

Alternatives for epoxides in Graphene Oxide

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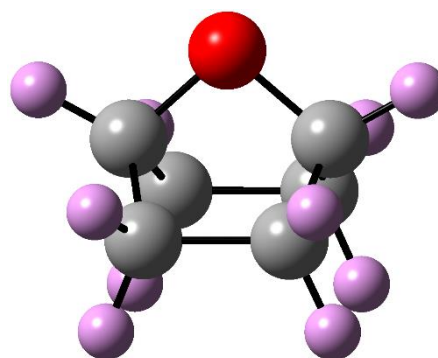
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1. Input Coordinates of Cyclohexane isomers hosting epoxides or ether bridges.

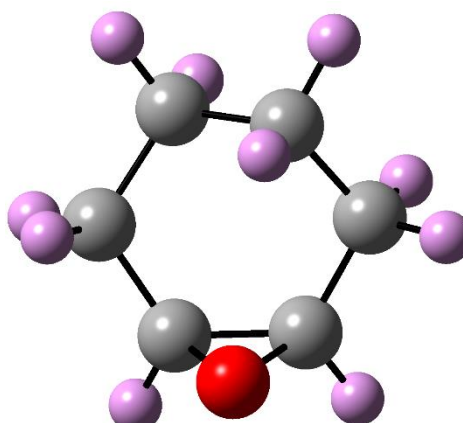
A. C_{2v}

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	0.61698946	-0.54504724	0.48174436
C	0.06335804	-0.05596974	1.28608546
C	-0.08353580	1.75005286	2.82347349
C	-1.74699260	-0.13296446	2.82347278
C	-0.40329608	0.35627156	3.36065739
C	-1.41741761	-0.42411034	1.35830402
C	0.24603919	1.45890699	1.35830473
H	0.80121781	2.16200611	3.32173354
H	-2.04666916	-1.06177493	3.32173233
H	-0.27312174	0.24127519	4.43885016
H	-2.03559582	0.14500260	0.65791037
H	-0.39497755	2.00216693	0.65791107
H	-0.90954677	2.45673633	2.94549587
H	-2.55016505	0.59957201	2.94549517
H	-1.55981202	-1.49186354	1.15734520
H	1.28807496	1.73191750	1.15734642
O	0.51844356	-0.45799262	2.59906804



B. C_1

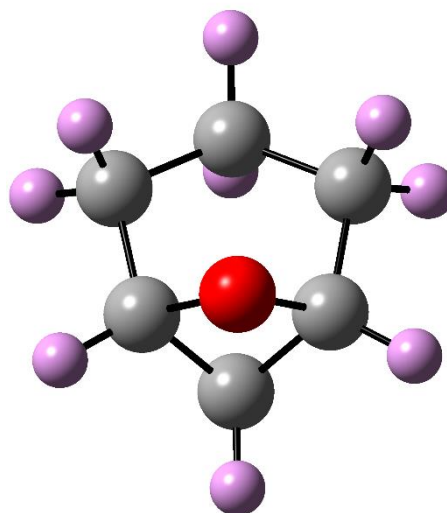
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	-1.31408576	2.13069418	-0.55868727
C	-0.78548766	1.32006931	-0.07649136
C	-0.66177261	-1.16989328	0.32529089
C	1.51606490	0.08859490	0.10128382
C	0.71656187	-1.13964735	-0.33293435
C	0.71964255	1.35135781	-0.00282147
C	-1.51451425	0.01621654	-0.12617192
H	-0.54655342	-1.15340335	1.41612012
H	1.86296650	-0.03996285	1.13380437
H	0.59817748	-1.13606302	-1.42369185



H	1.26777074	2.18944014	-0.40915293
H	-1.84099921	-0.15382418	-1.15928075
H	-1.17610983	-2.10389536	0.07238108
H	2.41327644	0.16916081	-0.52303656
H	1.27423839	-2.04654213	-0.07351844
H	-2.42043780	0.07486016	0.48727327
O	-0.10873828	1.60283772	1.14963328

