Supporting Information:

Exhaustive Product Analysis of Three Benzene Discharges by Microwave Spectroscopy

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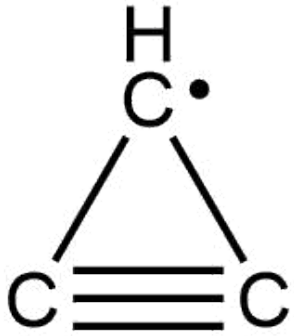
Contents

Molecule 1

IUPAC Name: cyclopropa-1-yn-3-ylradical

Common name: cyclic-C3H, c-C3H

SMILES: [CH]1C#C1

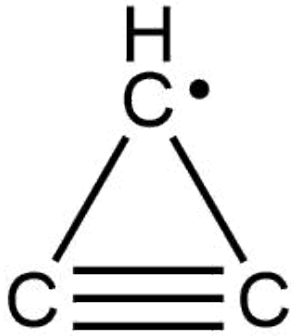


Molecule 2

IUPAC Name: cyclopropa-1-yn-3-ylradical (ve1)

Common name: cyclic-C3H, c-C3H (ve1)

SMILES: [CH]1C#C1



2: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	1	1	0	1	1	1	1	1	1	1	14714.48800	14714.48758	0.00042	0.00500	0.00000
2:	1	1	0	1	0	1	1	1	1	1	14718.44430	14718.44618	-0.00188	0.00500	0.00000
3:	1	1	0	1	1	1	1	1	1	0	14723.75430	14723.75393	0.00037	0.00500	0.00000
4:	1	1	0	1	0	1	1	1	2	1	14787.63700	14787.63497	0.00203	0.00500	0.00000
5:	1	1	0	1	1	1	1	1	2	2	14797.17410	14797.17447	-0.00037	0.00500	0.00000
6:	1	1	0	2	2	1	1	1	1	1	14836.07200	14836.07046	0.00154	0.00500	0.00000
7:	1	1	0	2	1	1	1	1	1	0	14859.64910	14859.64921	-0.00011	0.00500	0.00000
8:	1	1	0	2	2	1	1	1	2	1	14905.25670	14905.25925	-0.00255	0.00500	0.00000
9:	1	1	0	2	2	1	1	1	2	2	14918.75790	14918.75735	0.00055	0.00500	0.00000
10:	1	1	0	2	1	1	1	1	2	1	14919.57300	14919.57166	0.00134	0.00500	0.00000
11:	1	1	0	2	1	1	1	1	2	2	14933.06910	14933.06976	-0.00066	0.00500	0.00000
12:	2	1	2	3	3	1	1	1	2	2	90016.00000	90016.04162	-0.04162	0.10000	0.00000
13:	2	1	2	3	2	1	1	1	2	2	90032.00000	90032.07181	-0.07181	0.10000	0.00000
14:	2	1	2	2	2	1	1	1	2	2	90283.00000	90282.93868	0.06132	0.10000	0.00000
15:	2	1	1	2	2	1	1	0	2	2	119716.80000	119716.91146	-0.11146	0.10000	0.00000
16:	2	1	1	3	3	1	1	0	2	2	119785.20000	119785.16134	0.03866	0.10000	0.00000
17:	2	1	1	3	2	1	1	0	2	2	119800.40000	119800.38911	0.01089	0.10000	0.00000
18:	2	1	2	3	2	1	1	1	2	1	90018.68000	90018.57371	0.10629	0.10000	0.00000
19:	2	1	1	3	2	1	1	0	2	1	119786.00000	119786.07670	-0.07670	0.10000	0.00000
20:	2	1	2	3	2	1	1	1	1	1	89949.42000	89949.38492	0.03508	0.10000	0.00000
21:	2	1	2	2	1	1	1	1	1	1	90184.55000	90184.54886	0.00114	0.10000	0.00000
22:	2	1	2	2	2	1	1	1	1	1	90200.30000	90200.25179	0.04821	0.10000	0.00000

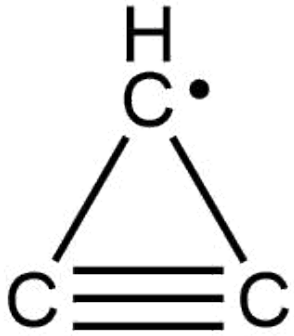
```
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.97483E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   1.00000E+00   10   1.03356E-01   11   7.19285E-01   12   9.85030E-01
   13   4.66204E-01   14   9.56370E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A  44185.950000000(  0)      0.000000000
   2         20000          B       33664.2104( 76)          -0.0000
   3         30000          C       18810.7104( 76)          -0.0000
   4           200       -D_N     -0.054930000(  0)     -0.000000000
   5          1100      -D_NK     -0.590210000(  0)      0.000000000
   6          2000       -D_K      0.414200000(  0)      0.000000000
   7         40100       -d_N     -0.020640000(  0)     -0.000000000
   8         41000       -d_K     -0.359700000(  0)      0.000000000
   9      10010000     eps_aa           96.134( 38)            0.000
  10      10020000     eps_bb           70.050( 38)           -0.000
  11      10030000     eps_cc         -193.815( 38)           -0.000
  12     120000000     a_F(H)         -22.8176( 58)          -0.0000
  13     120010000    T_aa(H)          15.6638(136)           0.0000
  14     120020000    T_bb(H)          -0.0828(109)          -0.0000
 MICROWAVE AVG =        0.000031 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.045448 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.49191         0.49191
```

Molecule 3

IUPAC Name: cyclopropa-1-yn-3-ylradical (ve2)

Common name: cyclic-C3H, c-C3H (ve2)

SMILES: [CH]1C#C1



3: Fit file

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EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  1  0  1  1  1  1  1  1  1         14396.65960   14396.65733    0.00227    0.00500   0.00000
    2:   1  1  0  1  0  1  1  1  1  1         14398.51300   14398.51300   -0.00000    0.00500   0.00000
    3:   1  1  0  1  1  1  1  1  1  0         14407.17740   14407.17815   -0.00075    0.00500   0.00000
    4:   1  1  0  1  0  1  1  1  2  1         14470.70580   14470.70527    0.00053    0.00500   0.00000
    5:   1  1  0  1  1  1  1  1  2  2         14484.33570   14484.33557    0.00013    0.00500   0.00000
    6:   1  1  0  2  2  1  1  1  1  1         14512.52210   14512.52272   -0.00062    0.00500   0.00000
    7:   1  1  0  2  1  1  1  1  1  0         14540.78830   14540.78702    0.00128    0.00500   0.00000
    8:   1  1  0  2  2  1  1  1  2  1         14584.71550   14584.71498    0.00052    0.00500   0.00000
    9:   1  1  0  2  2  1  1  1  2  2         14600.20240   14600.20096    0.00144    0.00500   0.00000
   10:   1  1  0  2  1  1  1  1  2  1         14602.45820   14602.45846   -0.00026    0.00500   0.00000
   11:   2  1  2  3  3  1  1  1  2  2         91609.00000   91608.81383    0.18617    0.10000   0.00000
   12:   2  1  2  3  2  1  1  1  2  2         91627.10000   91626.95296    0.14704    0.10000   0.00000
   13:   2  1  2  2  2  1  1  1  2  2         91897.68000   91897.51015    0.16985    0.10000   0.00000
   14:   2  1  2  3  2  1  1  1  2  1         91611.70000   91611.46699    0.23301    0.10000   0.00000
   15:   2  1  2  2  1  1  1  1  2  1         91865.30000   91865.12839    0.17161    0.10000   0.00000
   16:   2  1  1  2  2  1  1  0  2  2        120695.95000  120696.15746   -0.20746    0.10000   0.00000
   17:   2  1  1  3  3  1  1  0  2  2        120741.20000  120741.42000   -0.22000    0.10000   0.00000
   18:   2  1  1  3  2  1  1  0  2  2        120760.51000  120760.65244   -0.14244    0.10000   0.00000
   19:   2  1  1  2  1  1  1  0  2  1        120669.70000  120669.82882   -0.12882    0.10000   0.00000
   20:   2  1  1  3  2  1  1  0  2  1        120742.70000  120742.90896   -0.20896    0.10000   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.97304E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
```

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   7   1.00000E+00    8   1.00000E+00    9   1.00000E+00   10   1.00726E-01   11   7.04540E-01   12   9.65437E-01
  13   4.10695E-01   14   9.42626E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A  44185.950000000(  0)      0.000000000
  2         20000          B       33825.6321( 80)          -0.0000
  3         30000          C       19290.1633( 80)           0.0000
  4           200       -D_N     -0.054930000(  0)     -0.000000000
  5          1100      -D_NK     -0.590210000(  0)      0.000000000
  6          2000       -D_K      0.414200000(  0)      0.000000000
  7         40100       -d_N     -0.020640000(  0)     -0.000000000
  8         41000       -d_K     -0.359700000(  0)      0.000000000
  9      10010000     eps_aa          102.644( 40)           -0.000
 10      10020000     eps_bb           57.748( 40)            0.000
 11      10030000     eps_cc         -204.548( 40)            0.000
 12     120000000     a_F(H)         -27.0491( 74)           0.0000
 13     120010000    T_aa(H)          15.2729(155)          -0.0000
 14     120020000    T_bb(H)          -1.3191(124)          -0.0000
 MICROWAVE AVG =        0.000227 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.130551 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.31348         1.31348
```
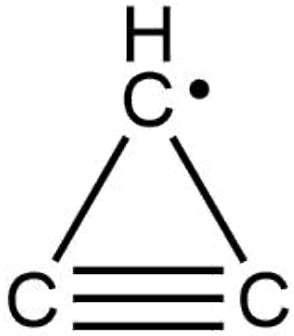

Molecule 4

IUPAC Name: cyclopropa-1-yn-3-ylradical (ve3)

Common name: cyclic-C3H, c-C3H (ve3)

SMILES: [CH]1C#C1



4: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	1	1	0	1	1	1	1	1	1	1	15424.64230		15424.65094		-0.00864	0.00500	0.00000
2:	1	1	0	1	0	1	1	1	1	1	15427.87740		15427.87470		0.00270	0.00500	0.00000
3:	1	1	0	1	1	1	1	1	1	0	15433.60410		15433.60187		0.00223	0.00500	0.00000
4:	1	1	0	1	0	1	1	1	2	1	15693.25900		15693.26118		-0.00218	0.00500	0.00000
5:	1	1	0	1	1	1	1	1	2	2	15707.25120		15707.24535		0.00585	0.00500	0.00000
6:	1	1	0	2	2	1	1	1	1	1	15552.08590		15552.08030		0.00560	0.00500	0.00000
7:	1	1	0	2	1	1	1	1	1	0	15578.29310		15578.29469		-0.00159	0.00500	0.00000
8:	1	1	0	2	2	1	1	1	2	1	15817.46770		15817.46677		0.00093	0.00500	0.00000
9:	1	1	0	2	1	1	1	1	2	2	15851.93790		15851.93817		-0.00027	0.00500	0.00000
10:	1	1	0	2	2	1	1	1	2	2	15834.66530		15834.67470		-0.00940	0.00500	0.00000
11:	1	1	0	2	1	1	1	1	2	1	15834.73500		15834.73024		0.00476	0.00500	0.00000
12:	2	1	2	3	3	1	1	1	2	2	88197.85000		88197.80310		0.04690	0.10000	0.00000
13:	2	1	2	3	2	1	1	1	2	1	88199.30000		88199.31950		-0.01950	0.10000	0.00000
14:	2	1	2	3	2	1	1	1	2	2	88216.50000		88216.52744		-0.02744	0.10000	0.00000
15:	2	1	2	2	1	1	1	1	2	2	88894.25000		88894.22630		0.02370	0.10000	0.00000
16:	2	1	2	2	2	1	1	1	2	2	88911.60000		88911.58249		0.01751	0.10000	0.00000
17:	2	1	2	2	1	1	1	1	2	1	88877.10000		88877.01837		0.08163	0.10000	0.00000
18:	2	1	2	2	1	1	1	1	1	1	88611.48000		88611.63190		-0.15190	0.10000	0.00000
19:	2	1	2	2	1	1	1	1	1	0	88620.65000		88620.58282		0.06718	0.10000	0.00000
20:	2	1	2	2	2	1	1	1	1	1	88628.95000		88628.98808		-0.03808	0.10000	0.00000

