58.080
IUPAC name	prop-1-en-2-ol
$\mu_{a,b,c}$	0.6, 0.3, 0.0
A, B, C	10128.3105, 9063.6191, 4930.0576
A_s, B_s, C_s	10098.9384, 9037.3346, 4915.7604
Charge, Multiplicity	0, 1
Predicted log column density	10.460±3.227
Electronic energy	-193.07411

geom1393



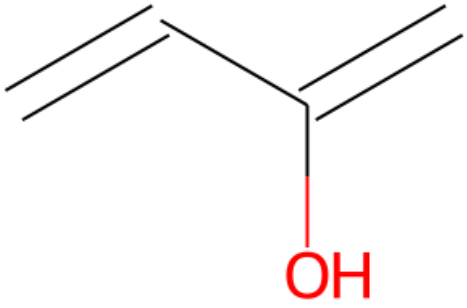
SMILES: C=CC(=O)O

Nearest TMC-1 molecule (distance): CC=C (4.46)

Is DFT optimized?: True

Property	Value
Formula	C3H4O2
Molecular weight	72.063
IUPAC name	prop-2-enoic acid
$\mu_{a,b,c}$	2.6, 3.9, 0.0
A, B, C	10912.9510, 4262.3227, 3065.1534
A_s, B_s, C_s	10881.3034, 4249.9619, 3056.2644
Charge, Multiplicity	0, 1
Predicted log column density	11.139±3.370
Electronic energy	-267.07513

geom1394



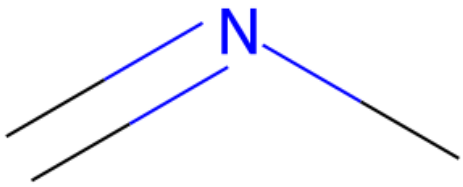
SMILES: C=CC(=C)O

Nearest TMC-1 molecule (distance): CC=C (4.52)

Is DFT optimized?: True

Property	Value
Formula	C4H6O
Molecular weight	70.091
IUPAC name	buta-1,3-dien-2-ol
$\mu_{a,b,c}$	1.7, 0.4, 0.6
A, B, C	9793.0040, 4219.8156, 2969.4289
A_s, B_s, C_s	9764.6043, 4207.5781, 2960.8175
Charge, Multiplicity	0, 1
Predicted log column density	9.979±3.199
Electronic energy	-231.13761

geom1395



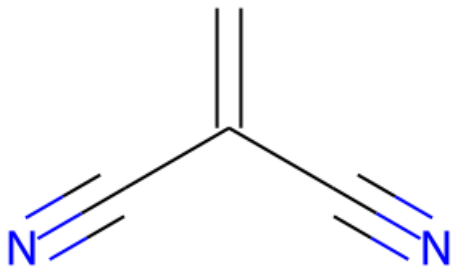
SMILES: C=NC

Nearest TMC-1 molecule (distance): C=[OH+] (3.40)

Is DFT optimized?: True

Property	Value
Formula	C2H5N
Molecular weight	43.069
IUPAC name	N-methylmethanimine
$\mu_{a,b,c}$	0.0, 1.9, 0.0
A, B, C	52615.4036, 10663.2237, 9392.5977
A_s, B_s, C_s	52462.8189, 10632.3003, 9365.3592
Charge, Multiplicity	0, 1
Predicted log column density	11.217±2.782
Electronic energy	-133.89478

geom1396



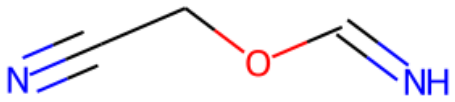
SMILES: C=C(C#N)C#N

Nearest TMC-1 molecule (distance): C=C=CC#N (5.80)

Is DFT optimized?: True

Property	Value
Formula	C4H2N2
Molecular weight	78.074
IUPAC name	2-methylidenepropanedinitrile
$\mu_{a,b,c}$	0.0, 4.5, 0.0
A, B, C	6553.3295, 2878.8523, 2000.1807
A_s, B_s, C_s	6534.3248, 2870.5036, 1994.3801
Charge, Multiplicity	0, 1
Predicted log column density	10.329±3.836
Electronic energy	-262.96875

geom1397



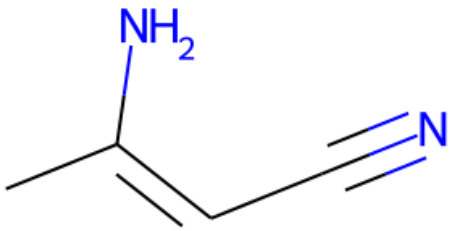
SMILES: N#CCOC=N

Nearest TMC-1 molecule (distance): CCC#N (5.80)

Is DFT optimized?: True

Property	Value
Formula	C3H4N2O
Molecular weight	84.078
IUPAC name	
$\mu_{a,b,c}$	0.6, 2.8, 0.0
A, B, C	21517.5056, 1571.2056, 1478.0331
A_s, B_s, C_s	21455.1049, 1566.6491, 1473.7468
Charge, Multiplicity	0, 1
Predicted log column density	13.734±4.647
Electronic energy	-301.30302

geom1398



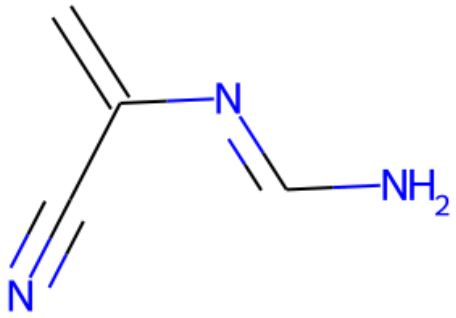
SMILES: CC(N)=CC#N

Nearest TMC-1 molecule (distance): C=CC#N (6.00)

Is DFT optimized?: True

Property	Value
Formula	C4H6N2
Molecular weight	82.106
IUPAC name	3-aminobut-2-enenitrile
$\mu_{a,b,c}$	5.8, 0.5, 0.5
A, B, C	9334.8749, 2235.1193, 1824.6969
A_s, B_s, C_s	9307.8037, 2228.6374, 1819.4053
Charge, Multiplicity	0, 1
Predicted log column density	10.743±4.030
Electronic energy	-265.43660

geom1399



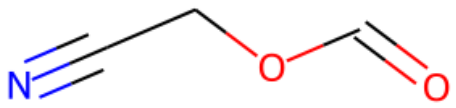
SMILES: C=C(C#N)N=CN

Nearest TMC-1 molecule (distance): C=C=CC#N (6.09)

Is DFT optimized?: True

Property	Value
Formula	C4H5N3
Molecular weight	95.105
IUPAC name	N'-(1-cyanoethenyl)methanimidamide
$\mu_{a,b,c}$	4.0, 1.0, 0.0
A, B, C	4491.0726, 1918.4137, 1344.2208
A_s, B_s, C_s	4478.0485, 1912.8503, 1340.3226
Charge, Multiplicity	0, 1
Predicted log column density	10.783±4.903
Electronic energy	-319.54111

geom1400



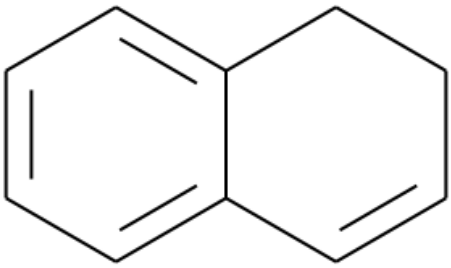
SMILES: N#CCOC=O

Nearest TMC-1 molecule (distance): CCC#N (5.19)

Is DFT optimized?: False

Property	Value
Formula	C3H3NO2
Molecular weight	85.062
IUPAC name	cyanomethyl formate
$\mu_{a,b,c}$	1.4, 0.6, 3.9
A, B, C	7170.5222, 2493.7054, 2103.7344
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.940±3.799
Electronic energy	-321.17297

geom1401



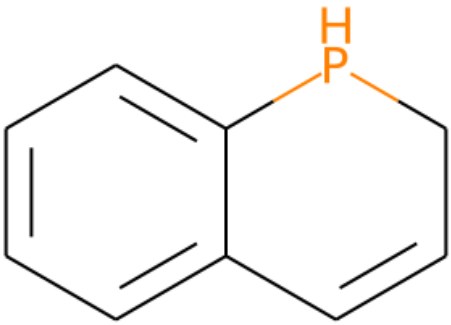
SMILES: C1=Cc2ccccc2CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (2.10)

Is DFT optimized?: False

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	1,2-dihydronaphthalene
$\mu_{a,b,c}$	0.0, 0.5, 0.7
A, B, C	2916.0379, 1166.3932, 841.7647
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.630±2.549
Electronic energy	-386.95606

geom1402



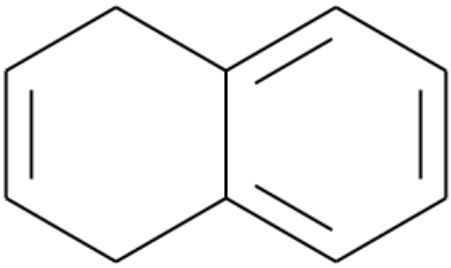
SMILES: C1=Cc2ccccc2PC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (2.20)

Is DFT optimized?: True

Property	Value
Formula	C9H9P
Molecular weight	148.145
IUPAC name	1,2-dihydrophosphinoline
$\mu_{a,b,c}$	0.1, 1.2, 0.1
A, B, C	2237.8843, 1012.2825, 717.3736
A_s, B_s, C_s	2231.3944, 1009.3469, 715.2932
Charge, Multiplicity	0, 1
Predicted log column density	12.861±2.535
Electronic energy	-689.58498

geom1403



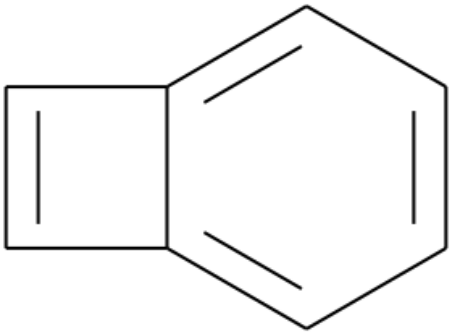
SMILES: C1=CCc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (2.82)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	1,4-dihydronaphthalene
$\mu_{a,b,c}$	0.3, 0.0, 0.0
A, B, C	2900.9513, 1172.9154, 843.8235
A_s, B_s, C_s	2892.5385, 1169.5140, 841.3764
Charge, Multiplicity	0, 1
Predicted log column density	12.434±2.653
Electronic energy	-386.95730

geom1404



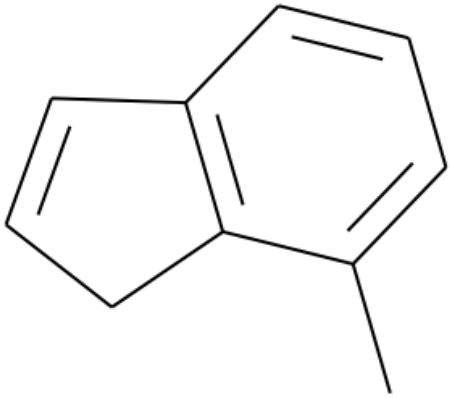
SMILES: C1=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (2.82)