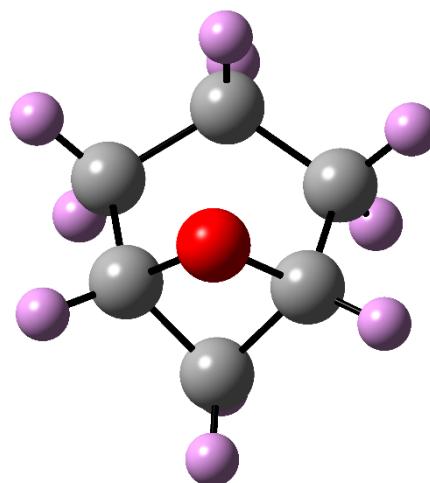
C. C_s

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	0.38934807	-0.65075113	0.51347989
C	-0.08034668	-0.08270576	1.32176786
C	-0.21064459	2.02254101	2.66937790
C	-1.48330380	-0.13005296	2.77787725
C	-1.10575906	1.13720039	3.54643617
C	-1.62380237	0.02549918	1.24286826
C	0.66033708	1.19680285	1.71342992
H	0.40174272	2.69356925	3.28123059
H	-2.00363691	1.69398813	3.83590276
H	-2.25443702	-0.73997396	3.25742710
H	-0.57955918	0.86621897	4.46903906
H	-2.11174662	-0.81850121	0.74529169
H	1.61043341	0.94012714	2.19607667
H	0.89751620	1.79189665	0.82483690
H	-2.04200390	0.96264228	0.87040467
H	-0.85910213	2.67136942	2.06568842
O	-0.25607079	-0.90999539	2.53025485



D. C_s

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	-0.12932772	-0.01140886	-0.08452269
C	-0.04341961	-0.04195740	1.00730840
C	-0.00523205	1.59958801	2.95124999
C	-1.31980857	-0.59414597	3.16411397
C	-1.36862441	0.94762826	3.18707734
C	-1.39898163	-0.35731916	1.64173992
C	0.45697741	1.31573112	1.51643015
H	0.72436148	1.21139720	3.67109320
H	-0.41184213	-1.06682182	3.54542474
H	0.03659543	2.09519421	0.86647714
H	0.67685607	-0.83068885	1.25282565

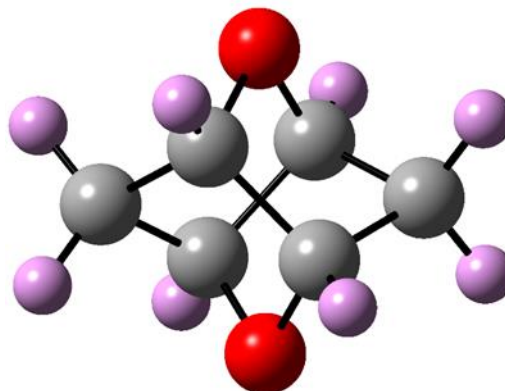


H	-0.06665792	2.68253946	3.10568950
H	-2.20005311	-1.08236175	3.59367563
H	-1.95038717	1.37158716	4.01057899
H	-2.00757368	-1.08665416	1.09949440
H	1.54530396	1.39727894	1.42618826
O	-2.13223167	0.89256132	1.92463585

2. Input Coordinates of Cyclohexane isomers hosting epoxides or ether bridges.

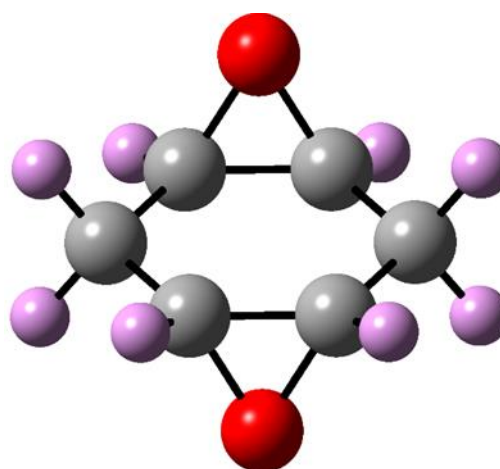
A. D_2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
C	-0.16958285	0.22438394	1.18697418
C	-0.54753967	1.74112939	2.67089454
C	-1.05954346	-0.54231993	3.30920520
C	-1.69020693	0.66581212	2.63909286
C	0.26146081	-0.24852713	2.62000019
C	-0.01339086	1.73371909	1.24927569
H	-1.02270107	-0.44934350	4.39854106
H	1.08539414	-0.95550611	2.71302357
H	-0.65934956	2.27638730	0.55292579
H	0.20531525	-0.31968019	0.32049602
H	-2.70088508	0.96650383	2.91377985
H	1.02918195	2.05393571	1.16467154
H	-1.49299996	-1.49818118	3.00082338
H	-0.73569295	2.69148080	3.16966233
O	0.54926734	1.01131161	3.28985423
O	-1.62220166	0.18008755	1.26862666