NORMALIZED DIAGONAL:

1 1.00000E+00 2 1.00000E+00 3 1.78577E-01 4 1.00000E+00 5 1.00000E+00 6 1.00000E+00

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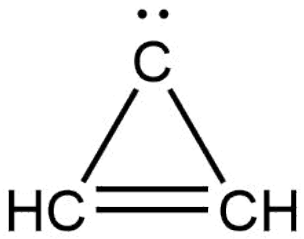
   7   1.00000E+00    8   1.00000E+00    9   7.85116E-02   10   8.92824E-01   11   9.72150E-01   12   1.00000E+00
  13   5.22812E-01   14   9.39080E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A  44536.821000000(  0)      0.000000000
  2         20000          B       33872.7080( 97)           0.0000
  3         30000          C       18172.3660( 96)          -0.0000
  4           200       -D_N     -0.054930000(  0)     -0.000000000
  5          1100      -D_NK     -0.590210000(  0)      0.000000000
  6          2000       -D_K      0.414200000(  0)      0.000000000
  7         40100       -d_N     -0.020640000(  0)     -0.000000000
  8         41000       -d_K     -0.359700000(  0)      0.000000000
  9      10010000     eps_aa           99.240( 43)            0.000
 10      10020000     eps_bb           76.003( 43)            0.000
 11      10030000     eps_cc         -462.938( 42)            0.000
 12     120000000     a_F(H)         -26.8826( 52)          -0.0000
 13     120010000    T_aa(H)          16.9934(121)           0.0000
 14     120020000    T_bb(H)          -0.9384( 94)          -0.0000
 MICROWAVE AVG =       -0.000000 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.044818 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.86210         0.86210
```

Molecule 5

IUPAC Name: cyclopropenylidene

Common name: cyclopropenylidene

SMILES: C1=C=C1

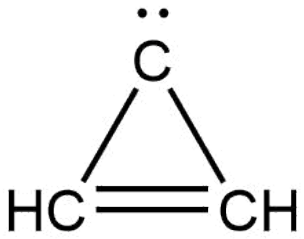


Molecule 6

IUPAC Name: cyclopropenylidene (1v2)

Common name: cyclopropenylidene (1v2)

SMILES: C1=C=C1



6: Line file

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cyclopropa-1,2-dien-2-ylidene (1v2)
  1  1  0  1  0  1                  18260.981  0.002  /CfA2016
  2  1  2  1  0  1                  85094.247  0.016  /Mollaaghababa1993
  6  2  4  6  1  5                 149810.664  0.049  /Mollaaghababa1993
  6  3  4  6  2  5                 149906.375  0.011  /Mollaaghababa1993
  4  1  4  3  0  3                 150404.201  0.025  /Mollaaghababa1993
  4  1  3  3  2  2                 182867.192  0.035  /Mollaaghababa1993
  5  0  5  4  1  4                 183796.955  0.027  /Mollaaghababa1993
  5  1  5  4  0  4                 183799.271  0.074  /Mollaaghababa1993
  4  2  3  3  1  2                 184989.032  0.036  /Mollaaghababa1993
  6  0  6  5  1  5                 217209.774  0.032  /Mollaaghababa1993
  6  1  6  5  0  5                 217209.774  0.032  /Mollaaghababa1993
  5  1  4  4  2  3                 217153.380  0.033  /Mollaaghababa1993
  5  2  4  4  1  3                 217395.789  0.045  /Mollaaghababa1993
  7  0  7  6  1  6                 250620.413  0.184  /Mollaaghababa1993
  7  1  7  6  0  6                 250620.413  0.184  /Mollaaghababa1993
  6  2  5  5  1  4                 250669.785  0.033  /Mollaaghababa1993
  6  2  4  5  3  3                 283777.906  0.100  /Mollaaghababa1993
  8  0  8  7  1  7                 284029.646  0.029  /Mollaaghababa1993
  8  1  8  7  0  7                 284029.646  0.029  /Mollaaghababa1993
  7  1  6  6  2  5                 284056.649  0.036  /Mollaaghababa1993
  7  2  6  6  1  5                 284058.229  0.090  /Mollaaghababa1993
  6  3  4  5  2  3                 284749.440  0.039  /Mollaaghababa1993
  8  1  7  7  2  6                 317458.778  0.034  /Mollaaghababa1993
  8  2  7  7  1  6                 317458.778  0.034  /Mollaaghababa1993
  9  0  9  8  1  8                 317437.340  0.030  /Mollaaghababa1993
  9  1  9  8  0  8                 317437.340  0.030  /Mollaaghababa1993
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 7  3  5  6  2  4                317618.961  0.022  /Mollaaghababa1993
 8  2  6  7  3  5                350923.357  0.103  /Mollaaghababa1993
 8  3  6  7  2  5                350932.847  0.029  /Mollaaghababa1993
 9  1  8  8  2  7                350859.759  0.034  /Mollaaghababa1993
 9  2  8  8  1  7                350859.759  0.034  /Mollaaghababa1993
10  0 10  9  1  9                350842.945  0.033  /Mollaaghababa1993
10  1 10  9  0  9                350842.945  0.033  /Mollaaghababa1993
10  1  9  9  2  8                384259.389  0.045  /Mollaaghababa1993
10  2  9  9  1  8                384259.389  0.045  /Mollaaghababa1993
11  0 11 10  1 10                384246.309  0.021  /Mollaaghababa1993
11  1 11 10  0 10                384246.309  0.021  /Mollaaghababa1993
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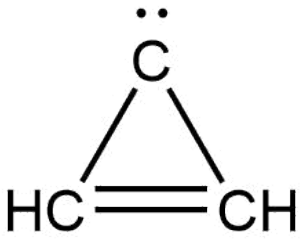
Molecule 7

IUPAC Name: cyclopropenylidene (1v3)

Common name: cyclopropenylidene (1v3)

SMILES: C1=C=C1



7: Line file

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cyclopropa-1,2-dien-2-ylidene (1v3)
  1  1  0  1  0  1                  18241.7207 0.002  /CfA2016
  2  1  2  1  0  1                  85269.797  0.029  /Mollaaghababa1993
  6  2  4  6  1  5                 150597.623  0.013  /Mollaaghababa1993
  6  3  4  6  2  5                 150671.447  0.010  /Mollaaghababa1993
  4  0  4  3  1  3                 150841.525  0.034  /Mollaaghababa1993
  4  1  4  3  0  3                 150869.622  0.024  /Mollaaghababa1993
  4  1  3  3  2  2                 183618.056  0.036  /Mollaaghababa1993
  5  0  5  4  1  4                 184363.409  0.030  /Mollaaghababa1993
  5  1  5  4  0  4                 184365.192  0.091  /Mollaaghababa1993
  4  2  3  3  1  2                 185472.101  0.027  /Mollaaghababa1993
  6  0  6  5  1  5                 217873.176  0.020  /Mollaaghababa1993
  6  1  6  5  0  5                 217873.176  0.020  /Mollaaghababa1993
  5  1  4  4  2  3                 217894.288  0.015  /Mollaaghababa1993
  5  2  4  4  1  3                 218092.608  0.023  /Mollaaghababa1993
  7  1  6  7  0  7                 218165.939  0.029  /Mollaaghababa1993
  7  0  7  6  1  6                 251380.782  0.010  /Mollaaghababa1993
  7  1  7  6  0  6                 251380.782  0.010  /Mollaaghababa1993
  6  2  5  5  1  4                 251486.793  0.015  /Mollaaghababa1993
  6  2  4  5  3  3                 284817.468  0.039  /Mollaaghababa1993
  8  0  8  7  1  7                 284886.883  0.015  /Mollaaghababa1993
  8  1  8  7  0  7                 284886.883  0.015  /Mollaaghababa1993
  7  1  6  6  2  5                 284975.039  0.029  /Mollaaghababa1993
  7  2  6  6  1  5                 284976.280  0.099  /Mollaaghababa1993
  6  3  4  5  2  3                 285612.023  0.031  /Mollaaghababa1993
  8  1  7  7  2  6                 318474.948  0.010  /Mollaaghababa1993
  8  2  7  7  1  6                 318474.948  0.010  /Mollaaghababa1993
```

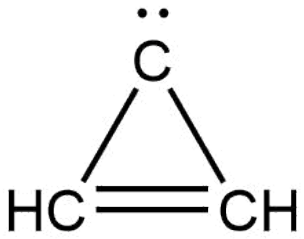
```
 9  0  9  8  1  8                318390.987  0.010  /Mollaaghababa1993
 9  1  9  8  0  8                318390.987  0.010  /Mollaaghababa1993
 7  2  5  6  3  4                318585.940  0.042  /Mollaaghababa1993
 7  3  5  6  2  4                318667.220  0.046  /Mollaaghababa1993
 8  3  6  7  2  5                352094.371  0.044  /Mollaaghababa1993
 9  1  8  8  2  7                351973.888  0.010  /Mollaaghababa1993
 9  2  8  8  1  7                351973.888  0.010  /Mollaaghababa1993
10  0 10  9  1  9                351892.831  0.034  /Mollaaghababa1993
10  1 10  9  0  9                351892.831  0.034  /Mollaaghababa1993
```

Molecule 8

IUPAC Name: cyclopropenylidene (1v5)

Common name: cyclopropenylidene (1v5)

SMILES: C1=C=C1



8: Line file

```
cyclopropa-1,2-dien-2-ylidene (1v5)
  2  1  2  1  0  1                  85293.282  0.029  /Mollaaghababa1993
  3  0  3  2  1  2                 117282.486  0.012  /Mollaaghababa1993
  8  3  5  8  2  6                 183601.810  0.010  /Mollaaghababa1993
  8  4  5  8  3  6                 183623.633  0.010  /Mollaaghababa1993
  5  0  5  4  1  4                 184556.042  0.021  /Mollaaghababa1993
  5  1  5  4  0  4                 184557.669  0.065  /Mollaaghababa1993
  6  0  6  5  1  5                 218109.762  0.020  /Mollaaghababa1993
  6  1  6  5  0  5                 218109.762  0.020  /Mollaaghababa1993
  7  0  7  6  1  6                 251661.765  0.022  /Mollaaghababa1993
  7  1  7  6  0  6                 251661.765  0.022  /Mollaaghababa1993
  6  2  5  5  1  4                 251661.765  0.022  /Mollaaghababa1993
  8  0  8  7  1  7                 285212.585  0.027  /Mollaaghababa1993
  8  1  8  7  0  7                 285212.585  0.027  /Mollaaghababa1993
  7  1  6  6  2  5                 285192.690  0.031  /Mollaaghababa1993
  7  2  6  6  1  5                 285193.900  0.100  /Mollaaghababa1993
  8  1  7  7  2  6                 318733.541  0.036  /Mollaaghababa1993
  8  2  7  7  1  6                 318733.541  0.036  /Mollaaghababa1993
  9  0  9  8  1  8                 318761.970  0.043  /Mollaaghababa1993
  9  1  9  8  0  8                 318761.970  0.043  /Mollaaghababa1993
  7  3  5  6  2  4                 318820.571  0.021  /Mollaaghababa1993
  9  1  8  8  2  7                 352272.881  0.033  /Mollaaghababa1993
  9  2  8  8  1  7                 352272.881  0.033  /Mollaaghababa1993
 10  0 10  9  1  9                 352309.608  0.026  /Mollaaghababa1993
 10  1 10  9  0  9                 352309.608  0.026  /Mollaaghababa1993
 10  1  9  9  2  8                 385810.485  0.032  /Mollaaghababa1993
 10  2  9  9  1  8                 385810.485  0.032  /Mollaaghababa1993
```