Is DFT optimized?: True

Property	Value
Formula	C8H6
Molecular weight	102.136
IUPAC name	bicyclo[4.2.0]octa-1,3,5,7-tetraene
$\mu_{a,b,c}$	0.7, 0.0, 0.0
A, B, C	4840.8492, 2198.9340, 1512.0790
A_s, B_s, C_s	4826.8107, 2192.5570, 1507.6940
Charge, Multiplicity	0, 1
Predicted log column density	12.637±2.574
Electronic energy	-308.25956

geom1405



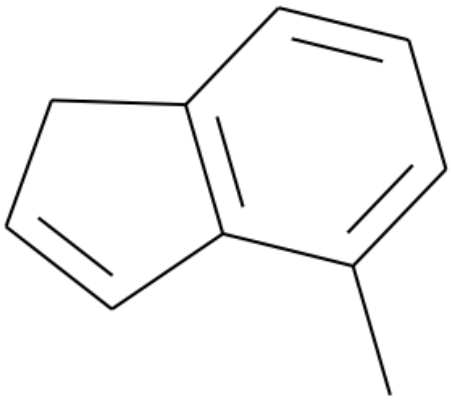
SMILES: `Cc1cccc2c1CC=C2`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (2.82)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	7-methyl-1H-indene
$\mu_{a,b,c}$	0.2, 0.9, 0.0
A, B, C	2121.3427, 1461.8232, 874.8264
A_s, B_s, C_s	2115.1908, 1457.5839, 872.2894
Charge, Multiplicity	0, 1
Predicted log column density	13.447±3.109
Electronic energy	-386.96079

geom1406



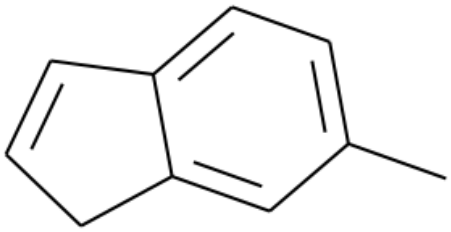
SMILES: `Cc1cccc2c1C=CC2`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (2.88)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	4-methyl-1H-indene
$\mu_{a,b,c}$	0.6, 0.1, 0.0
A, B, C	2124.6599, 1453.7014, 872.4868
A_s, B_s, C_s	2118.4984, 1449.4857, 869.9566
Charge, Multiplicity	0, 1
Predicted log column density	12.560±3.030
Electronic energy	-386.96012

geom1407



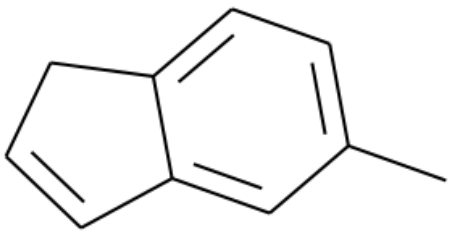
SMILES: `Cc1ccc2c(c1)CC=C2`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (2.90)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	6-methyl-1H-indene
$\mu_{a,b,c}$	0.1, 0.7, 0.0
A, B, C	3349.3682, 1016.8112, 787.6418
A_s, B_s, C_s	3339.6551, 1013.8625, 785.3577
Charge, Multiplicity	0, 1
Predicted log column density	13.198±2.924
Electronic energy	-386.95896

geom1408



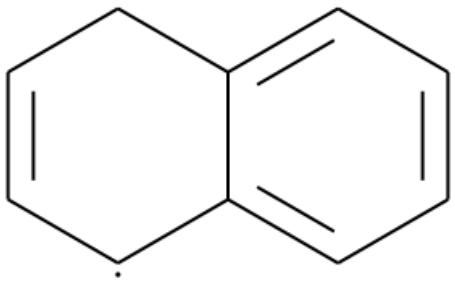
SMILES: Cc1ccc2c(c1)C=CC2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (2.90)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	5-methyl-1H-indene
$\mu_{a,b,c}$	0.3, 0.2, 0.0
A, B, C	3357.6973, 1014.9944, 787.0098
A_s, B_s, C_s	3347.9600, 1012.0509, 784.7274
Charge, Multiplicity	0, 1
Predicted log column density	13.198±2.924
Electronic energy	-386.95905

geom1409



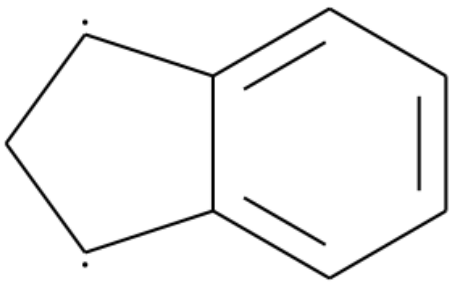
SMILES: [CH]1C=CCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.02)

Is DFT optimized?: True

Property	Value
Formula	C10H9
Molecular weight	129.182
IUPAC name	1,4-dihydronaphthalene
$\mu_{a,b,c}$	0.2, 0.5, 0.0
A, B, C	3012.1922, 1193.6810, 859.3529
A_s, B_s, C_s	3003.4569, 1190.2193, 856.8607
Charge, Multiplicity	0, 2
Predicted log column density	13.356±2.472
Electronic energy	-386.32633

geom1410



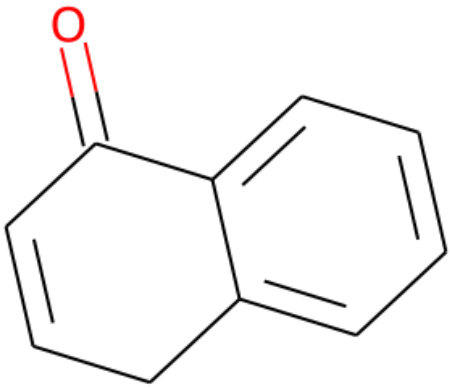
SMILES: `[CH]1C[CH]c2ccccc21`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (3.17)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	2,3-dihydro-1H-indene
$\mu_{a,b,c}$	0.8, 0.0, 0.0
A, B, C	3823.3604, 1547.8843, 1109.3218
A_s, B_s, C_s	3812.2726, 1543.3954, 1106.1047
Charge, Multiplicity	0, 3
Predicted log column density	12.480±3.109
Electronic energy	-347.57253

geom1411



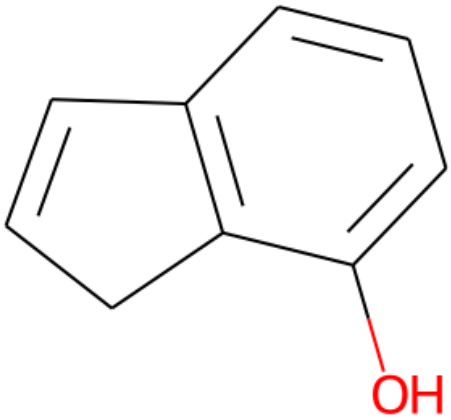
SMILES: O=C1C=CCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.20)

Is DFT optimized?: False

Property	Value
Formula	C10H8O
Molecular weight	144.173
IUPAC name	4H-naphthalen-1-one
$\mu_{a,b,c}$	0.0, 0.5, 4.4
A, B, C	1964.6308, 1104.7726, 710.2867
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.897±3.008
Electronic energy	-460.95877

geom1412



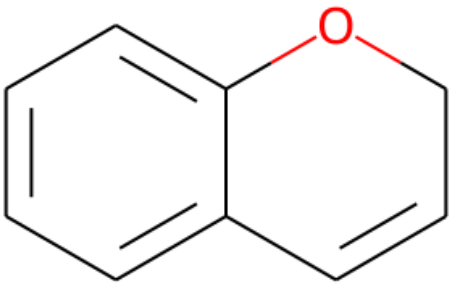
SMILES: Oc1cccc2c1CC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.21)

Is DFT optimized?: True

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	3H-inden-4-ol
$\mu_{a,b,c}$	0.9, 0.1, 0.0
A, B, C	2189.5773, 1465.3230, 882.6257
A_s, B_s, C_s	2183.2275, 1461.0736, 880.0661
Charge, Multiplicity	0, 1
Predicted log column density	13.310±3.209
Electronic energy	-422.85356

geom1413



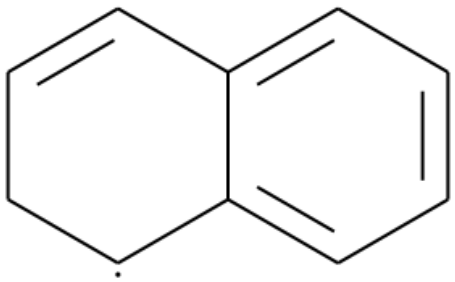
SMILES: C1=Cc2ccccc2OC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.28)

Is DFT optimized?: True

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	2H-chromene
$\mu_{a,b,c}$	0.7, 0.9, 0.6
A, B, C	3024.5369, 1229.8214, 889.1754
A_s, B_s, C_s	3015.7658, 1226.2549, 886.5968
Charge, Multiplicity	0, 1
Predicted log column density	13.153±4.029
Electronic energy	-422.84410

geom1414



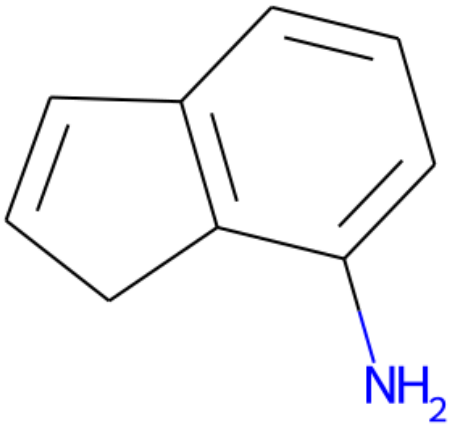
SMILES: `[CH]1CC=Cc2ccccc21`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (3.28)

Is DFT optimized?: True

Property	Value
Formula	C10H9
Molecular weight	129.182
IUPAC name	1,2-dihydronaphthalene
$\mu_{a,b,c}$	0.7, 0.2, 0.0
A, B, C	3039.4423, 1181.1268, 854.9779
A_s, B_s, C_s	3030.6279, 1177.7015, 852.4985
Charge, Multiplicity	0, 2
Predicted log column density	12.311±2.710
Electronic energy	-386.31747

geom1415



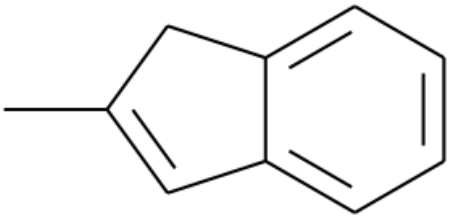
SMILES: Nc1cccc2c1CC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.42)

Is DFT optimized?: False

Property	Value
Formula	C9H9N
Molecular weight	131.178
IUPAC name	3H-inden-4-amine
$\mu_{a,b,c}$	0.9, 0.4, 1.4
A, B, C	2175.0589, 1478.8873, 886.2990
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.448±3.544
Electronic energy	-402.99204

geom1416



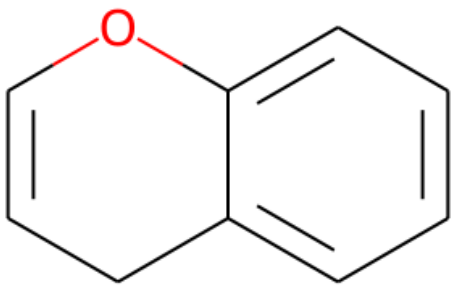
SMILES: CC1=Cc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.54)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	2-methyl-1H-indene
$\mu_{a,b,c}$	1.1, 0.5, 0.0
A, B, C	3708.6703, 956.5035, 767.6269
A_s, B_s, C_s	3697.9152, 953.7296, 765.4008
Charge, Multiplicity	0, 1
Predicted log column density	11.933±3.422
Electronic energy	-386.96236

geom1417



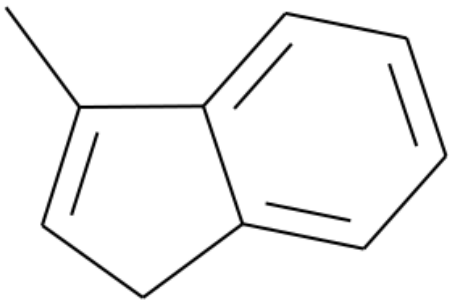
SMILES: C1=COc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.59)

Is DFT optimized?: True

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	4H-chromene
$\mu_{a,b,c}$	0.2, 1.1, 0.0
A, B, C	2989.4175, 1233.7195, 878.0196
A_s, B_s, C_s	2980.7482, 1230.1418, 875.4734
Charge, Multiplicity	0, 1
Predicted log column density	13.343±4.009
Electronic energy	-422.84633

geom1418



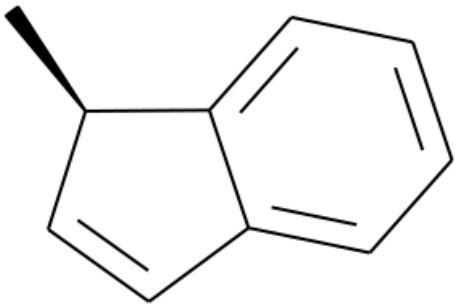
SMILES: CC1=CCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.60)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	3-methyl-1H-indene
$\mu_{a,b,c}$	0.5, 0.3, 0.0
A, B, C	2512.1226, 1260.1862, 848.0394
A_s, B_s, C_s	2504.8375, 1256.5317, 845.5801
Charge, Multiplicity	0, 1
Predicted log column density	11.582±3.435
Electronic energy	-386.96301

geom1419



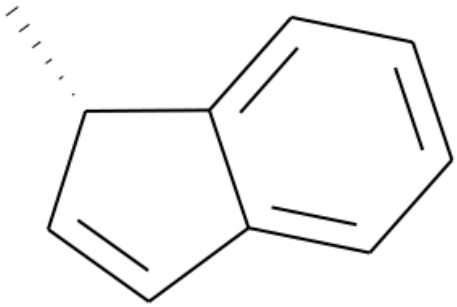
SMILES: C[C@@H]1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.62)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	(1R)-1-methyl-1H-indene
$\mu_{a,b,c}$	0.7, 0.2, 0.1
A, B, C	2596.7164, 1247.7600, 886.3686
A_s, B_s, C_s	2589.1860, 1244.1415, 883.7981
Charge, Multiplicity	0, 1
Predicted log column density	11.223±3.674
Electronic energy	-386.95744

geom1420



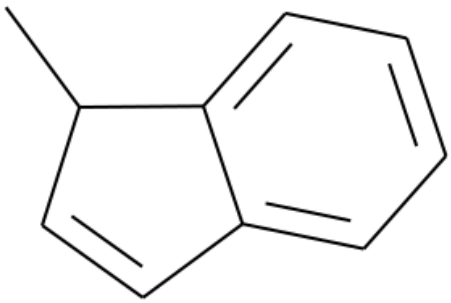
SMILES: C[C@H]1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.62)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	(1S)-1-methyl-1H-indene
$\mu_{a,b,c}$	0.7, 0.2, 0.1
A, B, C	2596.9914, 1247.8600, 886.7376
A_s, B_s, C_s	2589.4601, 1244.2412, 884.1661
Charge, Multiplicity	0, 1
Predicted log column density	11.223±3.674
Electronic energy	-386.95744

geom1421



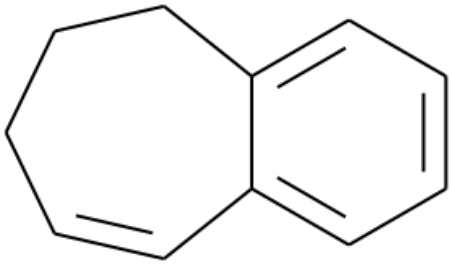
SMILES: CC1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.62)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	1-methyl-1H-indene
$\mu_{a,b,c}$	0.7, 0.2, 0.1
A, B, C	2596.7687, 1247.8562, 886.5771
A_s, B_s, C_s	2589.2381, 1244.2374, 884.0060
Charge, Multiplicity	0, 1
Predicted log column density	11.223±3.674
Electronic energy	-386.95744

geom1422



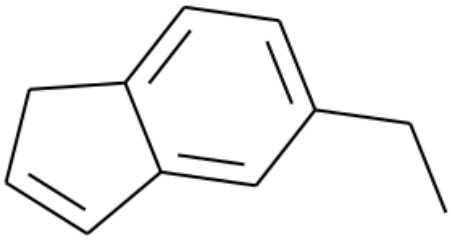
SMILES: C1=Cc2ccccc2CCC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.73)