B. C_{2h}

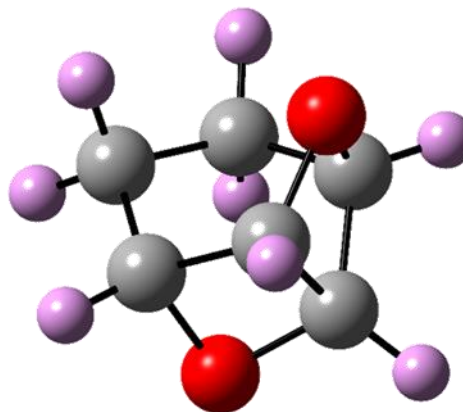
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	-0.38245548	0.52929340	-0.22917145
C	-0.29548398	0.46552315	0.84683692
C	0.11980872	1.86682174	3.03593170
C	-1.63496254	-0.09081175	2.90673942
C	-0.92714867	1.00477748	3.66289950
C	-1.34244137	-0.39652111	1.47380472
C	0.41232989	1.56111238	1.60299700
H	1.04912274	1.77389409	3.61018311
H	-2.04952982	-0.93088848	3.44695213
H	-2.27175539	-0.30359346	0.89955330
H	0.82689717	2.40118911	1.06278429
H	-0.19283485	2.91426233	3.12047151



H	-0.84017717	0.94100723	4.73890787
H	-1.02979780	-1.44396170	1.38926490
O	1.02213763	0.27831195	1.38775794
O	-2.24477028	1.19198868	3.12197848

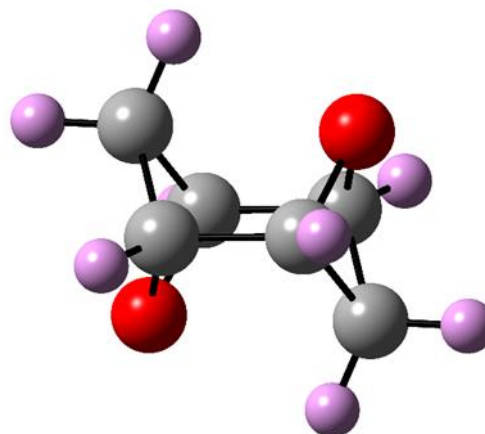
C. C_2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
C	0.95490959	0.52869767	2.38320626
C	-0.77994011	1.59020790	2.24713332
C	-1.08420670	-0.63301483	3.33523287
C	-1.79490221	0.67744214	2.94012269
C	0.15667736	-0.79705513	2.45385826
C	0.03407312	0.79956661	1.19259281
H	-0.77826197	-0.58337464	4.38693089
H	-2.23184776	1.15875485	3.82120835
H	0.48262321	1.30367283	0.33572625
H	-1.76433080	-1.48508796	3.23375457
H	-2.61619357	0.45675610	2.24808713
H	0.75093236	-1.69791095	2.62675577
O	0.43226758	1.70820290	3.06879396
H	-1.15557789	2.56362376	1.92166197
H	2.02633517	0.52907819	2.17927576
O	-0.20664783	-0.63330221	1.03975915



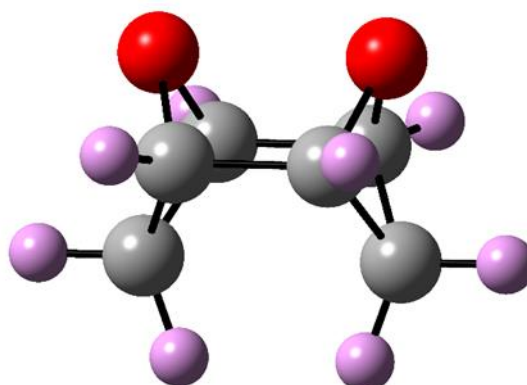
D. C_{2h}

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	-1.03049599	0.26634589	0.18754263
C	-0.11825731	0.09432065	0.76197766
C	-0.95822304	1.74780587	2.52463997
C	-1.53683097	-0.13872561	2.87854858
C	-1.06652240	0.96941761	3.87640958
C	-0.22655667	-0.68406761	2.11374727
C	0.35205125	1.20246386	1.75983866
H	-1.10649235	2.82833012	2.56474324
H	-2.24324782	-0.87802247	3.26004576
H	-1.84655901	1.33560323	4.55309653
H	-0.07828737	-1.76459186	2.07364400
H	1.05846810	1.94176072	1.37834148
H	0.66177929	-0.27186497	0.08529071
H	-0.15428373	0.79739237	4.45084461
O	1.02604639	0.06766532	2.49072077
O	-2.21082610	0.99607294	2.14766647