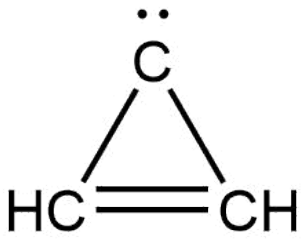
```
11  0 11 10  1 10                385855.612  0.031  /Mollaaghababa1993
11  1 11 10  0 10                385855.612  0.031  /Mollaaghababa1993
```

Molecule 9

IUPAC Name: cyclopropenylidene (1v5+1v6)

Common name: cyclopropenylidene (1v5+1v6)

SMILES: C1=C=C1



9: Line file

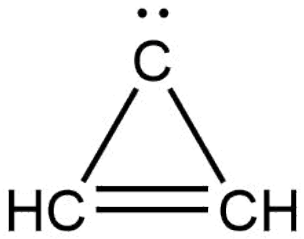
```
cyclopropa-1,2-dien-2-ylidene (1v5+1v6)
  1   1   0   1   0   1                       17273.3365      0.0020  \1-dr1913,dr1914
  2   1   2   1   0   1                       84417.0750      0.0500  \1-dr1913,dr1914
```

Molecule 10

IUPAC Name: cyclopropenylidene (1v6)

Common name: cyclopropenylidene (1v6)

SMILES: C1=C=C1



10: Line file

```
cyclopropa-1,2-dien-2-ylidene (1v6)
  1  1  0  1  0  1                    17435.7694     0.0020    2.956E-04
  2  2  0  2  1  1                    20002.0651     0.0020    5.194E-04
  2  1  1  2  0  2                    45598.3800     0.0250    1.248E-03
  3  1  3  2  2  0                    51442.2930     0.0250    3.496E-06
  2  0  2  1  1  1                    81982.7240     0.0250    6.114E-03
  2  1  2  1  0  1                    84547.2250     0.0250    7.408E-03
  2  2  1  1  1  0                   119419.9870     0.0250    1.326E-02
  2  2  0  1  1  1                   147583.1580     0.0250  8.260E-03
  3  2  2  2  1  1                   152972.9240     0.0600  1.970E-02
  3  3  1  2  2  0                   188909.9440     0.0220  3.516E-02
  6  5  2  6  4  3                    85491.357    900.0000  6.528E-03
  3  0  3  2  1  2                   116791.782    900.0000  5.599E-02
  6  2  4  6  1  5                   145767.572    900.0000  5.556E-03
  4  1  3  3  2  2                   182391.982    900.0000  3.164E-02
  5  0  5  4  1  4                   184009.283    900.0000  1.567E-01
  5  1  5  4  0  4                   184010.229    900.0000  5.223E-02
  6  0  6  5  1  5                   217560.029    900.0000  6.494E-02
  6  1  6  5  0  5                   217560.029    900.0000  1.948E-01
  6  1  5  5  2  4                   250033.194    900.0000  5.411E-02
  5  3  3  4  2  2                   251033.194    900.0000  3.890E-02
  7  0  7  6  1  6                   251108.912    900.0000  2.114E-01
  7  1  7  6  0  6                   251108.912    900.0000  7.049E-02
  8  0  8  7  1  7                   284656.236    900.0000  6.828E-02
  8  1  8  7  0  7                   284656.236    900.0000  2.048E-01
  8  1  7  7  2  6                   317115.455    900.0000  5.103E-02
  8  2  7  7  1  6                   317115.455    900.0000  1.531E-01
```

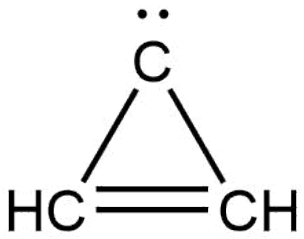
9	0	9	8	1	8	318201.315	900.0000	1.796E-01
9	1	9	8	0	8	318201.315	900.0000	5.987E-02
8	2	6	7	3	5	349608.498	900.0000	3.868E-02
8	3	6	7	2	5	349611.562	900.0000	1.161E-01
9	1	8	8	2	7	350652.972	900.0000	1.270E-01
9	2	8	8	1	7	350652.972	900.0000	4.233E-02
10	0	10	9	1	9	351744.215	900.0000	4.800E-02
10	1	10	9	0	9	351744.215	900.0000	1.440E-01
10	1	9	9	2	8	384187.925	900.0000	3.210E-02
10	2	9	9	1	8	384187.925	900.0000	9.629E-02
11	0	11	10	1	10	385284.523	900.0000	1.062E-01
11	1	11	10	0	10	385284.523	900.0000	3.541E-02

Molecule 11

IUPAC Name: cyclopropenylidene (2v6)

Common name: cyclopropenylidene (2v6)

SMILES: C1=C=C1



11: Line file

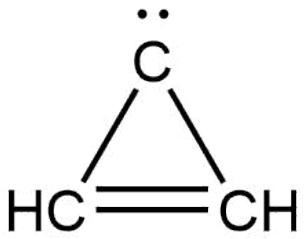
```
cyclopropa-1,2-dien-2-ylidene (2v6)
  1  1  0  1  0  1                    16828.2152      0.0020  2.956E-04
  2  2  0  2  1  1                    19005.3654      0.0020  4.750E-04
  2  1  1  2  0  2                    44701.9600      0.0250  1.176E-03
  2  0  2  1  1  1                    81856.4600      0.0200  6.114E-03
  2  1  2  1  0  1                    84032.7120      0.0250  7.408E-03
  2  2  1  1  1  0                    117689.5580     0.0400  1.292E-02
  2  2  0  1  1  1                    145563.9210     0.0250  7.881E-03
  3  2  2  2  1  1                    151288.5860     0.0800  1.934E-02
  3  3  1  2  2  0                    185867.4090     0.0250  3.412E-02
  7  3  4  6  4  3                    345556.219      0.2000  2.484E-02
  8  2  6  7  3  5                    347791.719      0.2000  1.206E-02
  8  3  6  7  2  5                    347793.625      0.2000  3.619E-02
  9  1  8  8  2  7                    349759.688      0.2000  4.739E-02
  9  2  8  8  1  7                    349759.688      0.2000  1.580E-02
 10  0 10  9  1  9                    351768.562      0.2000  1.977E-02
 10  1 10  9  0  9                    351768.562      0.2000  5.932E-02
  6  5  2  5  4  1                    358937.938      0.2000  2.118E-02
```

Molecule 12

IUPAC Name: cyclopropenylidene (3v6)

Common name: cyclopropenylidene (3v6)

SMILES: C1=C=C1



12: Line file

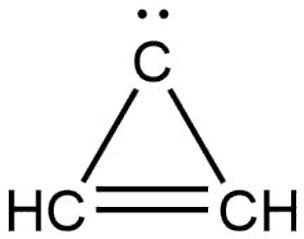
```
cyclopropa-1,2-dien-2-ylidene (3v6)
  1  1  0  1  0  1                      16296.6072     0.0020  2.956E-04
  2  2  0  2  1  1                      18170.4450     0.0020  4.430E-04
  2  1  2  1  0  1                      83631.8257     0.0500  7.408E-03
  2  2  1  1  1  0                     116301.8090     0.0500  1.263E-02
```

Molecule 13

IUPAC Name: cyclopropenylidene (4v6)

Common name: cyclopropenylidene (4v6)

SMILES: C1=C=C1



13: Line file

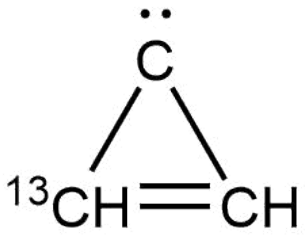
```
cyclopropa-1,2-dien-2-ylidene (4v6)
  1  1  0  1  0  1                      15931.7423     0.0020  2.956E-04
  2  1  2  1  0  1                      83305.3050     0.0500  /1-DR1906
```

Molecule 14

IUPAC Name: cyclopropenylidene (H13CCCH)

Common name: cyclopropenylidene (H13CCCH)

SMILES: C1=C=C1



14: Line file

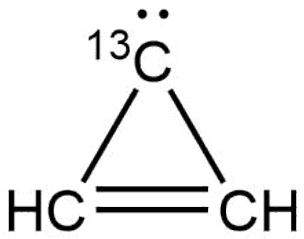
```
cyclopropa-1,2-dien-2-ylidene (H13CCCH)
  1  1  0  1  0  1  1  1  1  2  0  2     14845.0647    0.0020 0.124E-05
  1  1  0  1  0  1  1  1  1  1  0  1     14845.0821    0.0020 0.247E-05
  1  1  0  2  0  2  1  1  1  2  0  2     14845.0939    0.0020 0.618E-05
  1  1  0  2  0  2  1  1  1  1  0  1     14845.1115    0.0020 0.124E-05
  1  1  0  1  0  1  1  0  1  2  0  2     18413.8000    0.0020 0.782E-04
  1  1  0  1  0  1  1  0  1  1  0  1     18413.8000    0.0020 0.156E-03
  1  1  0  2  0  2  1  0  1  2  0  2     18413.8281    0.0020 0.391E-03
  1  1  0  2  0  2  1  0  1  1  0  1     18413.8281    0.0020 0.782E-04
  2  2  0  2  0  2  2  1  1  2  0  2     22550.8216    0.0020 0.171E-03
  2  2  0  3  0  3  2  1  1  3  0  3     22550.8216    0.0020 0.266E-03
  3  3  0  3  0  3  3  2  1  3  0  3     29699.4190    0.0020 0.258E-03
  3  3  0  4  0  4  3  2  1  4  0  4     29699.4190    0.0020 0.348E-03
```

Molecule 15

IUPAC Name: cyclopropenylidene (HC13CCH)

Common name: cyclopropenylidene (HC13CCH)

SMILES: C1=C=C1



15: Line file

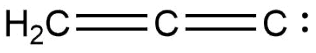
```
cyclopropa-1,2-dien-2-ylidene (HC13CCH)
  1  1  0  1  0  1  1  0  1  2  0  2   16978.936200   0.00200 0.665E-04
  1  1  0  1  0  1  1  0  1  1  0  1   16978.947800   0.00200 0.133E-03
  1  1  0  2  0  2  1  0  1  2  0  2   16978.977400   0.00200 0.332E-03
  1  1  0  2  0  2  1  0  1  1  0  1   16978.993200   0.00200 0.665E-04
  2  2  0  2  0  2  2  1  1  2  0  2   18130.879000   0.00200 0.111E-03
  2  2  0  3  0  3  2  1  1  3  0  3   18130.903700   0.00200 0.172E-03
```

Molecule 16

IUPAC Name: propadienylidene

Common name: propadienylidene

SMILES: C=C=[C]

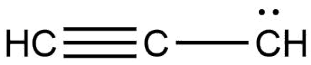


Molecule 17

IUPAC Name: cyanometh-1,1-diyl

Common name: cyanomethyl carbene

SMILES: [CH]C#N



Molecule 18

IUPAC Name: 2-oxoethenylidene

Common name: dicarbonmonoxide, ketenylidene

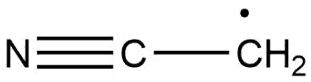
SMILES: [C]=C=O

Molecule 19

IUPAC Name: cyanomethyl radical

Common name: cyanomethyl radical

SMILES: [CH2]C#N

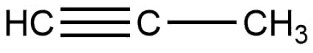


Molecule 20

IUPAC Name: propyne

Common name: propyne, methyl acetylene

SMILES: CC#C

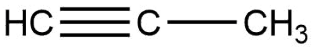


Molecule 21

IUPAC Name: propyne (ve1)

Common name: propyne, methyl acetylene (ve1)