Is DFT optimized?: False

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	8,9-dihydro-7H-benzo[7]annulene
$\mu_{a,b,c}$	0.0, 0.3, 0.5
A, B, C	2172.2775, 946.3718, 716.4006
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.300±3.369
Electronic energy	-426.25505

geom1423



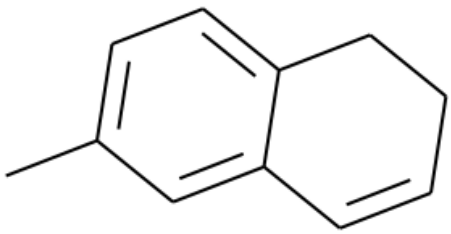
SMILES: CCc1ccc2c(c1)C=CC2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.77)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	5-ethyl-1H-indene
$\mu_{a,b,c}$	0.3, 0.2, 0.1
A, B, C	2803.4494, 701.0213, 593.3186
A_s, B_s, C_s	2795.3194, 698.9883, 591.5980
Charge, Multiplicity	0, 1
Predicted log column density	11.848±3.890
Electronic energy	-426.26295

geom1424



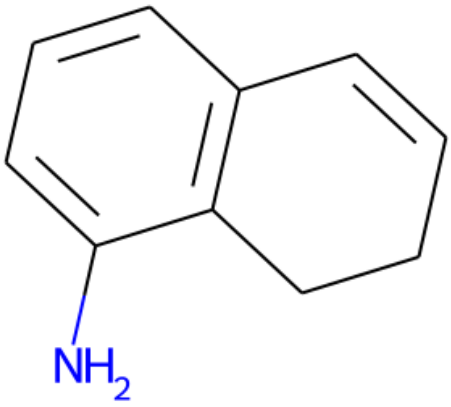
SMILES: `Cc1ccc2c(c1)C=CCC2`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (3.80)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	6-methyl-1,2-dihydronaphthalene
$\mu_{a,b,c}$	0.2, 0.1, 0.1
A, B, C	2632.7383, 792.9671, 624.5185
A_s, B_s, C_s	2625.1034, 790.6675, 622.7074
Charge, Multiplicity	0, 1
Predicted log column density	12.229±3.370
Electronic energy	-426.26903

geom1425



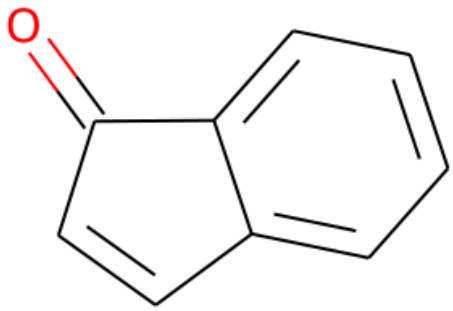
SMILES: Nc1cccc2c1CCC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.80)

Is DFT optimized?: True

Property	Value
Formula	C10H11N
Molecular weight	145.205
IUPAC name	7,8-dihydronaphthalen-1-amine
$\mu_{a,b,c}$	0.2, 1.3, 1.0
A, B, C	1856.7483, 1080.9219, 698.4224
A_s, B_s, C_s	1851.3637, 1077.7872, 696.3970
Charge, Multiplicity	0, 1
Predicted log column density	13.489±3.847
Electronic energy	-442.30289

geom1426



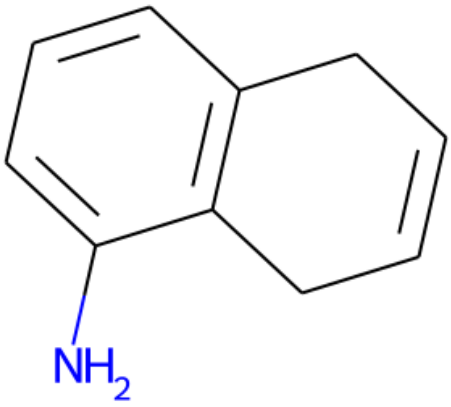
SMILES: O=C1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.81)

Is DFT optimized?: False

Property	Value
Formula	C9H6O
Molecular weight	130.146
IUPAC name	inden-1-one
$\mu_{a,b,c}$	0.0, 0.7, 3.6
A, B, C	2798.1457, 1327.3455, 900.2822
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	11.973±3.197
Electronic energy	-421.63636

geom1427



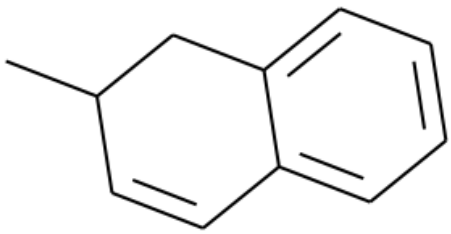
SMILES: Nc1cccc2c1CC=CC2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.83)

Is DFT optimized?: True

Property	Value
Formula	C10H11N
Molecular weight	145.205
IUPAC name	5,8-dihydronaphthalen-1-amine
$\mu_{a,b,c}$	0.2, 0.9, 1.1
A, B, C	1851.7186, 1079.3154, 688.5741
A_s, B_s, C_s	1846.3486, 1076.1854, 686.5772
Charge, Multiplicity	0, 1
Predicted log column density	14.323±3.657
Electronic energy	-442.29931

geom1428



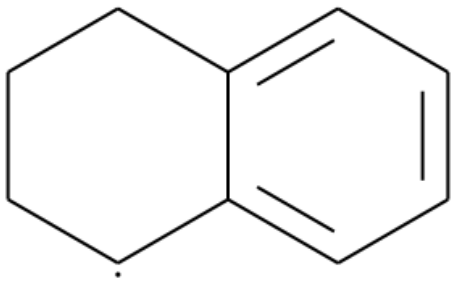
SMILES: CC1C=Cc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.86)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	2-methyl-1,2-dihydronaphthalene
$\mu_{a,b,c}$	0.6, 0.3, 0.0
A, B, C	2250.3125, 905.1960, 736.8412
A_s, B_s, C_s	2243.7866, 902.5709, 734.7044
Charge, Multiplicity	0, 1
Predicted log column density	10.650±3.681
Electronic energy	-426.26783

geom1429



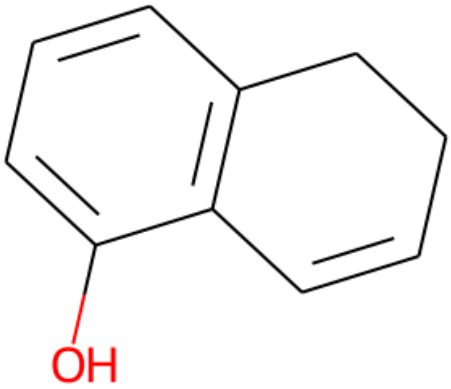
SMILES: [CH]1CCCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.87)

Is DFT optimized?: False

Property	Value
Formula	C10H11
Molecular weight	131.198
IUPAC name	1,2,3,4-tetrahydronaphthalene
$\mu_{a,b,c}$	0.1, 0.2, 0.7
A, B, C	2874.5041, 1139.0641, 838.5917
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 2
Predicted log column density	11.461±3.528
Electronic energy	-387.53907

geom1430



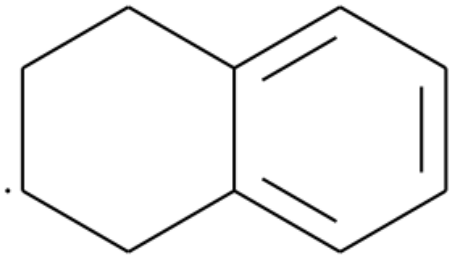
SMILES: Oc1cccc2c1C=CCC2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (3.90)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	5,6-dihydronaphthalen-1-ol
$\mu_{a,b,c}$	0.8, 0.6, 0.2
A, B, C	1871.8992, 1082.2600, 701.1525
A_s, B_s, C_s	1866.4707, 1079.1215, 699.1192
Charge, Multiplicity	0, 1
Predicted log column density	11.451±3.563
Electronic energy	-462.16211

geom1431



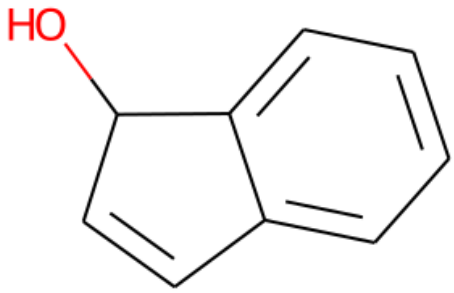
SMILES: [CH]1CCc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.02)

Is DFT optimized?: True

Property	Value
Formula	C10H11
Molecular weight	131.198
IUPAC name	1,2,3,4-tetrahydronaphthalene
$\mu_{a,b,c}$	0.6, 0.1, 0.1
A, B, C	2763.3703, 1166.1025, 862.5400
A_s, B_s, C_s	2755.3565, 1162.7208, 860.0387
Charge, Multiplicity	0, 2
Predicted log column density	11.346±3.849
Electronic energy	-387.52414

geom1432



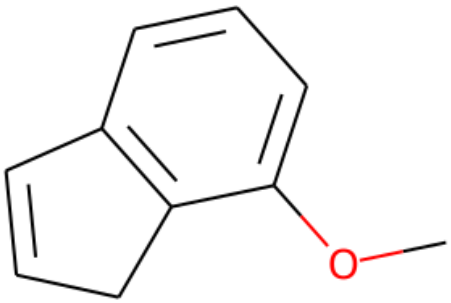
SMILES: OC1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.02)

Is DFT optimized?: True

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	1H-inden-1-ol
$\mu_{a,b,c}$	1.1, 0.8, 1.2
A, B, C	2638.2969, 1253.9262, 879.7349
A_s, B_s, C_s	2630.6458, 1250.2898, 877.1837
Charge, Multiplicity	0, 1
Predicted log column density	10.863±4.039
Electronic energy	-422.83833

geom1433



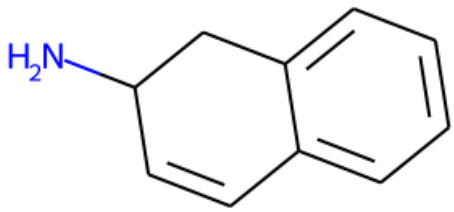
SMILES: COc1cccc2c1CC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.02)

Is DFT optimized?: False

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	7-methoxy-1H-indene
$\mu_{a,b,c}$	0.4, 0.2, 1.0
A, B, C	1898.8809, 1019.9469, 673.9123
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	16.074±3.730
Electronic energy	-462.14115

geom1434



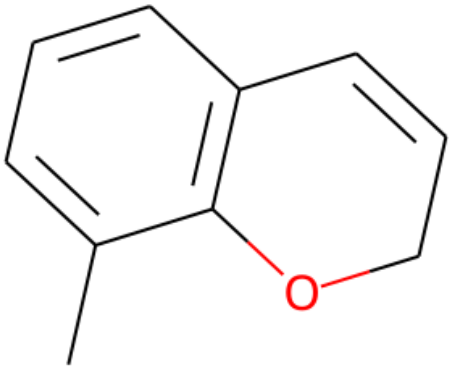
SMILES: NC1C=Cc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.03)