E. C_{2v}

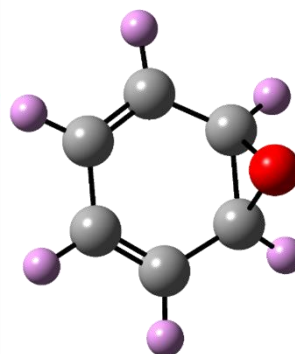
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	-1.21443430	1.34785791	0.57769161
C	-0.60899098	0.46062686	0.74927229
C	-0.16130215	1.00052934	3.26945105
C	-1.77768491	-0.15309463	3.00774996
C	-1.65860100	1.40069598	3.08814402
C	-1.15708751	-0.70892435	1.62485757
C	0.45929525	0.44469961	1.88655866
H	-1.96327501	2.01854703	2.24635170
H	-1.71340951	-1.49501048	1.11080240
H	1.46665185	0.77462212	1.62567149
H	-0.22411757	0.14322665	-0.22872225
H	0.46387815	1.67274291	3.86017670
H	-2.71618322	-0.59688968	3.34530761
H	-2.11551493	1.83723127	3.98592481
O	0.30885158	-1.06152323	1.79016953
O	-0.72943360	-0.13159706	4.10380583



3. Input coordinates of the cyclohexadiene isomers hosting epoxides and 1,4 bridges.

A. C_s

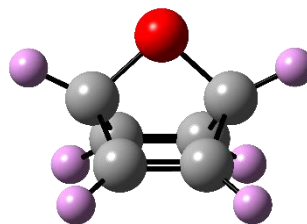
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
H	0.44218196	-1.87061750	1.24252416
C	0.01123637	-1.04537429	0.71511584
C	0.37191048	1.42960367	0.77462552
C	0.23571461	0.26528472	-1.47116363
C	0.37890005	1.42643852	-0.77644087
C	-0.02309260	-1.03972363	-0.70707365
C	0.23888743	0.26930683	1.47357684
H	0.30129964	0.26259281	-2.53914835
H	0.50243471	2.34774682	-1.30637500
H	0.43569007	-1.82929781	-1.26473939
H	0.29470134	0.27338401	2.54211237
H	0.47970492	2.35456673	1.30162050
O	-1.34541300	-1.27061486	0.01536571



B. C_{2v}

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

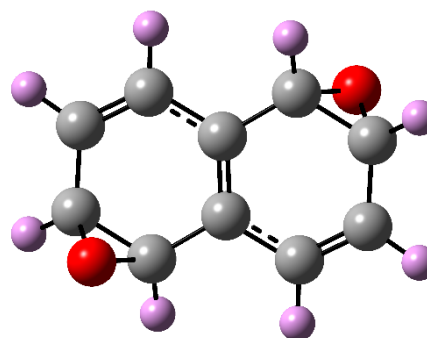
H	-0.47886681	0.25711355	-0.11571863
C	-0.33067045	0.46658379	0.92983986
C	0.08212829	1.38274574	2.97650403
C	-1.82608552	0.13947598	2.86884681
C	-1.35390082	1.27331878	3.42428626
C	-0.67768443	-0.44176951	2.08272250
C	0.14151425	1.60042659	1.48527931
H	-1.89180116	1.98612520	4.02562037
H	-0.65633531	-1.51809861	1.91761229
H	0.45494778	2.49945419	0.98274445
H	0.78016213	1.93131910	3.60739034
H	-2.82561575	-0.25621544	2.92715729
O	0.40051157	-0.04179309	2.98173215



4. Input coordinates of the most stable isomer of $C_{10}H_8O_2$.

A. C_i

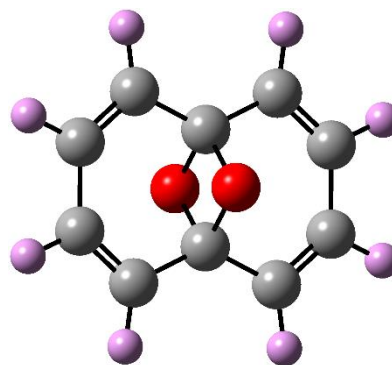
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.537735453	-0.020177278	0.962268697
1	-0.166904453	0.788567425	1.582546295
6	0.061014305	-0.076710228	-0.381888055
1	0.241461491	0.868919962	-0.884602499
6	0.393483163	-1.225250932	-0.997583415
1	0.842446887	-1.207953277	-1.986011267
6	0.149182517	-2.518522978	-0.367749243
6	0.523271358	-3.726382185	-1.139524259
1	0.293877071	-3.678255216	-2.199409527
6	-0.408079809	-2.571189617	0.870413730
6	0.278838161	-5.069535317	-0.459604210
1	-0.091992839	-5.878280021	-1.079881807
6	-0.652380455	-3.864461663	1.500247903
1	-1.101344179	-3.881759318	2.488675755
6	-0.782168650	-1.363330410	1.642188746
1	-0.552774364	-1.411457380	2.702074014
6	-0.319911597	-5.013002367	0.884552543
1	-0.500358783	-5.958632557	1.387266986
8	1.600254528	-4.591248164	-0.745107047
8	-1.859151820	-0.498464431	1.247771534