SMILES: CC#C



21: Fit file

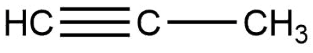
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  0  2  1  0  0  0  2  2         17016.22210   17016.22069    0.00141    0.00200   0.00171
    2:   1  0  0  2  3  0  0  0  2  2         17016.23810   17016.23811   -0.00001    0.00200   0.00116
    3:   1  0  0  2  2  0  0  0  2  2         17016.25850   17016.25989   -0.00139    0.00200   0.00178
    4:   2 -1  0  2  4  1  1  0  2  3         34032.06500   34032.06273    0.00227    0.00200   0.00200   34032.06500   -0.00000
    5:   2  1  0  2  4  1 -1  0  2  3         34032.06500   34032.06273    0.00227    0.00200   0.00200   34032.06500   -0.00000
    6:   2 -1  4  1  3  1  1  4  1  2         34032.06500   34032.06802   -0.00302    0.00200   0.00200   34032.06500   -0.00000
    7:   2  1  4  1  3  1 -1  4  1  2         34032.06500   34032.06802   -0.00302    0.00200   0.00200   34032.06500   -0.00000
    8:   2  0  0  2  2  1  0  0  2  2         34032.40730   34032.41082   -0.00352    0.00200   0.00151
    9:   2  0  0  2  4  1  0  0  2  3         34032.42990   34032.42638    0.00352    0.00200   0.00151
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   3.15913E-01    4   8.45711E-01    5   9.10829E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1          1000        A-B  147255.20000000(  0)      -0.00000000
   2           100          B       8508.12596( 78)         -0.00000
   3           200       -D_J           -2.362(113)E-03        0.000E-03
   4          1100      -D_JK         -0.09006( 62)          0.00000
   5     120020000     3S(HH)          -0.0871( 58)           0.0000
 MICROWAVE AVG =       -0.000000 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002188 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        1.09416         1.09416
```

Molecule 22

IUPAC Name: propyne (ve2)

Common name: propyne, methyl acetylene (ve2)

SMILES: CC#C



22: Fit file

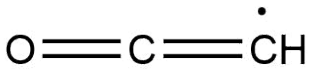
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  0  2  1  0  0  0  2  2         17114.98310   17114.97891    0.00419    0.00200   0.00000
    2:   1  0  0  2  3  0  0  0  2  2         17114.99680   17114.99633    0.00047    0.00200   0.00000
    3:   1  0  0  2  2  0  0  0  2  2         17115.01720   17115.01811   -0.00091    0.00200   0.00000
    4:   2  0  0  2  2  1  0  0  2  2         34229.92320   34229.92726   -0.00406    0.00200   0.00000
    5:   2  0  0  2  4  1  0  0  2  3         34229.94500   34229.94281    0.00219    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.00000E+00    4   1.00000E+00    5   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1          1000        A-B  147255.20000000(  0)      -0.00000000
   2           100          B      8557.505069(302)         0.000000
   3           200       -D_J     -2.362355727(100)E-03 -0.000000000E-03
   4          1100      -D_JK     -0.090055385(  0)     -0.000000000
   5     120020000     3S(HH)     -0.087105494(  0)      0.000000000
 MICROWAVE AVG =        0.000375 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002823 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.41140         1.41140
```

Molecule 23

IUPAC Name: ethenonyl radical

Common name: ketenyl radical

SMILES: O=C=[CH]

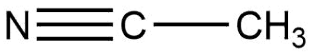


Molecule 24

IUPAC Name: methylcyanide

Common name: acetonitrile

SMILES: CC#N

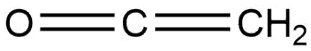


Molecule 25

IUPAC Name: ethenone

Common name: ketene

SMILES: C=C=O

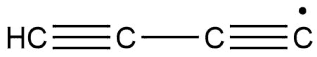


Molecule 26

IUPAC Name: 1,3-butadiynyl radical

Common name: butadiynyl radical

SMILES: [C]#C-C#C

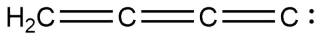


Molecule 27

IUPAC Name: butatrienylidene

Common name: butatrienylidene

SMILES: C=C=C=[C]

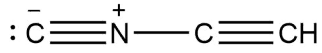


Molecule 28

IUPAC Name: isocyanoethyne

Common name: isocyanoacetylene

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

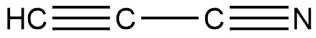


Molecule 29

IUPAC Name: 2-propynenitrile

Common name: cyanoacetylene, propiolonitrile

SMILES: C#CC#N

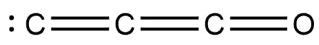


Molecule 30

IUPAC Name: 3-oxo-1,2-propadienylidene

Common name: tricarbonmonoxide

SMILES: [C]=C=C=O

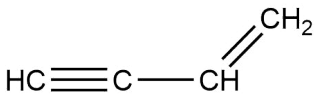


Molecule 31

IUPAC Name: 1-buten-3-yne

Common name: vinylacetylene

SMILES: C=CC#C

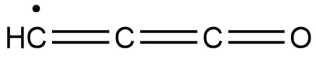


Molecule 32

IUPAC Name: 1,2-pentadien-1-on-3-yl

Common name: 1,2-pentadien-1-on-3-yl

SMILES: [CH]=C=C=O

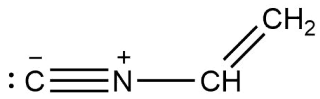


Molecule 33

IUPAC Name: isocyanoethene

Common name: vinylisocyanide

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



33: Fit file

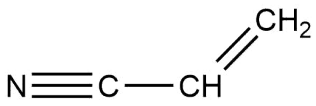
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0  0  0  0  1         10255.45940   10255.46032   -0.00092    0.00200   0.00126
    2:   1  0  1  0  2  0  0  0  0  1         10255.56810   10255.56701    0.00109    0.00200   0.00013
    3:   1  0  1  0  1  0  0  0  0  1         10255.64140   10255.63814    0.00326    0.00200   0.00063
    4:   2  0  2  0  1  1  0  1  0  1         20506.64580   20506.64068    0.00512    0.00200   0.00126
    5:   2  0  2  0  3  1  0  1  0  2         20506.76230   20506.75776    0.00454    0.00200   0.00003   20506.76354   -0.00124
    6:   2  0  2  0  2  1  0  1  0  1         20506.76230   20506.76932   -0.00702    0.00200   0.00003   20506.76354   -0.00124
    7:   2  0  2  0  1  1  0  1  0  0         20506.82270   20506.81851    0.00419    0.00200   0.00063
    8:   3  0  3  0  4  2  0  2  0  3         30749.16890   30749.16061    0.00829    0.00200   0.00003
    9:   3  0  3  0  3  2  0  2  0  2         30749.18900   30749.17376    0.01524    0.00200   0.00006   30749.17338    0.01562
   10:   3  0  3  0  2  2  0  2  0  1         30749.18900   30749.17301    0.01599    0.00200   0.00006   30749.17338    0.01562
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.00000E+00    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   1.00000E+00   10   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10099          A  51479.457800000(  0)      0.000000000
   2         20099          B   5386.648560000(  0)     -0.000000000
   3         30099          C   4868.940210000(  0)     -0.000000000
   4           299     -Del_J     -2.476150000(  0)E-03 -0.000000000E-03
   5          1199    -Del_JK      0.100008200(  0)      0.000000000
   6          2099     -Del_K     -3.421080000(  0)      0.000000000
   7         40199     -del_J     -0.549200000(  0)E-03  0.000000000E-03
   8         41099     -del_K     -0.027203000(  0)     -0.000000000
   9     110010000     chi_aa          0.23710(252)          0.00000
  10     110020000     chi_bb      1.690000000(  0)      0.000000000
 MICROWAVE AVG =        0.004426 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.006805 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        3.40265         3.40265
```

Molecule 34

IUPAC Name: 2-propenenitrile

Common name: acrylonitrile, vinylcyanide

SMILES: C=CC#N

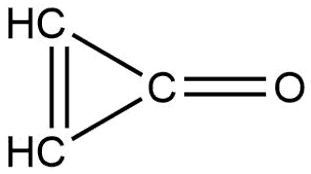


Molecule 35

IUPAC Name: 2-cyclopropen-1-one

Common name: cyclopropenone

SMILES: C1=CC1=O



35: Fit file

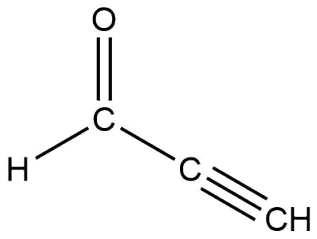
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                    14105.72400   14105.72887   -0.00487    0.00200   0.00000
    2:   4  1  3  4  1  4                    15427.87640   15427.88091   -0.00451    0.00200   0.00000
    3:   2  1  2  1  1  1                    26667.00880   26667.02992   -0.02112    0.00200   0.00000
    4:   2  0  2  1  0  1                    28139.88580   28139.88339    0.00241    0.00200   0.00000
    5:   2  1  1  1  1  0                    29755.52900   29755.50640    0.02260    0.00200   0.00000
    6:   3  1  3  2  1  2                    39956.73450   39956.73547   -0.00097    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.25639E-01    3   9.98557E-01    4   1.76750E-01    5   8.29273E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         32035.58(215)            -0.00
   2         20000          B       7824.98649( 99)          0.00000
   3         30000          C       6280.74825( 80)          0.00000
   4           200  -\Delta_J           -1.468( 93)E-03        0.000E-03
   5          1100 -\Delta_JK         -0.03859(152)         -0.00000
   6          2000  -\Delta_K      0.017525575(  0)E-18 -0.000000000E-18
   7         40100         d1     -9.616010536(  0)E-24 -0.000000000E-24
   8         50000         d2     -0.019798083(  0)E-21  0.000000000E-21
 MICROWAVE AVG =       -0.001077 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.012959 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        6.47934         6.47934
```

Molecule 36

IUPAC Name: 2-propynal

Common name: propiolaldehyde

SMILES: C#CC=O

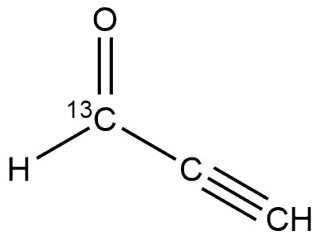


Molecule 37

IUPAC Name: 2-propynal (13C1)

Common name: propiolaldehyde (13C1)

SMILES: C#CC=O



37: Fit file

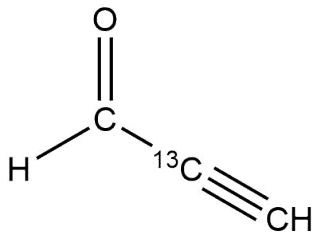
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                      9027.73380    9027.73255    0.00125    0.00200   0.00000
    2:   2  1  2  1  1  1                     17748.92100   17748.91813    0.00287    0.00200   0.00000
    3:   2  0  2  1  0  1                     18054.30560   18054.30546    0.00014    0.00200   0.00000
    4:   2  1  1  1  1  0                     18363.07360   18363.08222   -0.00862    0.00200   0.00000
    5:   3  1  3  2  1  2                     26622.59450   26622.59369    0.00081    0.00200   0.00000
    6:   3  0  3  2  0  2                     27078.55820   27078.55924   -0.00104    0.00200   0.00000
    7:   3  1  2  2  1  1                     27543.84300   27543.83725    0.00575    0.00200   0.00000
    8:   4  1  4  3  1  3                     35495.33070   35495.33274   -0.00204    0.00200   0.00000
    9:   4  0  4  3  0  3                     36099.33550   36099.33510    0.00040    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.92656E-01    3   3.46565E-01    4   1.82810E-01    5   9.86471E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            67232( 48)               0
   2         20000          B       4667.40997( 56)         0.00000
   3         30000          C       4360.32792( 59)        -0.00000
   4           200  -\Delta_J          -1.3336(266)E-03       0.0000E-03
   5          1100 -\Delta_JK          0.14177( 63)        -0.00000
   6          2000  -\Delta_K      0.017525575(  0)E-18 -0.000000000E-18
   7         40100         d1      1.733765744(  0)E-24 -0.000000000E-24
   8         50000         d2      0.028609447(  0)E-21  0.000000000E-21
 MICROWAVE AVG =       -0.000054 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.003701 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.85061         1.85061
```

Molecule 38

IUPAC Name: 2-propynal (13C2)

Common name: propiolaldehyde (13C2)

SMILES: C#CC=O



38: Fit file

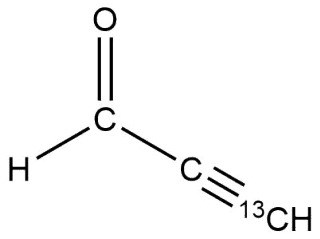
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                      9281.53440    9281.53301    0.00139    0.00200   0.00000
    2:   2  1  2  1  1  1                     18239.75220   18239.76591   -0.01371    0.00200   0.00000
    3:   2  0  2  1  0  1                     18561.77850   18561.77880   -0.00030    0.00200   0.00000
    4:   2  1  1  1  1  0                     18887.48190   18887.47854    0.00336    0.00200   0.00000
    5:   3  1  3  2  1  2                     27358.75380   27358.74466    0.00914    0.00200   0.00000
    6:   3  0  3  2  0  2                     27839.44970   27839.45037   -0.00067    0.00200   0.00000
    7:   3  1  2  2  1  1                     28330.31340   28330.31068    0.00272    0.00200   0.00000
    8:   4  0  4  3  0  3                     37113.26180   37113.26149    0.00031    0.00200   0.00000
    9:   4  1  3  3  1  2                     37772.04650   37772.05022   -0.00372    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.49858E-01    3   4.86664E-01    4   1.81875E-01    5   9.86217E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            68423( 45)               0
   2         20000          B       4802.69916( 59)         -0.00000
   3         30000          C       4478.84284( 56)         -0.00000
   4           200  -\Delta_J          -2.2480(267)E-03      -0.0000E-03
   5          1100 -\Delta_JK          0.15254( 64)          0.00000
   6          2000  -\Delta_K      0.017525575(  0)E-18 -0.000000000E-18
   7         40100         d1     -3.347590483(  0)E-24  0.000000000E-24
   8         50000         d2     -0.019798083(  0)E-21 -0.000000000E-21
 MICROWAVE AVG =       -0.000165 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005834 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        2.91718         2.91718
```