Is DFT optimized?: True

Property	Value
Formula	C10H11N
Molecular weight	145.205
IUPAC name	1,2-dihydronaphthalen-2-amine
$\mu_{a,b,c}$	0.2, 1.1, 0.0
A, B, C	2288.2825, 901.2584, 731.2953
A_s, B_s, C_s	2281.6464, 898.6448, 729.1745
Charge, Multiplicity	0, 1
Predicted log column density	12.387±3.679
Electronic energy	-442.29653

geom1435



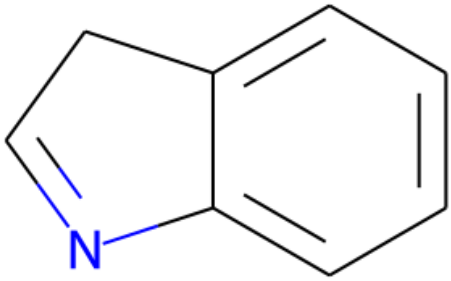
SMILES: Cc1cccc2c1OCC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.03)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	8-methyl-2H-chromene
$\mu_{a,b,c}$	0.9, 0.3, 0.5
A, B, C	1852.0837, 1144.2265, 720.5584
A_s, B_s, C_s	1846.7126, 1140.9082, 718.4688
Charge, Multiplicity	0, 1
Predicted log column density	13.557±4.139
Electronic energy	-462.15219

geom1436



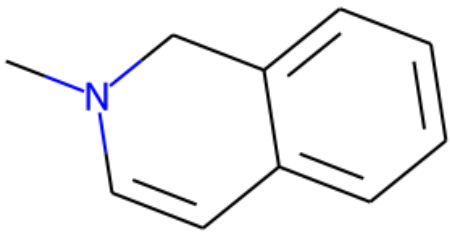
SMILES: C1=Nc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.08)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	3H-indole
$\mu_{a,b,c}$	0.1, 2.5, 0.0
A, B, C	3832.8491, 1628.5549, 1151.1130
A_s, B_s, C_s	3821.7338, 1623.8321, 1147.7748
Charge, Multiplicity	0, 1
Predicted log column density	12.779±5.812
Electronic energy	-363.69072

geom1437



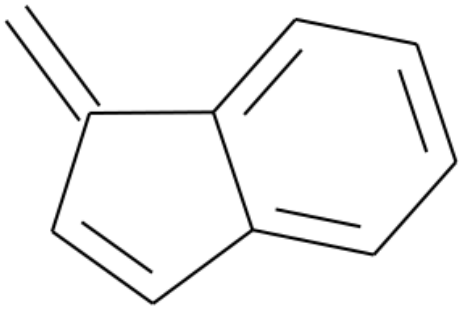
SMILES: CN1C=Cc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.08)

Is DFT optimized?: True

Property	Value
Formula	C10H11N
Molecular weight	145.205
IUPAC name	2-methyl-1H-isoquinoline
$\mu_{a,b,c}$	1.7, 0.7, 0.2
A, B, C	2753.9949, 819.9157, 643.7515
A_s, B_s, C_s	2746.0084, 817.5379, 641.8846
Charge, Multiplicity	0, 1
Predicted log column density	14.820±3.829
Electronic energy	-442.29092

geom1438



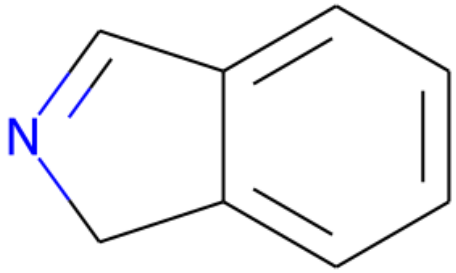
SMILES: C=C1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.11)

Is DFT optimized?: True

Property	Value
Formula	C10H8
Molecular weight	128.174
IUPAC name	1-methylideneindene
$\mu_{a,b,c}$	0.4, 0.2, 0.0
A, B, C	2748.0435, 1297.0556, 881.1567
A_s, B_s, C_s	2740.0741, 1293.2942, 878.6013
Charge, Multiplicity	0, 1
Predicted log column density	11.974±2.730
Electronic energy	-385.72677

geom1439



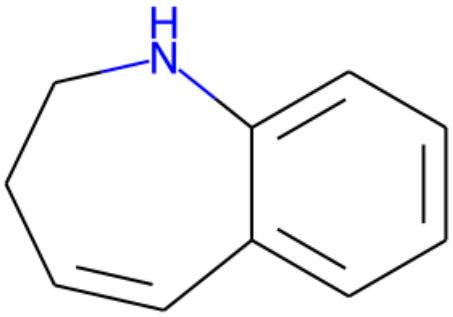
SMILES: C1=NCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.12)

Is DFT optimized?: True

Property	Value
Formula	C8H7N
Molecular weight	117.151
IUPAC name	1H-isoindole
$\mu_{a,b,c}$	2.3, 0.3, 0.0
A, B, C	3913.2810, 1575.2071, 1130.9916
A_s, B_s, C_s	3901.9325, 1570.6390, 1127.7117
Charge, Multiplicity	0, 1
Predicted log column density	11.463±4.873
Electronic energy	-363.69036

geom1440



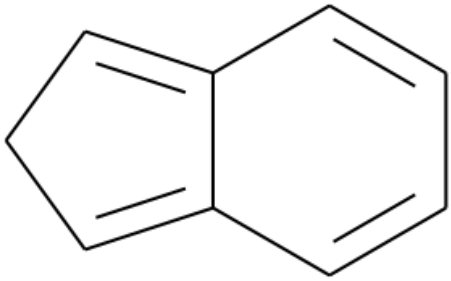
SMILES: C1=Cc2ccccc2NCC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.13)

Is DFT optimized?: True

Property	Value
Formula	C10H11N
Molecular weight	145.205
IUPAC name	2,3-dihydro-1H-1-benzazepine
$\mu_{a,b,c}$	1.0, 1.3, 0.6
A, B, C	2392.8685, 910.9005, 677.9404
A_s, B_s, C_s	2385.9292, 908.2589, 675.9744
Charge, Multiplicity	0, 1
Predicted log column density	11.938±4.551
Electronic energy	-442.29077

geom1441



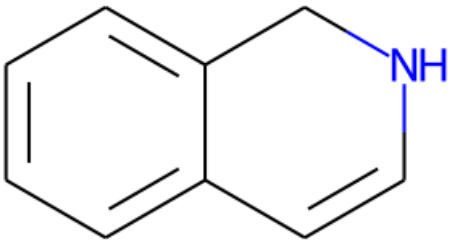
SMILES: C1=c2ccccc2=CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.16)

Is DFT optimized?: True

Property	Value
Formula	C9H8
Molecular weight	116.163
IUPAC name	2H-indene
$\mu_{a,b,c}$	0.6, 0.0, 0.0
A, B, C	3698.9412, 1594.8380, 1122.0701
A_s, B_s, C_s	3688.2143, 1590.2129, 1118.8161
Charge, Multiplicity	0, 1
Predicted log column density	13.212±4.146
Electronic energy	-347.61463

geom1442



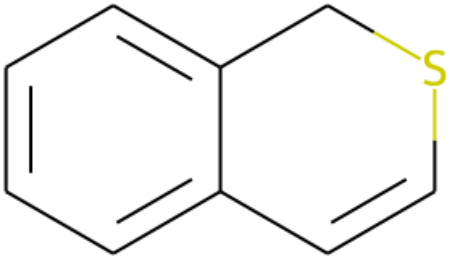
SMILES: C1=Cc2ccccc2CN1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.16)

Is DFT optimized?: True

Property	Value
Formula	C9H9N
Molecular weight	131.178
IUPAC name	1,2-dihydroisoquinoline
$\mu_{a,b,c}$	1.7, 1.0, 0.4
A, B, C	3016.3450, 1189.2370, 869.9797
A_s, B_s, C_s	3007.5976, 1185.7882, 867.4567
Charge, Multiplicity	0, 1
Predicted log column density	12.999±4.868
Electronic energy	-402.99160

geom1443



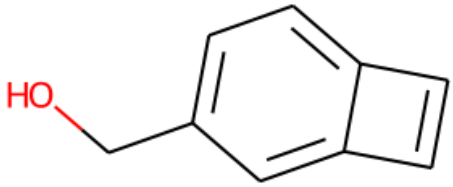
SMILES: C1=Cc2ccccc2CS1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.18)

Is DFT optimized?: True

Property	Value
Formula	C9H8S
Molecular weight	148.230
IUPAC name	1H-isothiochromene
$\mu_{a,b,c}$	1.0, 0.1, 0.7
A, B, C	2648.6961, 910.7480, 702.1274
A_s, B_s, C_s	2641.0149, 908.1069, 700.0912
Charge, Multiplicity	0, 1
Predicted log column density	13.060±5.078
Electronic energy	-745.82761

geom1444



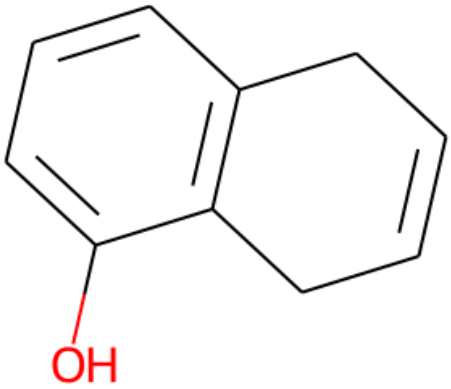
SMILES: OCc1ccc2c(c1)C=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.19)

Is DFT optimized?: True

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	3-bicyclo[4.2.0]octa-1(6),2,4,7-tetraenylmethanol
$\mu_{a,b,c}$	0.2, 1.7, 0.0
A, B, C	4111.8813, 847.6443, 705.8904
A_s, B_s, C_s	4099.9568, 845.1861, 703.8433
Charge, Multiplicity	0, 1
Predicted log column density	10.816±4.243
Electronic energy	-422.75423

geom1445



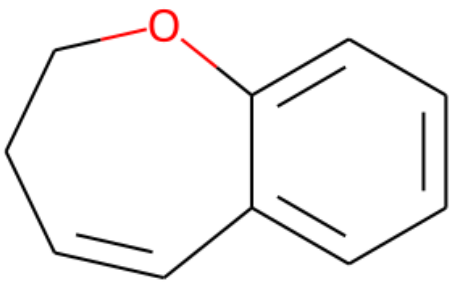
SMILES: Oc1cccc2c1CC=CC2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.20)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	5,8-dihydronaphthalen-1-ol
$\mu_{a,b,c}$	1.1, 0.3, 0.0
A, B, C	1862.0382, 1082.7981, 690.3994
A_s, B_s, C_s	1856.6382, 1079.6580, 688.3972
Charge, Multiplicity	0, 1
Predicted log column density	13.166±3.375
Electronic energy	-462.15866

geom1446



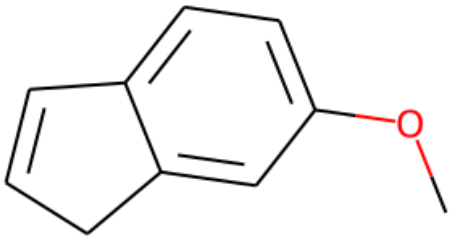
SMILES: C1=Cc2ccccc2OCC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.24)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	2,3-dihydro-1-benzoxepine
$\mu_{a,b,c}$	0.9, 0.4, 0.9
A, B, C	2411.7765, 933.7401, 692.6163
A_s, B_s, C_s	2404.7824, 931.0323, 690.6077
Charge, Multiplicity	0, 1
Predicted log column density	13.630±4.462
Electronic energy	-462.14689

geom1447



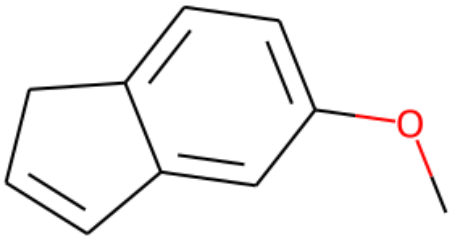
SMILES: COc1ccc2c(c1)CC=C2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.27)