B. D_{2H}

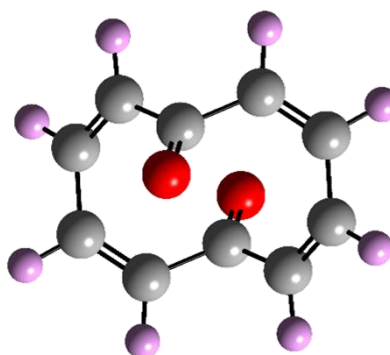
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
1	-0.276044511	-0.125497156	-0.112101322

6 -0.151011964 -0.1144441370 0.967407384
 1 -0.528987286 1.903304222 0.994875647
 6 -0.291587568 1.054597579 1.649221068
 6 0.300195535 -1.251007809 2.975564623
 6 -0.213664825 1.499369426 3.024518112
 6 0.142024618 -1.256121013 1.624180414
 6 0.243464725 -0.281621526 4.049067188
 6 -0.270395635 2.468755709 4.098020677
 1 0.252949629 -2.186474787 1.073515441
 1 0.558787186 -0.685556322 6.078709653
 1 0.535437154 -2.243726524 3.380534324
 6 -0.112224718 2.473868913 5.449404886
 1 -0.505637254 3.461474424 3.693050976
 1 -0.223149729 3.404222687 6.000069859
 6 0.180811864 1.332189270 6.106177916
 1 0.305844411 1.343245056 7.185686622
 6 0.321387468 0.163150321 5.424364232
 8 0.961383927 0.787691887 3.425336138
 8 -0.931584027 0.430056013 3.648249162



C. C_{2H}

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
1	0.106823771	-0.006400146	0.090851594
6	-0.012655161	0.076384586	1.175051390
1	0.033255395	2.239381092	1.025162749
6	-0.181161875	1.392483731	1.670396363
6	0.192712930	-1.400931092	3.281869396
6	-0.692800923	1.629050579	2.953183721
6	0.008026898	-1.171969510	1.896464842
6	0.722600823	-0.411302679	4.120401579
6	-0.162913030	2.618678992	3.791715904
1	-0.126037191	-2.069205734	1.285226996
1	-0.003455495	-1.021633192	6.048422551
6	0.021773002	2.389717410	5.177120458
1	0.155837091	3.286953634	5.788358304
6	0.042455061	1.141363314	5.898533910
1	-0.077023871	1.224148046	6.982733706
6	0.210961775	-0.174735831	5.403188937
8	-1.660814917	1.109596114	3.261773600
8	1.690614817	0.108151786	3.811811700
1	0.053488261	3.598888759	3.377112941
1	-0.023688361	-2.381140859	3.696472359



D. C_2

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

1	0.767836827	0.423039943	0.375656098
6	0.353298965	0.215743688	1.358339578
1	-0.342381362	2.222355611	1.590219907
6	-0.286526441	1.236785047	2.052391875
6	-0.025692233	-1.333291906	3.161181540
6	-0.973210913	0.989251299	3.275743154
6	0.420478536	-1.065809939	1.875474993
6	-0.468986467	-0.289317412	4.010136120
6	-0.933668294	2.178060581	4.045343876
1	0.836791932	-1.870880452	1.277049157
1	1.187998926	-0.836154319	5.319658777
1	0.020490294	-2.354027316	3.540221908
6	-0.058948255	2.306801355	5.113963056
1	-1.556934884	3.025690215	3.761146821
1	0.013856553	3.258590851	5.632002698
6	0.728441842	1.241286622	5.512732436
1	1.456658626	1.376778261	6.307605086
6	0.566802299	-0.020167220	4.950400275
8	-2.063202573	0.863972489	2.956023585
8	-1.303855348	-0.741431915	4.646205009