Molecule 39

IUPAC Name: 2-propynal (13C3)

Common name: propiolaldehyde (13C3)

SMILES: C#CC=O



39: Fit file

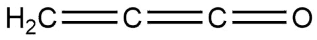
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                      9278.78970    9278.78960    0.00010    0.00200   0.00000
    2:   2  1  2  1  1  1                     18226.15260   18226.15807   -0.00547    0.00200   0.00000
    3:   2  0  2  1  0  1                     18556.19200   18556.19251   -0.00051    0.00200   0.00000
    4:   2  1  1  1  1  0                     18890.00300   18890.00299    0.00001    0.00200   0.00000
    5:   3  1  3  2  1  2                     27338.31810   27338.31186    0.00624    0.00200   0.00000
    6:   3  0  3  2  0  2                     27830.82450   27830.82399    0.00051    0.00200   0.00000
    7:   3  1  2  2  1  1                     28333.85190   28333.85191   -0.00001    0.00200   0.00000
    8:   4  1  4  3  1  3                     36449.35910   36449.36104   -0.00194    0.00200   0.00000
    9:   4  0  4  3  0  3                     37101.30350   37101.30366   -0.00016    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.02956E-01    3   2.22355E-01    4   1.13994E-01    5   9.86467E-01    6   1.00000E+00
    7   8.45797E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            68464( 58)               0
   2         20000          B       4805.39358(122)         -0.00000
   3         30000          C       4473.41135(111)          0.00000
   4           200  -\Delta_J           -3.832( 43)E-03        0.000E-03
   5          1100 -\Delta_JK          0.14832( 72)         -0.00000
   6          2000  -\Delta_K      0.017525575(  0)E-18 -0.000000000E-18
   7         40100         d1           -1.868( 32)E-03        0.000E-03
   8         50000         d2     -0.019798083(  0)E-21  0.000000000E-21
 MICROWAVE AVG =       -0.000136 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002852 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.42601         1.42601
```

Molecule 40

IUPAC Name: 1,2-propadien-1-one

Common name: propadienone, methylene ketene

SMILES: C=C=C=O

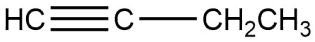


Molecule 41

IUPAC Name: 1-butyne

Common name: ethylacetylene

SMILES: CCC#C

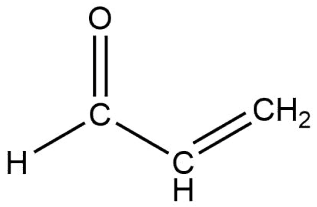


Molecule 42

IUPAC Name: 2-propenal (syn)

Common name: acrolein (syn), acrolein (cis), acrylaldehyde (syn)

SMILES: C=CC=O



42: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	3	1	2	3	1	3				8029.50700		8029.50911		-0.00211		0.00200		0.00000
2:	1	0	1	0	0	0				11143.23480		11143.23454		0.00026		0.00200		0.00000
3:	4	1	3	4	1	4				13366.98500		13366.98582		-0.00082		0.00200		0.00000
4:	3	0	3	2	1	2				17790.09540		17790.09653		-0.00113		0.00200		0.00000
5:	1	1	0	1	0	1				17929.34490		17929.34600		-0.00110		0.00200		0.00000
6:	2	1	1	2	0	2				19345.99780		19345.99761		0.00019		0.00200		0.00000
7:	5	1	4	5	1	5				20000.46540		20000.46325		0.00215		0.00200		0.00000
8:	2	1	2	1	1	1				20947.71570		20947.71581		-0.00011		0.00200		0.00000
9:	3	1	2	3	0	3				21613.49850		21613.49812		0.00038		0.00200		0.00000
10:	2	0	2	1	0	1				22208.55770		22208.55813		-0.00043		0.00200		0.00000
11:	2	2	0	3	1	3				22490.76350		22490.76353		-0.00003		0.00200		0.00000
12:	2	1	1	1	1	0				23625.20850		23625.20974		-0.00124		0.00200		0.00000
13:	4	1	3	4	0	4				24889.01290		24889.01177		0.00113		0.00200		0.00000
14:	1	1	1	0	0	0				27733.79760		27733.79795		-0.00035		0.00200		0.00000
15:	5	1	4	5	0	5				29346.49460		29346.50041		-0.00581		0.00200		0.00000
16:	4	0	4	3	1	3				30225.32810		30225.32827		-0.00017		0.00200		0.00000
17:	3	1	3	2	1	2				31374.08640		31374.08554		0.00086		0.00200		0.00000
18:	3	0	3	2	0	2				33119.81770		33119.81763		0.00007		0.00200		0.00000
19:	3	2	2	2	2	1				33429.91230		33429.91160		0.00070		0.00200		0.00000
20:	3	2	1	2	2	0				33739.30580		33739.30605		-0.00025		0.00200		0.00000
21:	6	1	5	6	0	6				35131.24920		35131.24622		0.00298		0.00200		0.00000
22:	3	1	2	2	1	1				35387.31840		35387.31814		0.00026		0.00200		0.00000
23:	2	1	2	1	0	1				37538.28060		37538.27923		0.00137		0.00200		0.00000

NORMALIZED DIAGONAL:

1 1.00000E+00 2 9.90001E-01 3 2.19057E-01 4 8.31855E-01 5 5.24777E-01 6 6.58741E-01
7 1.00000E+00 8 1.00000E+00

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

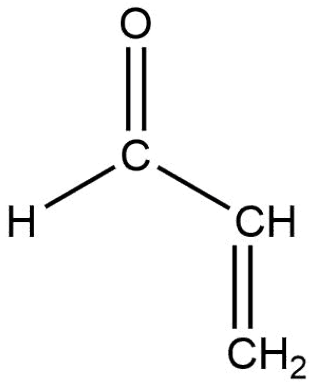
```
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A      22831.63152(112)          0.00000
  2         20000          B       6241.04745( 32)         -0.00000
  3         30000          C      4902.207561(296)        -0.000000
  4           200    Delta_J          -5.1200(156)E-03       0.0000E-03
  5          2000    Delta_K        -0.107593(260)        -0.000000
  6          1100   Delta_JK         0.029146( 51)         0.000000
  7         40100     -del_J     -1.484000000(  0)E-03 -0.000000000E-03
  8         41000     -del_K     -0.011360000(  0)      0.000000000
MICROWAVE AVG =       -0.000140 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001635 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.81754         0.81754
```

Molecule 43

IUPAC Name: 2-propenal (anti)

Common name: acrolein (anti), acrolein (trans), acrylaldehyde (anti), 2-propenal

SMILES: C=CC=O



43: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
 ***** NEXT LINE NOT USED IN FIT
    1:   2  0  2  1  0  1                     8092.18510   17801.30889 -999.99999    0.00200   0.00000
    2:   6  0  6  5  1  5                    13444.26960   13444.26981   -0.00021    0.00200   0.00000
    3:   2  1  2  3  0  3                    15585.86240   15585.86157    0.00083    0.00200   0.00000
    4:   2  1  2  1  1  1                    17387.59730   17387.59701    0.00029    0.00200   0.00000
    5:   2  0  2  1  0  1                    17801.30800   17801.30889   -0.00089    0.00200   0.00000
    6:   2  1  1  1  1  0                    18221.16190   18221.16340   -0.00150    0.00200   0.00000
    7:   1  1  1  2  0  2                    24892.57440   24892.57544   -0.00104    0.00200   0.00000
    8:   3  1  3  2  1  2                    26079.44850   26079.44959   -0.00109    0.00200   0.00000
    9:   3  0  3  2  0  2                    26694.31180   26694.31087    0.00093    0.00200   0.00000
   10:   3  2  2  2  2  1                    26706.66700   26706.66490    0.00210    0.00200   0.00000
   11:   3  2  1  2  2  0                    26718.80770   26718.80868   -0.00098    0.00200   0.00000
   12:   3  1  2  2  1  1                    27329.77070   27329.77083   -0.00013    0.00200   0.00000
   13:   4  1  4  3  1  3                    34768.98650   34768.98654   -0.00004    0.00200   0.00000
   14:   4  0  4  3  0  3                    35578.13750   35578.13684    0.00066    0.00200   0.00000
   15:   4  2  3  3  2  2                    35606.40850   35606.40955   -0.00105    0.00200   0.00000
   16:   4  2  2  3  2  1                    35636.76110   35636.76111   -0.00001    0.00200   0.00000
   17:   4  1  3  3  1  2                    36435.99120   36435.98992    0.00128    0.00200   0.00000
    1 Lines rejected from fit
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.83620E-01    3   9.83219E-01    4   7.19785E-01    5   1.05379E-03    6   6.54424E-01
    7   1.00000E+00    8   1.00000E+00
```

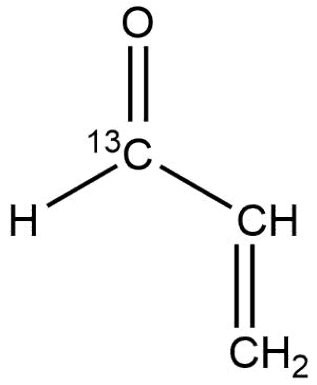
```
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         47353.13(110)            -0.00
   2         20000          B       4659.49968( 37)          -0.00000
   3         30000          C      4242.689724(280)          0.000000
   4           200    Delta_J          -1.0515(123)E-03      -0.0000E-03
   5          2000    Delta_K             0.23(110)             0.00
   6          1100   Delta_JK            8.760( 85)E-03        0.000E-03
   7         40100     -del_J     -0.121055275(  0)E-03 -0.000000000E-03
   8         41000     -del_K     -5.721825992(  0)E-03  0.000000000E-03
 MICROWAVE AVG =       -0.000053 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000987 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.49339         0.49339
```

Molecule 44

IUPAC Name: 2-propenal (anti) (13C1)

Common name: acrolein (anti), acrolein (trans), acrylaldehyde (anti), 2-propenal (13C1)