Is DFT optimized?: False

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	6-methoxy-1H-indene
$\mu_{a,b,c}$	0.2, 0.5, 0.7
A, B, C	3240.1328, 706.1040, 587.9766
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	15.519±4.143
Electronic energy	-462.13925

geom1448



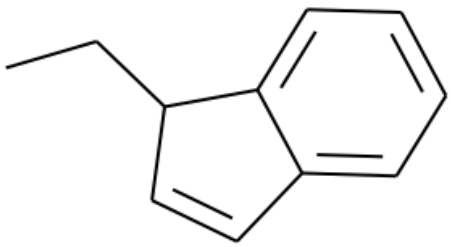
SMILES: COc1ccc2c(c1)C=CC2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.27)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	5-methoxy-1H-indene
$\mu_{a,b,c}$	0.5, 1.1, 0.0
A, B, C	2764.3214, 750.0691, 594.4027
A_s, B_s, C_s	2756.3049, 747.8939, 592.6789
Charge, Multiplicity	0, 1
Predicted log column density	15.519±4.143
Electronic energy	-462.14365

geom1449



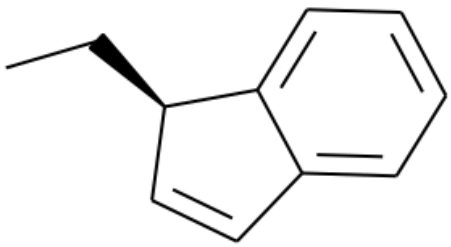
SMILES: CCC1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.34)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	1-ethyl-1H-indene
$\mu_{a,b,c}$	0.8, 0.2, 0.0
A, B, C	2368.8269, 814.5364, 632.5258
A_s, B_s, C_s	2361.9573, 812.1743, 630.6914
Charge, Multiplicity	0, 1
Predicted log column density	10.533±4.436
Electronic energy	-426.26116

geom1450



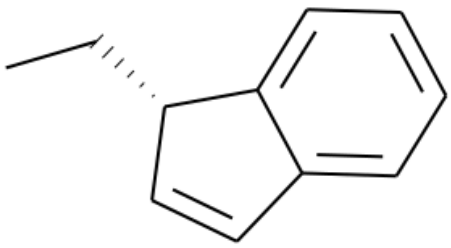
SMILES: CC[C@@H]1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.34)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	(1R)-1-ethyl-1H-indene
$\mu_{a,b,c}$	0.7, 0.1, 0.1
A, B, C	1946.1859, 971.1471, 767.7491
A_s, B_s, C_s	1940.5419, 968.3308, 765.5226
Charge, Multiplicity	0, 1
Predicted log column density	10.533±4.436
Electronic energy	-426.26164

geom1451



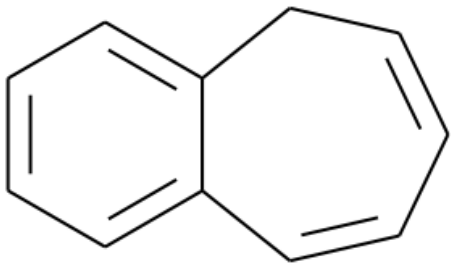
SMILES: CC[C@H]1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.34)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	(1S)-1-ethyl-1H-indene
$\mu_{a,b,c}$	0.8, 0.2, 0.0
A, B, C	2370.0407, 814.4063, 632.5411
A_s, B_s, C_s	2363.1676, 812.0445, 630.7067
Charge, Multiplicity	0, 1
Predicted log column density	10.533±4.436
Electronic energy	-426.26116

geom1452



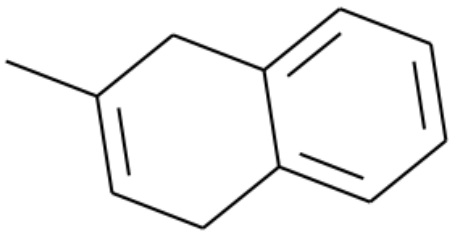
SMILES: C1=CCc2ccccc2C=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.35)

Is DFT optimized?: False

Property	Value
Formula	C11H10
Molecular weight	142.201
IUPAC name	9H-benzo[7]annulene
$\mu_{a,b,c}$	0.0, 0.6, 0.2
A, B, C	2395.2328, 921.0451, 668.1122
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.603±2.050
Electronic energy	-425.01922

geom1453



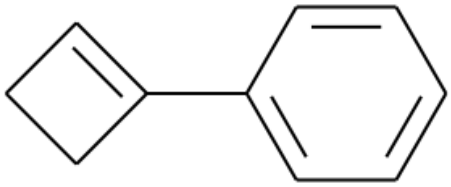
SMILES: CC1=CCc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.47)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	2-methyl-1,4-dihydronaphthalene
$\mu_{a,b,c}$	0.5, 0.1, 0.0
A, B, C	2618.4829, 793.2594, 615.7392
A_s, B_s, C_s	2610.8893, 790.9590, 613.9535
Charge, Multiplicity	0, 1
Predicted log column density	12.101±4.461
Electronic energy	-426.26643

geom1454



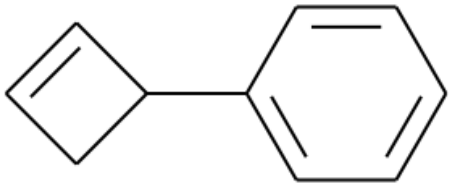
SMILES: C1=C(c2ccccc2)CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.48)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	cyclobuten-1-ylbenzene
$\mu_{a,b,c}$	0.1, 0.1, 0.0
A, B, C	3940.3293, 820.6626, 685.1060
A_s, B_s, C_s	3928.9023, 818.2827, 683.1192
Charge, Multiplicity	0, 1
Predicted log column density	12.198±4.478
Electronic energy	-386.91752

geom1455



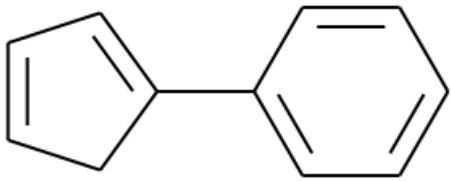
SMILES: C1=CC(c2ccccc2)C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.49)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	cyclobut-2-en-1-ylbenzene
$\mu_{a,b,c}$	0.3, 0.1, 0.1
A, B, C	3620.9389, 861.6981, 772.2841
A_s, B_s, C_s	3610.4382, 859.1992, 770.0445
Charge, Multiplicity	0, 1
Predicted log column density	11.810±4.869
Electronic energy	-386.90815

geom1456



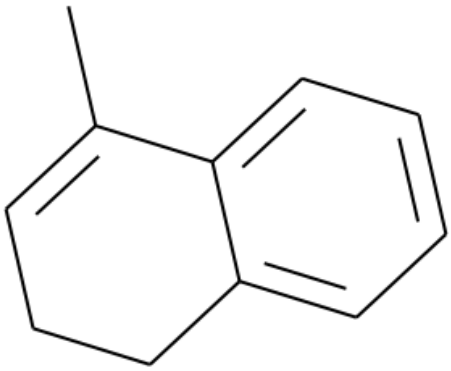
SMILES: C1=CCC(c2ccccc2)=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.50)

Is DFT optimized?: True

Property	Value
Formula	C11H10
Molecular weight	142.201
IUPAC name	cyclopenta-1,3-dien-1-ylbenzene
$\mu_{a,b,c}$	0.0, 0.4, 0.0
A, B, C	3423.6931, 668.7553, 561.4201
A_s, B_s, C_s	3413.7644, 666.8159, 559.7920
Charge, Multiplicity	0, 1
Predicted log column density	13.137±3.550
Electronic energy	-425.02844

geom1457



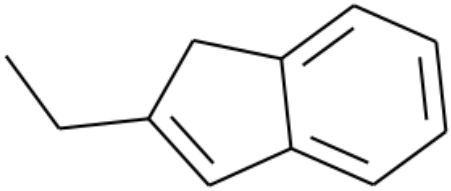
SMILES: CC1=CCCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.52)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	4-methyl-1,2-dihydronaphthalene
$\mu_{a,b,c}$	0.4, 0.2, 0.0
A, B, C	1790.3486, 1087.0600, 697.9691
A_s, B_s, C_s	1785.1566, 1083.9076, 695.9449
Charge, Multiplicity	0, 1
Predicted log column density	10.606±4.083
Electronic energy	-426.26997

geom1458



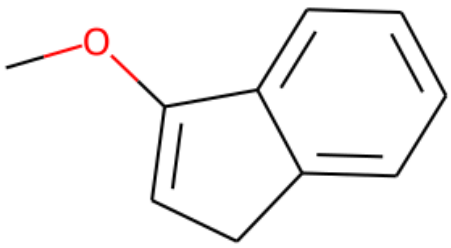
SMILES: CCC1=Cc2ccccc2C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.53)

Is DFT optimized?: False

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	2-ethyl-1H-indene
$\mu_{a,b,c}$	0.6, 1.1, 0.2
A, B, C	3211.1904, 664.3813, 572.4074
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.441±4.042
Electronic energy	-426.26315

geom1459



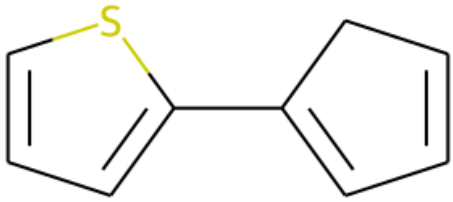
SMILES: COC1=CCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.58)

Is DFT optimized?: False

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	3-methoxy-1H-indene
$\mu_{a,b,c}$	0.6, 1.4, 0.7
A, B, C	2425.5203, 843.9865, 631.2908
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.870±4.298
Electronic energy	-462.14570

geom1460



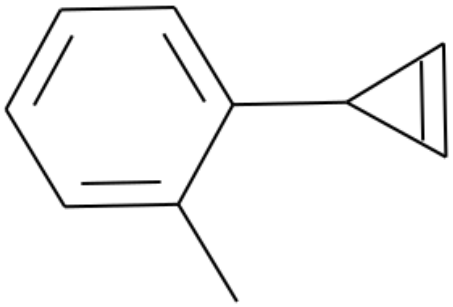
SMILES: C1=CCC(c2cccs2)=C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.58)

Is DFT optimized?: True

Property	Value
Formula	C9H8S
Molecular weight	148.230
IUPAC name	2-cyclopenta-1,3-dien-1-ylthiophene
$\mu_{a,b,c}$	0.0, 0.2, 0.0
A, B, C	3321.7030, 738.8921, 606.7151
A_s, B_s, C_s	3312.0701, 736.7493, 604.9556
Charge, Multiplicity	0, 1
Predicted log column density	12.920±5.452
Electronic energy	-745.79175

geom1461



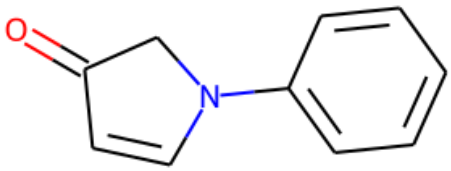
SMILES: `Cc1ccccc1C1C=C1`

Nearest TMC-1 molecule (distance): `c1ccc2c(c1)CC=C2` (4.58)

Is DFT optimized?: True

Property	Value
Formula	C10H10
Molecular weight	130.190
IUPAC name	1-cycloprop-2-en-1-yl-2-methylbenzene
$\mu_{a,b,c}$	0.9, 0.1, 0.2
A, B, C	2296.1445, 1145.9419, 805.0581
A_s, B_s, C_s	2289.4857, 1142.6187, 802.7234
Charge, Multiplicity	0, 1
Predicted log column density	12.014±4.785
Electronic energy	-386.87053

geom1462



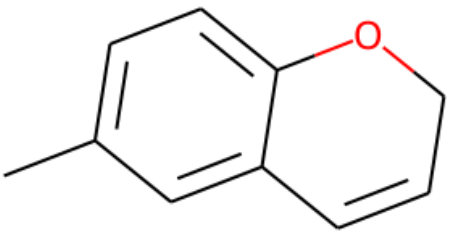
SMILES: O=C1C=CN(c2ccccc2)C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.59)

Is DFT optimized?: True

Property	Value
Formula	C10H9NO
Molecular weight	159.188
IUPAC name	1-phenyl-2H-pyrrol-3-one
$\mu_{a,b,c}$	4.5, 1.5, 0.4
A, B, C	3022.2647, 516.5502, 445.0428
A_s, B_s, C_s	3013.5002, 515.0522, 443.7522
Charge, Multiplicity	0, 1
Predicted log column density	13.060±3.893
Electronic energy	-516.28570

geom1463



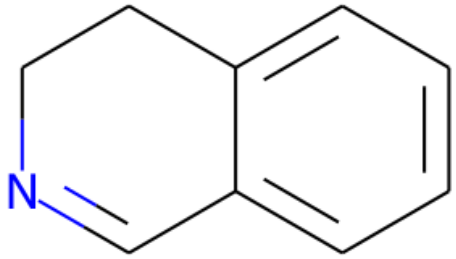
SMILES: Cc1ccc2c(c1)C=CCO2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.59)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	6-methyl-2H-chromene
$\mu_{a,b,c}$	0.2, 1.2, 0.6
A, B, C	2733.2755, 814.5133, 638.2112
A_s, B_s, C_s	2725.3490, 812.1512, 636.3604
Charge, Multiplicity	0, 1
Predicted log column density	13.769±4.440
Electronic energy	-462.15054

geom1464



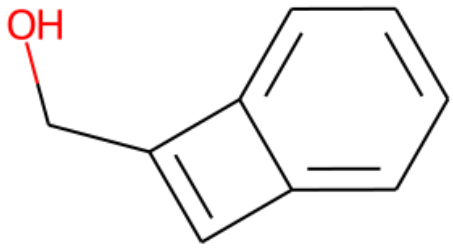
SMILES: C1=NCCc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.60)

Is DFT optimized?: True

Property	Value
Formula	C9H9N
Molecular weight	131.178
IUPAC name	3,4-dihydroisoquinoline
$\mu_{a,b,c}$	2.1, 1.3, 0.1
A, B, C	2989.4421, 1184.7225, 871.7266
A_s, B_s, C_s	2980.7727, 1181.2868, 869.1986
Charge, Multiplicity	0, 1
Predicted log column density	9.791±5.368
Electronic energy	-402.99651

geom1465



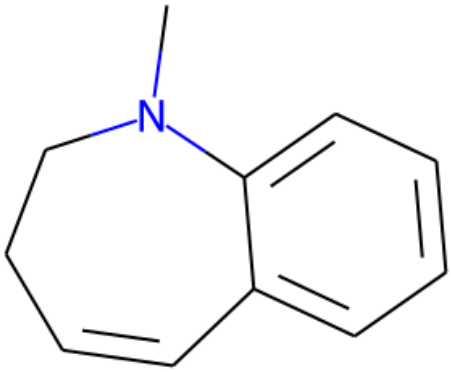
SMILES: OCC1=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.61)

Is DFT optimized?: True

Property	Value
Formula	C9H8O
Molecular weight	132.162
IUPAC name	7-bicyclo[4.2.0]octa-1,3,5,7-tetraenylmethanol
$\mu_{a,b,c}$	1.4, 1.7, 0.0
A, B, C	3977.1389, 822.8123, 684.6954
A_s, B_s, C_s	3965.6052, 820.4262, 682.7098
Charge, Multiplicity	0, 1
Predicted log column density	9.065±4.317
Electronic energy	-422.75933

geom1466



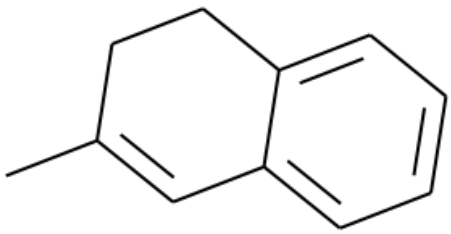
SMILES: CN1CCC=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.62)

Is DFT optimized?: True

Property	Value
Formula	C11H13N
Molecular weight	159.232
IUPAC name	1-methyl-2,3-dihydro-1-benzazepine
$\mu_{a,b,c}$	0.9, 0.6, 0.4
A, B, C	1465.3713, 929.9787, 631.7136
A_s, B_s, C_s	1461.1217, 927.2818, 629.8816
Charge, Multiplicity	0, 1
Predicted log column density	14.679±3.957
Electronic energy	-481.58064

geom1467



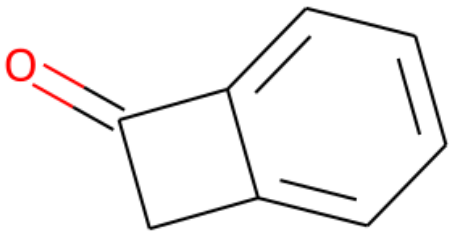
SMILES: CC1=Cc2ccccc2CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.66)

Is DFT optimized?: True

Property	Value
Formula	C11H12
Molecular weight	144.217
IUPAC name	3-methyl-1,2-dihydronaphthalene
$\mu_{a,b,c}$	1.0, 0.5, 0.1
A, B, C	2609.7079, 802.6124, 628.4040
A_s, B_s, C_s	2602.1397, 800.2848, 626.5817
Charge, Multiplicity	0, 1
Predicted log column density	10.410±4.263
Electronic energy	-426.27198

geom1468



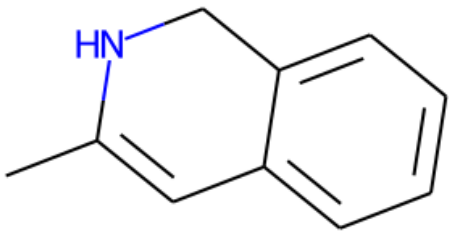
SMILES: O=C1Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.66)

Is DFT optimized?: True

Property	Value
Formula	C8H6O
Molecular weight	118.135
IUPAC name	bicyclo[4.2.0]octa-1,3,5-trien-7-one
$\mu_{a,b,c}$	3.5, 1.5, 0.0
A, B, C	3863.3992, 1423.5815, 1047.2127
A_s, B_s, C_s	3852.1953, 1419.4531, 1044.1758
Charge, Multiplicity	0, 1
Predicted log column density	11.719±4.176
Electronic energy	-383.52911

geom1469



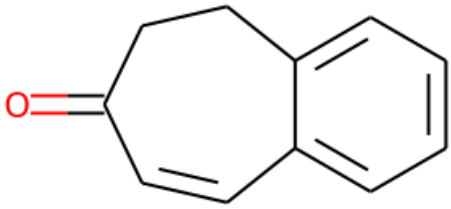
SMILES: CC1=Cc2ccccc2CN1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.71)

Is DFT optimized?: True

Property	Value
Formula	C10H11N
Molecular weight	145.205
IUPAC name	3-methyl-1,2-dihydroisoquinoline
$\mu_{a,b,c}$	1.9, 1.1, 0.4
A, B, C	2711.5953, 811.6661, 637.1528
A_s, B_s, C_s	2703.7317, 809.3123, 635.3051
Charge, Multiplicity	0, 1
Predicted log column density	12.338±4.666
Electronic energy	-442.30267

geom1470



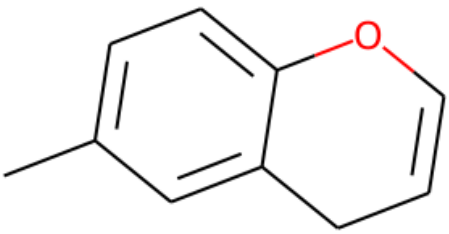
SMILES: O=C1C=Cc2ccccc2CC1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.73)

Is DFT optimized?: True

Property	Value
Formula	C11H10O
Molecular weight	158.200
IUPAC name	8,9-dihydrobenzo[7]annulen-7-one
$\mu_{a,b,c}$	4.2, 0.2, 0.4
A, B, C	2293.6841, 651.0444, 527.3751
A_s, B_s, C_s	2287.0324, 649.1564, 525.8457
Charge, Multiplicity	0, 1
Predicted log column density	10.496±4.178
Electronic energy	-500.25681

geom1471



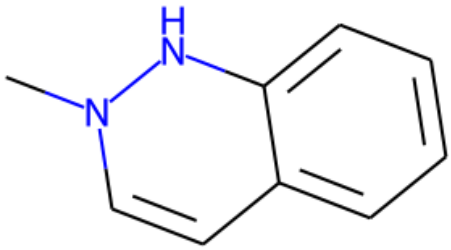
SMILES: Cc1ccc2c(c1)CC=CO2

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.75)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	6-methyl-4H-chromene
$\mu_{a,b,c}$	0.4, 1.2, 0.0
A, B, C	2706.5121, 816.6926, 632.2879
A_s, B_s, C_s	2698.6632, 814.3242, 630.4543
Charge, Multiplicity	0, 1
Predicted log column density	13.961±4.589
Electronic energy	-462.15294

geom1472



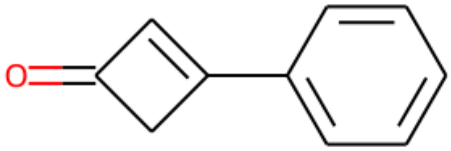
SMILES: CN1C=Cc2ccccc2N1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.75)

Is DFT optimized?: True

Property	Value
Formula	C9H10N2
Molecular weight	146.193
IUPAC name	2-methyl-1H-cinnoline
$\mu_{a,b,c}$	0.4, 0.5, 0.2
A, B, C	2438.9954, 909.6989, 723.4831
A_s, B_s, C_s	2431.9224, 907.0608, 721.3850
Charge, Multiplicity	0, 1
Predicted log column density	13.223±4.629
Electronic energy	-458.28987

geom1473



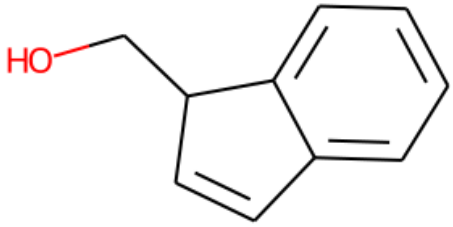
SMILES: O=C1C=C(c2ccccc2)C1

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.78)

Is DFT optimized?: False

Property	Value
Formula	C10H8O
Molecular weight	144.173
IUPAC name	3-phenylcyclobut-2-en-1-one
$\mu_{a,b,c}$	0.2, 0.5, 5.2
A, B, C	3943.0592, 573.5331, 502.3323
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.333±4.163
Electronic energy	-460.91442

geom1474



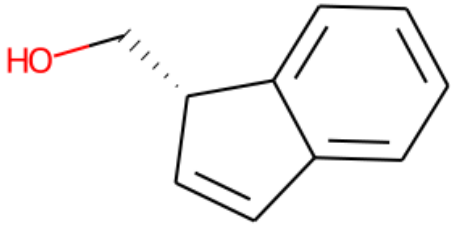
SMILES: OCC1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.78)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	1H-inden-1-ylmethanol
$\mu_{a,b,c}$	0.2, 1.0, 1.2
A, B, C	2410.3122, 813.8512, 633.6033
A_s, B_s, C_s	2403.3223, 811.4911, 631.7659
Charge, Multiplicity	0, 1
Predicted log column density	9.973±4.774
Electronic energy	-462.14796

geom1475



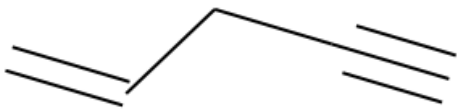
SMILES: OC[C@H]1C=Cc2ccccc21

Nearest TMC-1 molecule (distance): c1ccc2c(c1)CC=C2 (4.78)

Is DFT optimized?: True

Property	Value
Formula	C10H10O
Molecular weight	146.189
IUPAC name	[(1S)-1H-inden-1-yl]methanol
$\mu_{a,b,c}$	1.3, 0.5, 1.3
A, B, C	1865.5528, 1008.3174, 683.3436
A_s, B_s, C_s	1860.1427, 1005.3933, 681.3619
Charge, Multiplicity	0, 1
Predicted log column density	9.973±4.774
Electronic energy	-462.14781

geom1476



SMILES: C#CCC=C

Nearest TMC-1 molecule (distance): C=CC#C (3.13)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	pent-1-en-4-yne
$\mu_{a,b,c}$	0.5, 0.3, 0.1
A, B, C	19275.5119, 2561.1847, 2435.6897
A_s, B_s, C_s	19219.6130, 2553.7573, 2428.6262
Charge, Multiplicity	0, 1
Predicted log column density	11.339±2.364
Electronic energy	-193.97754

geom1477

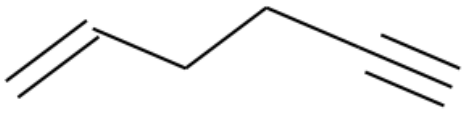
SMILES: C=CCC#CC

Nearest TMC-1 molecule (distance): C=CC#C (4.90)

Is DFT optimized?: False

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	hex-1-en-4-yne
$\mu_{a,b,c}$	0.1, 0.1, 0.3
A, B, C	12223.3390, 1317.4975, 1249.0399
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.253±2.582
Electronic energy	-233.27137

geom1478



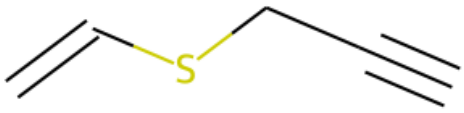
SMILES: C#CCCC=C

Nearest TMC-1 molecule (distance): C=CC#C (4.96)

Is DFT optimized?: False

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	hex-1-en-5-yne
$\mu_{a,b,c}$	0.0, 0.2, 0.8
A, B, C	16553.1699, 1376.9250, 1342.4427
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	10.155±2.965
Electronic energy	-233.26537

geom1479



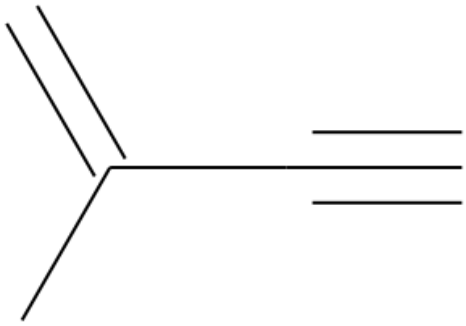
SMILES: C#CCSC=C

Nearest TMC-1 molecule (distance): C=CC#C (4.98)

Is DFT optimized?: False

Property	Value
Formula	C5H6S
Molecular weight	98.170
IUPAC name	3-ethenylsulfanylprop-1-yne
$\mu_{a,b,c}$	1.0, 1.0, 0.8
A, B, C	15947.1391, 1215.4622, 1137.5669
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	14.297±4.645
Electronic energy	-592.12061

geom1480



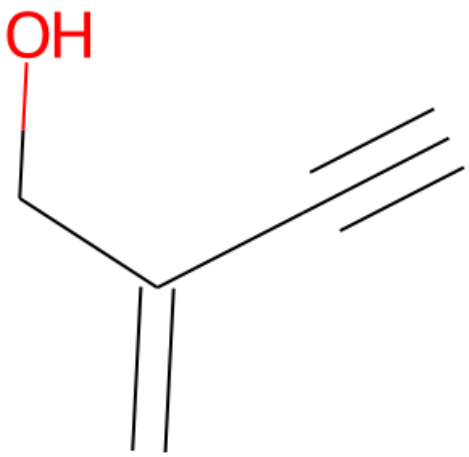
SMILES: C#CC(=C)C

Nearest TMC-1 molecule (distance): CC#C (5.18)