SMILES: C=CC=O



44: Line file

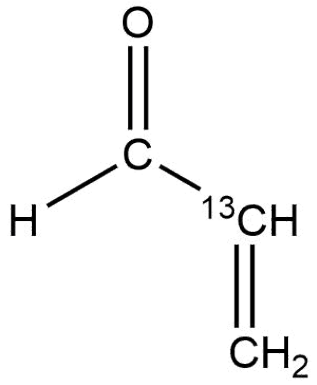
```
prop-2-enal (anti) (13C1)
  1  0  1  0  0  0                    8647.4263     0.002   \1-2484417
  2  0  2  1  0  1                   17292.1232     0.002   \1-2484419
  2  1  1  1  1  0                   17689.0367     0.002   \1-batch988
  3  1  3  2  1  2                   25349.3820     0.002   \1-batch988
  3  0  3  2  0  2                   25931.3788     0.002   \1-batch988
  3  1  2  2  1  1                   26531.7345     0.002   \1-batch988
```

Molecule 45

IUPAC Name: 2-propenal (anti) (13C2)

Common name: acrolein (anti), acrolein (trans), acrylaldehyde (anti), 2-propenal (13C2)

SMILES: C=CC=O



45: Line file

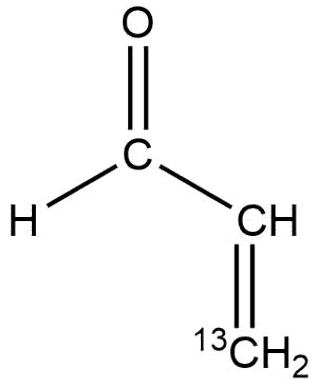
```
prop-2-enal (anti) (13C2)
  1  0  1  0  0  0                    8864.1793     0.002   \1-batch989
  2  0  2  1  0  1                   17725.1783     0.002   \1-batch989
  2  1  1  1  1  0                   18149.0411     0.002   \1-batch989
  3  0  3  2  0  2                   26579.8247     0.002   \1-batch989
```

Molecule 46

IUPAC Name: 2-propenal (anti) (13C3)

Common name: acrolein (anti), acrolein (trans), acrylaldehyde (anti), 2-propenal (13C3)

SMILES: C=CC=O



46: Line file

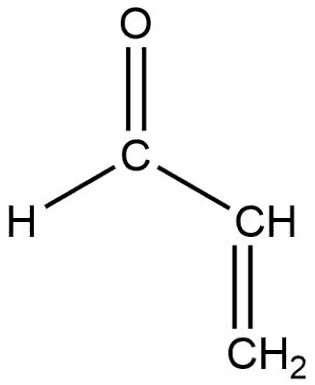
```
prop-2-enal (anti) (13C3)
  1  0  1  0  0  0                    8870.5744     0.002   \1-batch989
  2  0  2  1  0  1                   17738.0150     0.002   \1-batch989
  2  1  1  1  1  0                   18160.0365     0.002   \1-batch989
  3  0  3  2  0  2                   26599.1932     0.002   \1-batch989
```

Molecule 47

IUPAC Name: 2-propenal (anti) (ve1)

Common name: acrolein (anti), acrolein (trans), acrylaldehyde (anti), 2-propenal

SMILES: C=CC=O



47: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                     8892.53450    8892.53424    0.00026    0.00200   0.00000
    2:   2  1  2  1  1  1                    17368.75570   17368.76334   -0.00764    0.00200   0.00000
    3:   2  0  2  1  0  1                    17782.00890   17782.00838    0.00052    0.00200   0.00000
    4:   2  1  1  1  1  0                    18201.36800   18201.36120    0.00680    0.00200   0.00000
    5:   3  1  3  2  1  2                    26051.18640   26051.19118   -0.00478    0.00200   0.00000
    6:   3  0  3  2  0  2                    26665.36460   26665.36343    0.00117    0.00200   0.00000
    7:   3  1  2  2  1  1                    27300.07720   27300.07342    0.00378    0.00200   0.00000
    8:   4  1  4  3  1  3                    34731.30180   34731.29474    0.00706    0.00200   0.00000
    9:   4  0  4  3  0  3                    35539.54540   35539.54592   -0.00052    0.00200   0.00000
   10:   4  1  3  3  1  2                    36396.39660   36396.40318   -0.00658    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.63057E-01    3   6.46459E-01    4   3.19642E-01    5   3.26566E-02    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            47545( 41)               -0
   2         20000          B       4654.41710( 62)          0.00000
   3         30000          C       4238.11817( 68)          0.00000
   4           200    Delta_J           -0.259( 86)E-03       -0.000E-03
   5          2000    Delta_K           -134.4(161)              0.0
   6          1100   Delta_JK      0.041377332(  0)E-21  0.000000000E-21
   7         40100     -del_J     -1.158454703(  0)E-24 -0.000000000E-24
```

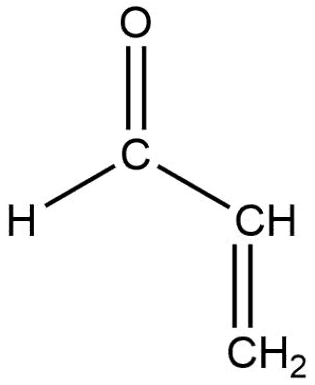
```
  8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
MICROWAVE AVG =        0.000009 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.004866 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        2.43291         2.43291
```

Molecule 48

IUPAC Name: 2-propenal (anti) (ve2)

Common name: acrolein (anti), acrolein (trans), acrylaldehyde (anti), 2-propenal

SMILES: C=CC=O



48: Fit file

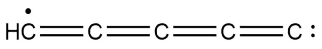
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                      8875.38220    8875.38259   -0.00039    0.00200   0.00000
    2:   2  0  2  1  0  1                     17747.81910   17747.81894    0.00016    0.00200   0.00000
    3:   3  0  3  2  0  2                     26614.36390   26614.36381    0.00009    0.00200   0.00000
    4:   4  0  4  3  0  3                     35472.07700   35472.07705   -0.00005    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   2.32614E-02    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A  47544.759517380(  0)      0.000000000
   2         20000          B        4643.4469(161)          -0.0000
   3         30000          C        4231.9357(153)           0.0000
   4           200    Delta_J     -2.584888171(  0)E-24 -0.000000000E-24
   5          2000    Delta_K     -0.134397676(  0)E-21  0.000000000E-21
   6          1100   Delta_JK      0.041377332(  0)E-21 -0.000000000E-21
   7         40100     -del_J     -1.158454703(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
 MICROWAVE AVG =       -0.000047 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000218 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.10903         0.10903
```

Molecule 50

IUPAC Name: 1,2,3,4-pentatetraene-1,1,5-trienyl radical

Common name: 1,2,3,4-pentatetraene-1,1,5-trienyl radical

SMILES: [C]=C=C=C=[CH]

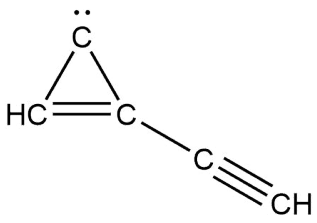


Molecule 51

IUPAC Name: 1-ethynyl-1-cyclopropen-2-ylidene

Common name: ethynyl cyclopropenylidene, acetyl cyclopropenylidene

SMILES: C1=[C](C1)C#C

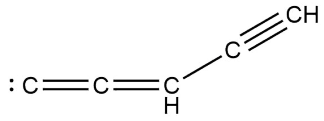


Molecule 52

IUPAC Name: 1,2-pentadien-4-yn-1-ylidene

Common name: 1,2-pentadien-4-yn-1-ylidene

SMILES: [C]=C=CC#C

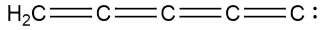


Molecule 53

IUPAC Name: pentatetraenylidene

Common name: pentatetraenylidene

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

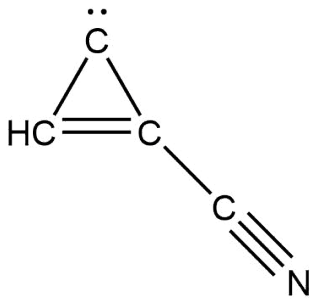


Molecule 54

IUPAC Name: 1-cyanocyclopropene-2,2-diyl

Common name: cyanocyclopropenylidene

SMILES: [C]1C=C1C#N

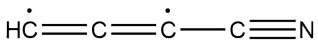


Molecule 55

IUPAC Name: cyanopropa-1,2-diene-1,3-diyl

Common name: cyanopropa-1,2-diene-1,3-diyl

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

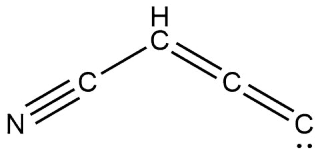


Molecule 56

IUPAC Name: cyanopropa-1,2-dienylidene

Common name: cyanoallenylidene

SMILES: [C]=C=CC#N

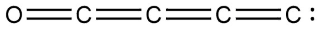


Molecule 57

IUPAC Name: 4-oxo-1,2,3-butatrienylidene

Common name: tetracarbonmonoxide

SMILES: [C]=C=C=C=O

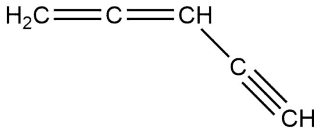


Molecule 58

IUPAC Name: 1,2-pentadien-4-yne

Common name: ethynylallene, allenylacetylene

SMILES: C=C=CC#C



58: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                     9854.40900    9854.41004   -0.00104    0.00200   0.00000
    2:   2  0  2  1  0  1                    10056.53200   10056.53304   -0.00104    0.00200   0.00000
    3:   2  1  1  1  1  0                    10261.99600   10261.99689   -0.00089    0.00200   0.00000
    4:   3  1  3  2  1  2                    14780.73600   14780.73523    0.00077    0.00200   0.00000
    5:   3  0  3  2  0  2                    15081.41100   15081.41038    0.00062    0.00200   0.00000
    6:   3  2  2  2  2  1                    15088.77500   15088.77531   -0.00031    0.00200   0.00000
    7:   3  1  2  2  1  1                    15392.07700   15392.07629    0.00071    0.00200   0.00000
    8:   4  1  4  3  1  3                    19706.01300   19706.01258    0.00042    0.00200   0.00000
    9:   4  0  4  3  0  3                    20102.22400   20102.22457   -0.00057    0.00200   0.00000
   10:   4  2  3  3  2  2                    20117.20600   20117.20481    0.00119    0.00200   0.00000
   11:   4  2  2  3  2  1                    20130.48100   20130.48129   -0.00029    0.00200   0.00000
   12:   4  1  3  3  1  2                    20521.04600   20521.04567    0.00033    0.00200   0.00000
   13:   5  1  5  4  1  4                    24629.90600   24629.90604   -0.00004    0.00200   0.00000
   14:   5  2  4  4  2  3                    25144.63800   25144.63870   -0.00070    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   5.01560E-01    3   2.19301E-01    4   2.59595E-01    5   9.95460E-01    6   1.00000E+00
    7   9.59381E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    25963.5( 35)              0.0
   2         20000                   2616.37580( 67)          0.00000
   3         30000                   2412.57336( 61)         -0.00000
   4           200                      -1.1546( 83)E-03      -0.0000E-03
   5          1100                     0.085522( 76)         0.000000
   6          2000                -0.073443248(  0)E-27 -0.000000000E-27
   7         40100                      -0.2816( 97)E-03      -0.0000E-03
   8         41000                 0.013582117(  0)E-27 -0.000000000E-27
 MICROWAVE AVG =       -0.000061 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000713 MHz, IR RMS =        0.00000
```

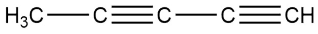
```
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.35638         0.35638
```

Molecule 59

IUPAC Name: 1,3-pentadiyne

Common name: methyldiacetylene, 1,3-pentadiyne

SMILES: CC#CC#C

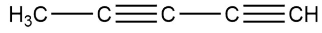


Molecule 60

IUPAC Name: 1,3-pentadiyne (ve1)

Common name: methyldiacetylene, 1,3-pentadiyne (ve1)

SMILES: CC#CC#C



60: Fit file

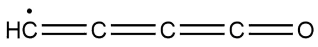
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  1  0                            8145.06690    8145.06817   -0.00127    0.00200   0.00000
    2:   3  0  2  0                           12217.59610   12217.59766   -0.00156    0.00200   0.00000
    3:   4  0  3  0                           16290.12140   16290.12164   -0.00024    0.00200   0.00000
    4:   5  0  4  0                           20362.63990   20362.63827    0.00163    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.00000E+00    4   1.00000E+00    5   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1          1000       A-B/  150000.00000000(  0)       0.00000000
   2           100       B  /      2036.267655(136)         0.000000
   3           200    -D_J  /     -0.076557900(  0)E-03  0.000000000E-03
   4          1100   -D_JK  /     -0.019800000(  0)      0.000000000
   5          2000   -D_JK  /     -2.926306000(  0)      0.000000000
 MICROWAVE AVG =       -0.000358 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001300 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.65019         0.65019
```

Molecule 61

IUPAC Name: 1,2,3-butatrien-1-on-4-yl

Common name: allyl ketene radical

SMILES: [CH]=C=C=C=O

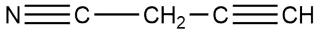


Molecule 62

IUPAC Name: 3-butynenitrile

Common name: propargyl cyanide

SMILES: C#CCC#N



62: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	AVG. CALC.FREQ.	- DIFF.	- WT.	
1:	1	0	1	1	0	0	0	1		5482.24200	5482.24344	-0.00144	0.00200	0.00000
2:	1	0	1	2	0	0	0	1		5482.92480	5482.92439	0.00041	0.00200	0.00000
3:	1	1	1	2	2	0	2	3		5949.11970	5949.12020	-0.00050	0.00200	0.00000
4:	2	1	2	2	1	1	1	1		10628.92350	10628.92847	-0.00497	0.00200	0.00000
5:	2	1	2	2	1	1	1	2		10628.99400	10628.99302	0.00098	0.00200	0.00000
6:	2	1	2	3	1	1	1	2		10629.65310	10629.65340	-0.00030	0.00200	0.00000
7:	2	1	2	1	1	1	1	1		10629.95370	10629.95578	-0.00208	0.00200	0.00000
8:	2	1	2	1	1	1	1	0		10630.11740	10630.11723	0.00017	0.00200	0.00000
9:	2	0	2	2	1	0	1	2		10959.92120	10959.92278	-0.00158	0.00200	0.00000
10:	2	0	2	1	1	0	1	0		10960.04500	10960.04518	-0.00018	0.00200	0.00000
11:	2	0	2	2	1	0	1	1		10960.60570	10960.60373	0.00197	0.00200	0.00000
12:	2	0	2	3	1	0	1	2		10960.65870	10960.65809	0.00061	0.00200	0.00000
13:	2	0	2	1	1	0	1	1		10961.74650	10961.74762	-0.00112	0.00200	0.00000
14:	2	1	1	2	1	1	0	1		11301.63380	11301.63211	0.00169	0.00200	0.00000
15:	2	1	1	1	1	1	0	1		11301.73640	11301.73990	-0.00350	0.00200	0.00000
16:	2	1	1	3	1	1	0	2		11302.31840	11302.31765	0.00075	0.00200	0.00000
17:	2	1	1	1	1	1	0	0		11303.27870	11303.28074	-0.00204	0.00200	0.00000
18:	5	0	5	4	4	1	4	3		11854.82510	11854.82247	0.00263	0.00200	0.00000
19:	5	0	5	6	4	1	4	5		11854.90460	11854.90463	-0.00003	0.00200	0.00000
20:	5	0	5	5	4	1	4	4		11855.05030	11855.05195	-0.00165	0.00200	0.00000
21:	3	1	3	3	2	1	2	2		15940.93730	15940.93631	0.00099	0.00200	0.00000
22:	3	1	3	2	2	1	2	1		15941.09010	15941.09140	-0.00130	0.00200	0.00000
23:	3	1	3	4	2	1	2	3		15941.15340	15941.15176	0.00164	0.00200	0.00000
24:	3	0	3	3	2	0	2	3		16427.64470	16427.64597	-0.00127	0.00200	0.00000
25:	3	0	3	2	2	0	2	1		16428.27760	16428.27887	-0.00127	0.00200	0.00000
26:	3	0	3	3	2	0	2	2		16428.38220	16428.38128	0.00092	0.00200	0.00000
27:	3	0	3	4	2	0	2	3		16428.41890	16428.41740	0.00150	0.00200	0.00000
28:	3	0	3	2	2	0	2	2		16429.41850	16429.42276	-0.00426	0.00200	0.00000
29:	3	1	2	3	2	1	1	2		16949.88150	16949.88308	-0.00158	0.00200	0.00000
30:	3	1	2	4	2	1	1	3		16950.07580	16950.07668	-0.00088	0.00200	0.00000
31:	3	1	2	2	2	1	1	1		16950.12890	16950.13015	-0.00125	0.00200	0.00000
32:	1	1	0	1	1	0	1	0		17245.64550	17245.64559	-0.00009	0.00200	0.00000

33:	1	1	0	0	1	0	1	1	17245.80690	17245.80719	-0.00029	0.00200	0.00000		
34:	1	1	0	2	1	0	1	2	17246.05360	17246.05074	0.00286	0.00200	0.00000		
35:	1	1	0	1	1	0	1	1	17247.34770	17247.34803	-0.00033	0.00200	0.00000		
36:	2	1	1	2	2	0	2	1	17587.23420	17587.23252	0.00168	0.00200	0.00000		
37:	2	1	1	1	2	0	2	1	17587.33940	17587.34031	-0.00091	0.00200	0.00000		
38:	2	1	1	3	2	0	2	3	17587.71280	17587.71030	0.00250	0.00200	0.00000		
39:	2	1	1	2	2	0	2	2	17588.37720	17588.37641	0.00079	0.00200	0.00000		
40:	3	1	2	2	3	0	3	2	18109.19480	18109.19160	0.00320	0.00200	0.00000		
41:	3	1	2	4	3	0	3	4	18109.37170	18109.36958	0.00212	0.00200	0.00000		
42:	4	1	3	3	4	0	4	3	18821.93610	18821.93532	0.00078	0.00200	0.00000		
43:	4	1	3	5	4	0	4	5	18822.05220	18822.05151	0.00069	0.00200	0.00000		
44:	4	1	3	4	4	0	4	4	18822.50110	18822.50344	-0.00234	0.00200	0.00000		
45:	4	1	4	4	3	1	3	3	21248.87490	21248.87287	0.00203	0.00200	0.00000		
46:	4	1	4	3	3	1	3	2	21248.91810	21248.91737	0.00073	0.00200	0.00000		
47:	4	1	4	5	3	1	3	4	21248.97520	21248.97297	0.00223	0.00200	0.00000		
48:	4	0	4	3	3	0	3	2	21881.14590	21881.14431	0.00159	0.00200	0.00000		
49:	4	0	4	4	3	0	3	3	21881.18010	21881.17873	0.00137	0.00200	0.00000		
50:	4	0	4	5	3	0	3	4	21881.20770	21881.20834	-0.00064	0.00200	0.00000		
51:	4	2	3	4	3	2	2	3	21928.87050	21928.87038	0.00012	0.00200	0.00000		
52:	4	2	3	5	3	2	2	4	21929.18140	21929.18133	0.00007	0.00200	0.00000		
53:	4	2	3	3	3	2	2	2	21929.26190	21929.26127	0.00063	0.00200	0.00000		
54:	4	2	2	4	3	2	1	3	21978.47550	21978.47774	-0.00224	0.00200	0.00000		
55:	4	2	2	5	3	2	1	4	21978.77570	21978.77627	-0.00057	0.00200	0.00000		
56:	1	1	1	0	0	0	0	1	22392.60270	22392.60579	-0.00309	0.00200	0.00000		
57:	1	1	1	2	0	0	0	1	22392.70130	22392.70268	-0.00138	0.00200	0.00000		
58:	1	1	1	1	0	0	0	1	22392.76560	22392.76724	-0.00164	0.00200	0.00000		
59:	4	1	3	4	3	1	2	3	22593.80250	22593.80396	-0.00146	0.00200	0.00000		
60:	4	1	3	3	3	1	2	2	22593.88920	22593.88804	0.00116	0.00200	0.00000	22593.88945	-0.0002
61:	4	1	3	5	3	1	2	4	22593.88920	22593.89027	-0.00107	0.00200	0.00000	22593.88945	-0.0002
62:	7	0	7	6	6	1	6	5	24279.34820	24279.34997	-0.00177	0.00200	0.00000		
63:	7	0	7	8	6	1	6	7	24279.40580	24279.40345	0.00235	0.00200	0.00000		
64:	5	1	5	5	4	1	4	4	26551.88360	26551.88568	-0.00208	0.00200	0.00000		
65:	5	1	5	4	4	1	4	3	26551.90790	26551.90325	0.00465	0.00200	0.00000		
66:	5	1	5	6	4	1	4	5	26551.94600	26551.94361	0.00239	0.00200	0.00000		
67:	5	0	5	4	4	0	4	3	27314.13580	27314.14001	-0.00421	0.00200	0.00000		
68:	5	0	5	5	4	0	4	4	27314.15450	27314.14965	0.00485	0.00200	0.00000		
69:	5	0	5	6	4	0	4	5	27314.17730	27314.17721	0.00009	0.00200	0.00000		
70:	5	2	4	6	4	2	3	5	27404.88300	27404.87704	0.00596	0.00200	0.00000		
71:	5	2	4	4	4	2	3	3	27404.89240	27404.89386	-0.00146	0.00200	0.00000		
72:	5	2	3	6	4	2	2	5	27503.85570	27503.84916	0.00654	0.00200	0.00000		
73:	2	1	2	2	1	0	1	2	27538.76840	27538.77131	-0.00291	0.00200	0.00000		
74:	2	1	2	3	1	0	1	2	27539.43160	27539.43169	-0.00009	0.00200	0.00000		
75:	2	1	2	2	1	0	1	1	27539.44850	27539.45226	-0.00376	0.00200	0.00000		
76:	2	1	2	1	1	0	1	1	27540.48160	27540.47958	0.00202	0.00200	0.00000		
77:	5	1	4	5	4	1	3	4	28232.24410	28232.24262	0.00148	0.00200	0.00000		
78:	5	1	4	4	4	1	3	3	28232.27600	28232.28243	-0.00643	0.00200	0.00000		
79:	5	1	4	6	4	1	3	5	28232.29370	28232.29120	0.00250	0.00200	0.00000		
80:	8	0	8	7	7	1	7	6	30590.89500	30590.89695	-0.00195	0.00200	0.00000		
81:	8	0	8	9	7	1	7	8	30590.93720	30590.94061	-0.00341	0.00200	0.00000		