Is DFT optimized?: True

Property	Value
Formula	C5H6
Molecular weight	66.103
IUPAC name	2-methylbut-1-en-3-yne
$\mu_{a,b,c}$	0.6, 0.2, 0.0
A, B, C	9381.3694, 3975.2480, 2841.7620
A_s, B_s, C_s	9354.1634, 3963.7198, 2833.5209
Charge, Multiplicity	0, 1
Predicted log column density	10.784±4.378
Electronic energy	-193.98329

geom1481



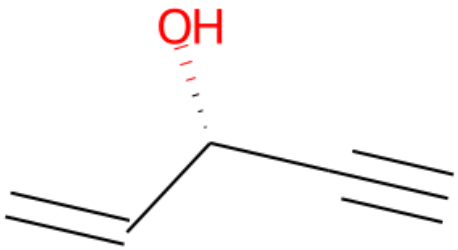
SMILES: C#CC(=C)CO

Nearest TMC-1 molecule (distance): C=CC#C (5.31)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	2-methylidenebut-3-yn-1-ol
$\mu_{a,b,c}$	0.7, 0.1, 1.3
A, B, C	8015.3246, 2254.0527, 1792.2419
A_s, B_s, C_s	7992.0802, 2247.5160, 1787.0444
Charge, Multiplicity	0, 1
Predicted log column density	9.969±5.272
Electronic energy	-269.17537

geom1482



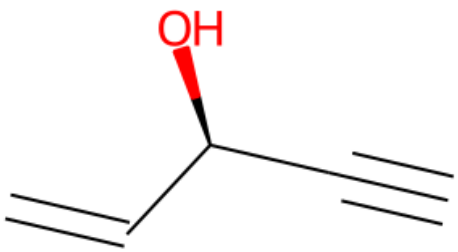
SMILES: C#C[C@@H](O)C=C

Nearest TMC-1 molecule (distance): C=CC#C (5.37)

Is DFT optimized?: False

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	(3S)-pent-1-en-4-yn-3-ol
$\mu_{a,b,c}$	1.1, 0.5, 0.7
A, B, C	5630.0609, 2491.2176, 1859.3721
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	9.674±4.718
Electronic energy	-269.14803

geom1483



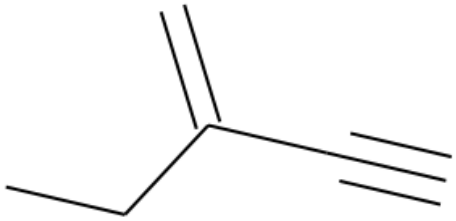
SMILES: C#C[C@H](O)C=C

Nearest TMC-1 molecule (distance): C=CC#C (5.37)

Is DFT optimized?: True

Property	Value
Formula	C5H6O
Molecular weight	82.102
IUPAC name	(3R)-pent-1-en-4-yn-3-ol
$\mu_{a,b,c}$	1.9, 0.8, 0.6
A, B, C	5759.2998, 2591.0415, 1925.7422
A_s, B_s, C_s	5742.5978, 2583.5275, 1920.1575
Charge, Multiplicity	0, 1
Predicted log column density	9.674±4.718
Electronic energy	-269.16564

geom1484



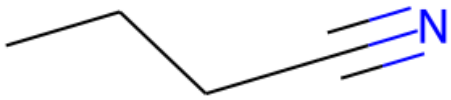
SMILES: C#CC(=C)CC

Nearest TMC-1 molecule (distance): CC#C (5.42)

Is DFT optimized?: True

Property	Value
Formula	C6H8
Molecular weight	80.130
IUPAC name	3-methylidenepent-1-yne
$\mu_{a,b,c}$	0.5, 0.0, 0.1
A, B, C	4614.1293, 3005.3432, 1995.2732
A_s, B_s, C_s	4600.7483, 2996.6277, 1989.4869
Charge, Multiplicity	0, 1
Predicted log column density	10.588±4.309
Electronic energy	-233.28994

geom1485



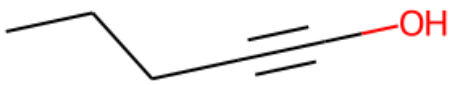
SMILES: CCCC#N

Nearest TMC-1 molecule (distance): CCC#N (2.79)

Is DFT optimized?: True

Property	Value
Formula	C4H7N
Molecular weight	69.107
IUPAC name	butanenitrile
$\mu_{a,b,c}$	4.2, 1.1, 0.0
A, B, C	23830.8614, 2257.6764, 2144.7124
A_s, B_s, C_s	23761.7519, 2251.1291, 2138.4927
Charge, Multiplicity	0, 1
Predicted log column density	10.623±3.614
Electronic energy	-211.31652

geom1486



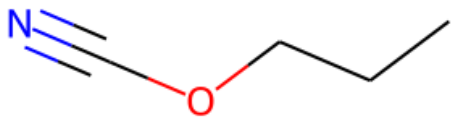
SMILES: CCCC#CO

Nearest TMC-1 molecule (distance): CCC#N (3.45)

Is DFT optimized?: True

Property	Value
Formula	C5H8O
Molecular weight	84.118
IUPAC name	pent-1-yn-1-ol
$\mu_{a,b,c}$	0.6, 1.5, 0.8
A, B, C	19763.2078, 1200.5620, 1157.2611
A_s, B_s, C_s	19705.8945, 1197.0804, 1153.9050
Charge, Multiplicity	0, 1
Predicted log column density	9.855±3.711
Electronic energy	-270.40450

geom1487



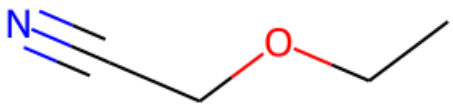
SMILES: CCCOC#N

Nearest TMC-1 molecule (distance): CCC#N (3.71)

Is DFT optimized?: True

Property	Value
Formula	C4H7NO
Molecular weight	85.106
IUPAC name	propyl cyanate
$\mu_{a,b,c}$	5.3, 0.1, 0.0
A, B, C	19533.0741, 1430.8963, 1367.5999
A_s, B_s, C_s	19476.4282, 1426.7467, 1363.6339
Charge, Multiplicity	0, 1
Predicted log column density	11.022±4.667
Electronic energy	-286.48819

geom1488



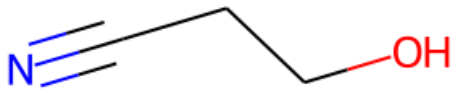
SMILES: CCOCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.07)

Is DFT optimized?: False

Property	Value
Formula	C4H7NO
Molecular weight	85.106
IUPAC name	2-ethoxyacetonitrile
$\mu_{a,b,c}$	4.8, 1.0, 0.8
A, B, C	16161.2259, 1456.8834, 1370.9364
A_s, B_s, C_s	- , - , -
Charge, Multiplicity	0, 1
Predicted log column density	12.345±4.770
Electronic energy	-286.48946

geom1489



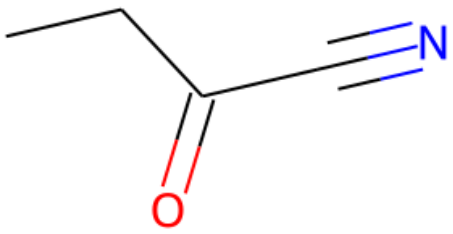
SMILES: N#CCCO

Nearest TMC-1 molecule (distance): CCC#N (4.08)

Is DFT optimized?: True

Property	Value
Formula	C3H5NO
Molecular weight	71.079
IUPAC name	3-hydroxypropanenitrile
$\mu_{a,b,c}$	2.9, 1.3, 1.5
A, B, C	26154.3217, 2306.8147, 2190.8541
A_s, B_s, C_s	26078.4741, 2300.1249, 2184.5007
Charge, Multiplicity	0, 1
Predicted log column density	10.600±3.942
Electronic energy	-247.20081

geom1490



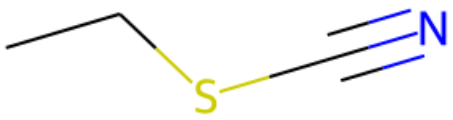
SMILES: CCC(=O)C#N

Nearest TMC-1 molecule (distance): CCC#N (4.14)

Is DFT optimized?: True

Property	Value
Formula	C4H5NO
Molecular weight	83.090
IUPAC name	propanoyl cyanide
$\mu_{a,b,c}$	3.2, 2.0, 0.0
A, B, C	8656.8548, 2230.5630, 1813.1475
A_s, B_s, C_s	8631.7500, 2224.0944, 1807.8894
Charge, Multiplicity	0, 1
Predicted log column density	10.386±4.239
Electronic energy	-285.29170

geom1491



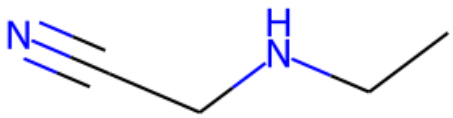
SMILES: CCSC#N

Nearest TMC-1 molecule (distance): CCC#N (4.14)

Is DFT optimized?: True

Property	Value
Formula	C3H5NS
Molecular weight	87.147
IUPAC name	ethyl thiocyanate
$\mu_{a,b,c}$	4.7, 0.2, 0.0
A, B, C	13441.6849, 2094.4901, 1854.5182
A_s, B_s, C_s	13402.7040, 2088.4160, 1849.1401
Charge, Multiplicity	0, 1
Predicted log column density	10.196±5.162
Electronic energy	-570.17233

geom1492



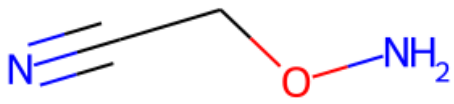
SMILES: CCNCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.17)

Is DFT optimized?: True

Property	Value
Formula	C4H8N2
Molecular weight	84.122
IUPAC name	2-(ethylamino)acetonitrile
$\mu_{a,b,c}$	4.0, 2.1, 1.0
A, B, C	15606.6373, 1416.8006, 1335.0994
A_s, B_s, C_s	15561.3780, 1412.6919, 1331.2277
Charge, Multiplicity	0, 1
Predicted log column density	12.526±4.687
Electronic energy	-266.63582

geom1493



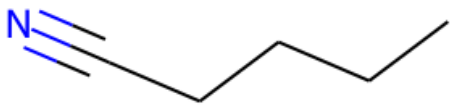
SMILES: N#CCON

Nearest TMC-1 molecule (distance): CCC#N (4.33)

Is DFT optimized?: True

Property	Value
Formula	C2H4N2O
Molecular weight	72.067
IUPAC name	2-aminooxyacetonitrile
$\mu_{a,b,c}$	4.3, 1.1, 0.0
A, B, C	31734.1380, 2454.9862, 2340.8279
A_s, B_s, C_s	31642.1090, 2447.8668, 2334.0395
Charge, Multiplicity	0, 1
Predicted log column density	10.928±4.031
Electronic energy	-263.17159

geom1494



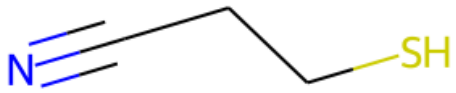
SMILES: CCCCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.36)

Is DFT optimized?: True

Property	Value
Formula	C5H9N
Molecular weight	83.134
IUPAC name	pentanenitrile
$\mu_{a,b,c}$	4.1, 1.7, 0.0
A, B, C	15178.3148, 1327.1705, 1258.5594
A_s, B_s, C_s	15134.2977, 1323.3217, 1254.9095
Charge, Multiplicity	0, 1
Predicted log column density	9.575±4.480
Electronic energy	-250.62026

geom1495



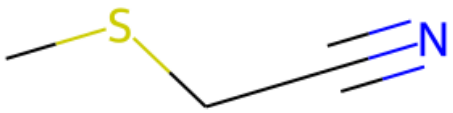
SMILES: N#CCCS

Nearest TMC-1 molecule (distance): CCC#N (4.36)

Is DFT optimized?: True

Property	Value
Formula	C3H5NS
Molecular weight	87.147
IUPAC name	3-sulfanylpropanenitrile
$\mu_{a,b,c}$	2.6, 1.1, 0.8
A, B, C	24892.7199, 1483.7350, 1437.0116
A_s, B_s, C_s	24820.5311, 1479.4322, 1432.8443
Charge, Multiplicity	0, 1
Predicted log column density	11.739±4.745
Electronic energy	-570.17706

geom1496



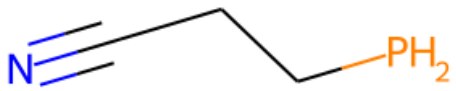
SMILES: CSCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.40)

Is DFT optimized?: True

Property	Value
Formula	C3H5NS
Molecular weight	87.147
IUPAC name	2-methylsulfanylacetonitrile
$\mu_{a,b,c}$	2.4, 0.8, 2.0
A, B, C	7721.0944, 2584.1815, 2141.0927
A_s, B_s, C_s	7698.7032, 2576.6874, 2134.8836
Charge, Multiplicity	0, 1
Predicted log column density	11.924±5.042
Electronic energy	-570.17450

geom1497



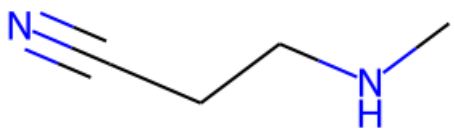
SMILES: N#CCCP

Nearest TMC-1 molecule (distance): CCC#N (4.41)

Is DFT optimized?: True

Property	Value
Formula	C3H6NP
Molecular weight	87.062
IUPAC name	3-phosphanylpropanenitrile
$\mu_{a,b,c}$	3.4, 0.4, 0.6
A, B, C	22906.5929, 1448.3010, 1399.6934
A_s, B_s, C_s	22840.1638, 1444.1009, 1395.6343
Charge, Multiplicity	0, 1
Predicted log column density	11.406±3.783
Electronic energy	-513.93218

geom1498



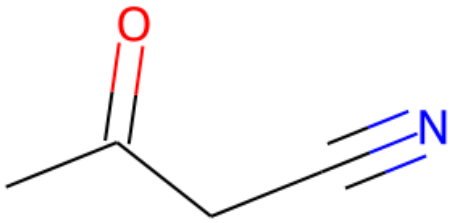
SMILES: CNCCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.45)

Is DFT optimized?: True

Property	Value
Formula	C4H8N2
Molecular weight	84.122
IUPAC name	3-(methylamino)propanenitrile
$\mu_{a,b,c}$	4.0, 1.2, 0.9
A, B, C	16711.6192, 1378.3477, 1309.6062
A_s, B_s, C_s	16663.1555, 1374.3505, 1305.8083
Charge, Multiplicity	0, 1
Predicted log column density	11.837±4.745
Electronic energy	-266.63843

geom1499



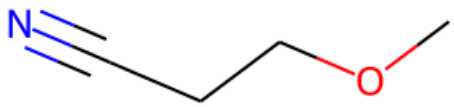
SMILES: CC(=O)CC#N

Nearest TMC-1 molecule (distance): CCC#N (4.49)

Is DFT optimized?: True

Property	Value
Formula	C4H5NO
Molecular weight	83.090
IUPAC name	3-oxobutanenitrile
$\mu_{a,b,c}$	0.9, 0.1, 0.8
A, B, C	8093.6757, 2344.2155, 1873.1184
A_s, B_s, C_s	8070.2040, 2337.4173, 1867.6863
Charge, Multiplicity	0, 1
Predicted log column density	11.291±4.087
Electronic energy	-285.30332

geom1500



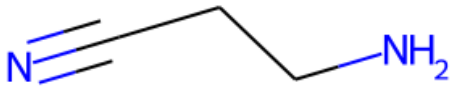
SMILES: COCCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.49)

Is DFT optimized?: True

Property	Value
Formula	C4H7NO
Molecular weight	85.106
IUPAC name	3-methoxypropanenitrile
$\mu_{a,b,c}$	3.9, 0.3, 0.0
A, B, C	18093.6330, 1419.5400, 1349.9338
A_s, B_s, C_s	18041.1614, 1415.4234, 1346.0190
Charge, Multiplicity	0, 1
Predicted log column density	12.111±4.623
Electronic energy	-286.49571

geom1501



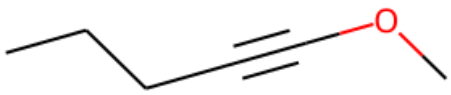
SMILES: N#CCCN

Nearest TMC-1 molecule (distance): CCC#N (4.52)

Is DFT optimized?: True

Property	Value
Formula	C3H6N2
Molecular weight	70.095
IUPAC name	3-aminopropanenitrile
$\mu_{a,b,c}$	4.2, 0.2, 0.9
A, B, C	25509.1933, 2295.1369, 2178.5646
A_s, B_s, C_s	25435.2166, 2288.4810, 2172.2467
Charge, Multiplicity	0, 1
Predicted log column density	8.609±3.834
Electronic energy	-227.34267

geom1502



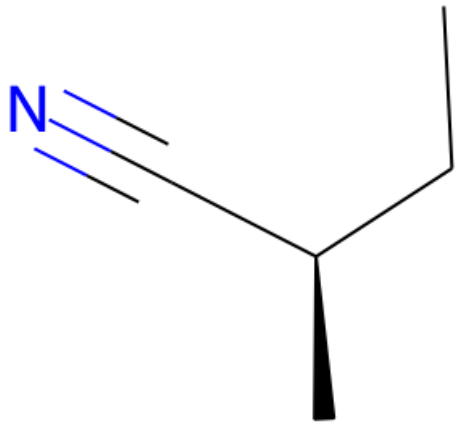
SMILES: CCCC#COC

Nearest TMC-1 molecule (distance): CCC#N (4.54)

Is DFT optimized?: True

Property	Value
Formula	C6H10O
Molecular weight	98.145
IUPAC name	1-methoxypent-1-yne
$\mu_{a,b,c}$	0.0, 1.8, 0.4
A, B, C	9624.2345, 871.2812, 819.7417
A_s, B_s, C_s	9596.3242, 868.7544, 817.3644
Charge, Multiplicity	0, 1
Predicted log column density	10.332±4.599
Electronic energy	-309.69768

geom1503



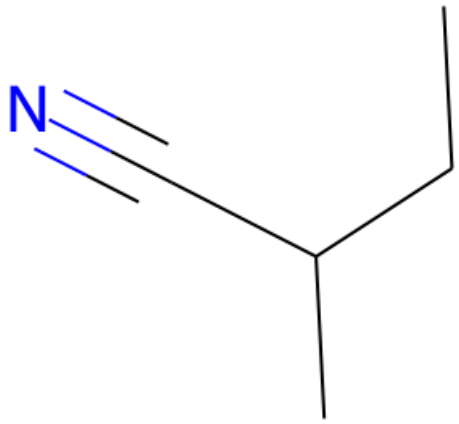
SMILES: CC[C@@H](C)C#N

Nearest TMC-1 molecule (distance): CCC#N (4.56)

Is DFT optimized?: True

Property	Value
Formula	C5H9N
Molecular weight	83.134
IUPAC name	(2R)-2-methylbutanenitrile
$\mu_{a,b,c}$	2.4, 3.4, 0.6
A, B, C	4067.2332, 3124.9866, 1911.0872
A_s, B_s, C_s	4055.4383, 3115.9241, 1905.5451
Charge, Multiplicity	0, 1
Predicted log column density	11.030±5.096
Electronic energy	-250.62164

geom1504



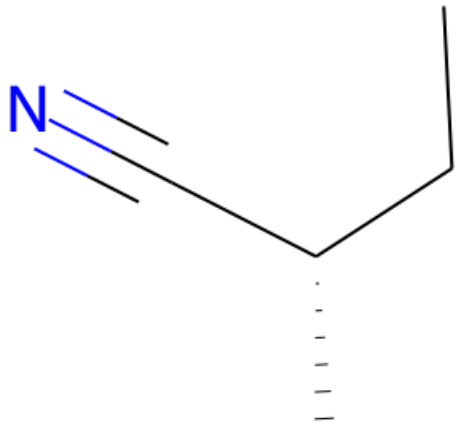
SMILES: CCC(C)C#N

Nearest TMC-1 molecule (distance): CCC#N (4.56)

Is DFT optimized?: True

Property	Value
Formula	C5H9N
Molecular weight	83.134
IUPAC name	2-methylbutanenitrile
$\mu_{a,b,c}$	2.4, 3.4, 0.6
A, B, C	4066.6459, 3125.0236, 1910.3670
A_s, B_s, C_s	4054.8526, 3115.9611, 1904.8270
Charge, Multiplicity	0, 1
Predicted log column density	11.030±5.096
Electronic energy	-250.62164

geom1505



SMILES: CC[C@H](C)C#N

Nearest TMC-1 molecule (distance): CCC#N (4.56)

Is DFT optimized?: True

Property	Value
Formula	C5H9N
Molecular weight	83.134
IUPAC name	(2S)-2-methylbutanenitrile
$\mu_{a,b,c}$	2.4, 3.4, 0.6
A, B, C	4064.5428, 3127.7847, 1911.2120
A_s, B_s, C_s	4052.7556, 3118.7141, 1905.6695
Charge, Multiplicity	0, 1
Predicted log column density	11.030±5.096
Electronic energy	-250.62164

geom1506

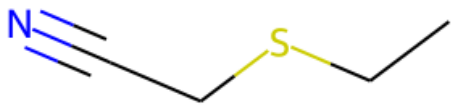
SMILES: CC#COCC

Nearest TMC-1 molecule (distance): CCC#N (4.59)

Is DFT optimized?: True

Property	Value
Formula	C5H8O
Molecular weight	84.118
IUPAC name	1-ethoxyprop-1-yne
$\mu_{a,b,c}$	0.8, 1.6, 0.0
A, B, C	23155.3575, 1294.8624, 1255.3768
A_s, B_s, C_s	23088.2069, 1291.1073, 1251.7362
Charge, Multiplicity	0, 1
Predicted log column density	11.762±4.292
Electronic energy	-270.39969

geom1507



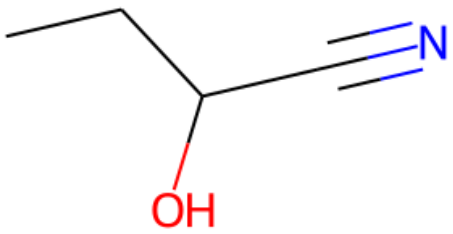
SMILES: CCSCC#N

Nearest TMC-1 molecule (distance): CCC#N (4.64)

Is DFT optimized?: True

Property	Value
Formula	C4H7NS
Molecular weight	101.174
IUPAC name	2-ethylsulfanylacetonitrile
$\mu_{a,b,c}$	2.2, 1.5, 2.0
A, B, C	5307.1120, 1642.2184, 1352.4639
A_s, B_s, C_s	5291.7214, 1637.4559, 1348.5418
Charge, Multiplicity	0, 1
Predicted log column density	11.308±5.336
Electronic energy	-609.47861

geom1508



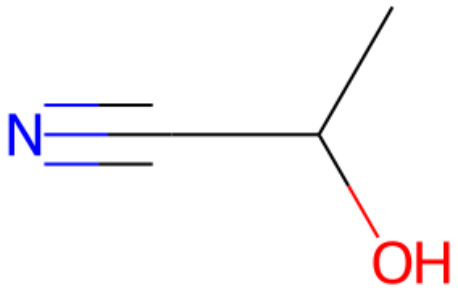
SMILES: CCC(O)C#N

Nearest TMC-1 molecule (distance): CCC#N (4.64)

Is DFT optimized?: True

Property	Value
Formula	C4H7NO
Molecular weight	85.106
IUPAC name	2-hydroxybutanenitrile
$\mu_{a,b,c}$	3.6, 0.4, 0.5
A, B, C	7075.8430, 2223.5256, 1806.0811
A_s, B_s, C_s	7055.3231, 2217.0774, 1800.8434
Charge, Multiplicity	0, 1
Predicted log column density	10.104±4.980
Electronic energy	-286.50378

geom1509



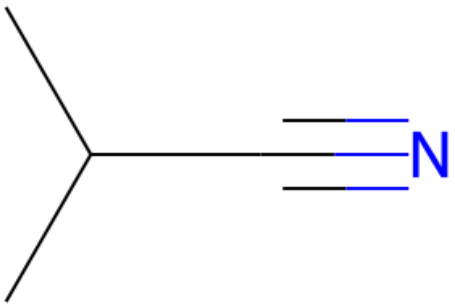
SMILES: CC(O)C#N

Nearest TMC-1 molecule (distance): OC#N (4.61)

Is DFT optimized?: True

Property	Value
Formula	C3H5NO
Molecular weight	71.079
IUPAC name	2-hydroxypropanenitrile
$\mu_{a,b,c}$	3.1, 1.4, 0.4
A, B, C	8586.0761, 4011.3551, 2979.8709
A_s, B_s, C_s	8561.1765, 3999.7221, 2971.2292
Charge, Multiplicity	0, 1
Predicted log column density	11.866±4.347
Electronic energy	-247.19990

geom1510



SMILES: CC(C)C#N

Nearest TMC-1 molecule (distance): CCC#N (4.72)

Is DFT optimized?: True

Property	Value
Formula	C4H7N
Molecular weight	69.107
IUPAC name	2-methylpropanenitrile
$\mu_{a,b,c}$	4.2, 0.0, 0.7
A, B, C	7935.1540, 3951.7330, 2890.9144
A_s, B_s, C_s	7912.1421, 3940.2730, 2882.5308
Charge, Multiplicity	0, 1
Predicted log column density	12.029±4.190
Electronic energy	-211.31733