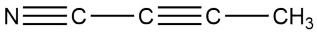
```
  82:   8  0  8  8  7  1  7  7              30591.13220   30591.12733    0.00487    0.00200   0.00000
  83:   6  1  6  6  5  1  5  5              31848.96790   31848.97029   -0.00239    0.00200   0.00000
  84:   6  1  6  5  5  1  5  4              31848.98500   31848.97928    0.00572    0.00200   0.00000
  85:   6  1  6  7  5  1  5  6              31849.00990   31849.00883    0.00107    0.00200   0.00000
  86:   6  0  6  6  5  0  5  5              32722.70030   32722.69988    0.00042    0.00200   0.00000   32722.70136   -0.00106
  87:   6  0  6  5  5  0  5  4              32722.70030   32722.70312   -0.00282    0.00200   0.00000   32722.70136   -0.00106
  88:   6  0  6  7  5  0  5  6              32722.72620   32722.72738   -0.00118    0.00200   0.00000
  89:   6  2  5  6  5  2  4  5              32876.13120   32876.13423   -0.00303    0.00200   0.00000
  90:   6  2  5  7  5  2  4  6              32876.23400   32876.23324    0.00076    0.00200   0.00000   32876.23330    0.00070
  91:   6  2  5  5  5  2  4  4              32876.23400   32876.23338    0.00062    0.00200   0.00000   32876.23330    0.00070
  92:   6  2  4  6  5  2  3  5              33048.68530   33048.68719   -0.00189    0.00200   0.00000
  93:   6  2  4  5  5  2  3  4              33048.76600   33048.76590    0.00010    0.00200   0.00000   33048.76679   -0.00079
  94:   6  2  4  7  5  2  3  6              33048.76600   33048.76743   -0.00143    0.00200   0.00000   33048.76679   -0.00079
  95:   6  1  5  6  5  1  4  5              33863.71620   33863.71312    0.00308    0.00200   0.00000
  96:   6  1  5  5  5  1  4  4              33863.72980   33863.73667   -0.00687    0.00200   0.00000
  97:   6  1  5  7  5  1  4  6              33863.74930   33863.74514    0.00416    0.00200   0.00000
  98:   7  1  7  7  6  1  6  6              37139.20490   37139.20224    0.00266    0.00200   0.00000   37139.20504   -0.00014
  99:   7  1  7  6  6  1  6  5              37139.20490   37139.20828   -0.00338    0.00200   0.00000   37139.20504   -0.00014
 100:   7  1  7  8  6  1  6  7              37139.22940   37139.23057   -0.00117    0.00200   0.00000
 101:   4  1  4  4  3  0  3  3              37340.27690   37340.27643    0.00047    0.00200   0.00000
 102:   4  1  4  3  3  0  3  2              37340.46310   37340.46186    0.00124    0.00200   0.00000
 103:   7  0  7  7  6  0  6  6              38102.69130   38102.69552   -0.00422    0.00200   0.00000
 104:   7  0  7  8  6  0  6  7              38102.72550   38102.72388    0.00162    0.00200   0.00000
 105:   7  2  6  7  6  2  5  6              38342.31080   38342.31277   -0.00197    0.00200   0.00000
 106:   7  2  6  6  6  2  5  5              38342.37540   38342.37369    0.00171    0.00200   0.00000   38342.37636   -0.00096
 107:   7  2  6  8  6  2  5  7              38342.37540   38342.37836   -0.00296    0.00200   0.00000   38342.37636   -0.00096
 108:   7  2  5  7  6  2  4  6              38616.69080   38616.69161   -0.00081    0.00200   0.00000
 109:   7  2  5  6  6  2  4  5              38616.72620   38616.72926   -0.00306    0.00200   0.00000
 110:   7  2  5  8  6  2  4  7              38616.73690   38616.73554    0.00136    0.00200   0.00000
 111:   7  1  6  7  6  1  5  6              39486.58770   39486.58462    0.00308    0.00200   0.00000
 112:   7  1  6  8  6  1  5  7              39486.61080   39486.60845    0.00235    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.27151E-02    3   9.99154E-01    4   4.93635E-01    5   7.71989E-01    6   5.30054E-03
    7   9.19767E-01    8   3.97041E-01    9   8.89320E-01   10   9.99884E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        19820.080( 70)           -0.000
   2         20000          B       2909.60624(119)          0.00000
   3         30000          C       2573.21226(116)         -0.00000
   4           200     -Del_J         -1.90456(137)E-03      0.00000E-03
   5          1100    -Del_JK        0.0679106(223)        0.0000000
   6          2000     -Del_K           -0.722( 69)            0.000
   7         40100     -del_J         -0.52354( 82)E-03      0.00000E-03
   8         41000     -del_K            -6.35( 58)E-03        -0.00E-03
   9     110010000     chi_aa         -2.26992(142)          0.00000
  10     110020000     chi_bb          0.21540(151)          0.00000
 MICROWAVE AVG =       -0.000036 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002466 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.23286         1.23286
```

Molecule 63

IUPAC Name: 2-butaynenitrile

Common name: methylcyanoacetylene, cyanoprop-1-yne

SMILES: CC#CC#N

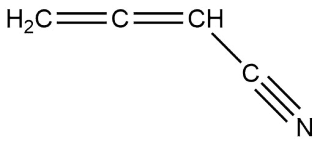


Molecule 64

IUPAC Name: 2,3-butadienenitrile

Common name: cyanoallene

SMILES: C=C=CC#N



64: Fit file

	EXP.FREQ.		CALC.FREQ.			DIFF.			EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	2	1	2	3	3	0	3	4			7590.97960	7590.98133	-0.00173	0.00200	0.00000
2:	2	1	2	1	3	0	3	2			7591.00790	7591.00930	-0.00140	0.00200	0.00000
3:	2	1	2	2	3	0	3	3			7591.26530	7591.26441	0.00089	0.00200	0.00000
4:	1	1	1	0	2	0	2	1			12962.21770	12962.21843	-0.00073	0.00200	0.00000
5:	1	1	1	1	2	0	2	1			12962.79130	12962.79400	-0.00270	0.00200	0.00000
6:	1	1	1	2	2	0	2	3			12963.04510	12963.04512	-0.00002	0.00200	0.00000
7:	3	1	2	2	3	0	3	2			24047.54390	24047.54496	-0.00106	0.00200	0.00000
8:	3	1	2	4	3	0	3	4			24047.69440	24047.69206	0.00234	0.00200	0.00000
9:	3	1	2	3	3	0	3	3			24048.11550	24048.11243	0.00307	0.00200	0.00000
10:	1	1	1	2	2	0	2	2			12963.91330	12963.91133	0.00197	0.00200	0.00000
11:	1	1	1	1	2	0	2	2			12964.14090	12964.14153	-0.00063	0.00200	0.00000
12:	2	1	2	2	1	1	1	1			10113.39020	10113.38924	0.00096	0.00200	0.00000
13:	2	1	2	2	1	1	1	2			10113.61920	10113.61944	-0.00024	0.00200	0.00000
14:	2	1	2	3	1	1	1	2			10114.23900	10114.23726	0.00174	0.00200	0.00000
15:	2	1	2	1	1	1	1	1			10114.35100	10114.35040	0.00060	0.00200	0.00000
16:	2	1	2	1	1	1	1	0			10114.92600	10114.92597	0.00003	0.00200	0.00000
17:	2	0	2	2	1	0	1	2			10325.87730	10325.87804	-0.00074	0.00200	0.00000
18:	2	0	2	1	1	0	1	0			10326.01550	10326.01515	0.00035	0.00200	0.00000
19:	2	0	2	2	1	0	1	1			10326.68500	10326.68492	0.00008	0.00200	0.00000
20:	2	0	2	3	1	0	1	2			10326.74490	10326.74424	0.00066	0.00200	0.00000
21:	2	0	2	1	1	0	1	1			10328.03190	10328.03245	-0.00055	0.00200	0.00000
22:	2	1	1	2	1	1	0	1			10542.27350	10542.27193	0.00157	0.00200	0.00000
23:	2	1	1	1	1	1	0	1			10542.65240	10542.65584	-0.00344	0.00200	0.00000
24:	2	1	1	2	1	1	0	2			10542.84490	10542.84854	-0.00364	0.00200	0.00000
25:	2	1	1	3	1	1	0	2			10543.09620	10543.09522	0.00098	0.00200	0.00000
26:	2	1	1	1	1	1	0	0			10544.09710	10544.09737	-0.00027	0.00200	0.00000
27:	3	1	3	3	2	1	2	3			15169.32890	15169.32955	-0.00065	0.00200	0.00000
28:	3	1	3	3	2	1	2	2			15169.94830	15169.94737	0.00093	0.00200	0.00000
29:	3	1	3	2	2	1	2	1			15170.15690	15170.15454	0.00236	0.00200	0.00000

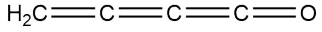
```
  30:   3  1  3  4  2  1  2  3              15170.19580   15170.19493    0.00087    0.00200   0.00000
  31:   3  1  3  2  2  1  2  2              15171.11510   15171.11570   -0.00060    0.00200   0.00000
  32:   3  0  3  3  2  0  2  3              15485.39900   15485.40015   -0.00115    0.00200   0.00000
  33:   3  0  3  2  2  0  2  1              15486.13590   15486.13510    0.00080    0.00200   0.00000
  34:   3  0  3  3  2  0  2  2              15486.26760   15486.26636    0.00124    0.00200   0.00000
  35:   3  0  3  4  2  0  2  3              15486.30160   15486.30105    0.00055    0.00200   0.00000
  36:   3  0  3  2  2  0  2  2              15487.48200   15487.48263   -0.00063    0.00200   0.00000
  37:   3  1  2  3  2  1  1  3              15812.97910   15812.98116   -0.00206    0.00200   0.00000
  38:   3  1  2  3  2  1  1  2              15813.22830   15813.22785    0.00045    0.00200   0.00000
  39:   3  1  2  4  2  1  1  3              15813.46260   15813.46169    0.00091    0.00200   0.00000
  40:   3  1  2  2  2  1  1  1              15813.48990   15813.49274   -0.00284    0.00200   0.00000
  41:   3  1  2  2  2  1  1  2              15813.87400   15813.87665   -0.00265    0.00200   0.00000
  42:   4  1  4  4  3  1  3  4              20224.07260   20224.07449   -0.00189    0.00200   0.00000
  43:   4  1  4  4  3  1  3  3              20224.94110   20224.93987    0.00123    0.00200   0.00000
  44:   4  1  4  3  3  1  3  2              20225.00250   20225.00054    0.00196    0.00200   0.00000
  45:   4  1  4  5  3  1  3  4              20225.05440   20225.05207    0.00233    0.00200   0.00000
  46:   4  1  4  3  3  1  3  3              20226.16370   20226.16887   -0.00517    0.00200   0.00000
  47:   4  0  4  4  3  0  3  4              20640.43690   20640.43828   -0.00138    0.00200   0.00000
  48:   4  0  4  3  3  0  3  2              20641.28600   20641.28570    0.00030    0.00200   0.00000
  49:   4  0  4  4  3  0  3  3              20641.34170   20641.33917    0.00253    0.00200   0.00000
  50:   4  0  4  5  3  0  3  4              20641.36350   20641.36320    0.00030    0.00200   0.00000
  51:   4  0  4  3  3  0  3  3              20642.50130   20642.50198   -0.00068    0.00200   0.00000
  52:   4  1  3  4  3  1  2  4              21082.06700   21082.06761   -0.00061    0.00200   0.00000
  53:   4  1  3  4  3  1  2  3              21082.54710   21082.54813   -0.00103    0.00200   0.00000
  54:   4  1  3  3  3  1  2  2              21082.63330   21082.63356   -0.00026    0.00200   0.00000
  55:   4  1  3  5  3  1  2  4              21082.65400   21082.65161    0.00239    0.00200   0.00000
  56:   4  1  3  3  3  1  2  3              21083.28240   21083.28237    0.00003    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.23886E-01    3   2.98510E-01    4   9.90569E-01    5   6.11698E-01    6   1.00000E+00
    7   9.94137E-01    8   1.00000E+00    9   9.99945E-01   10   9.30469E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A      25979.06566(110)          0.00000
   2         20000          B      2689.275982(262)         0.000000
   3         30000          C      2474.824698(276)        -0.000000
   4           200     -Del_J          -1.2841( 52)E-03       0.0000E-03
   5          1100    -Del_JK         0.085662( 92)        -0.000000
   6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
   7         40100     -del_J          -0.3103( 49)E-03      -0.0000E-03
   8         41000     -del_K     -6.135949147(  0)E-24 -0.000000000E-24
   9     110010000     chi_aa         -2.68973(126)         -0.00000
  10     110020000     chi_bb          0.76760(133)         -0.00000
 MICROWAVE AVG =       -0.000077 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001680 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.84002         0.84002
```

Molecule 65

IUPAC Name: 1,2,3-butatrien-1-one

Common name: butatrienone, allene ketone, vinylideneketene

SMILES: C=C=C=C=O



65: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                     8602.90430    8602.89933    0.00497    0.00200   0.00000
    2:   2  0  2  1  0  1                     8615.18400    8615.18435   -0.00035    0.00200   0.00000
    3:   2  1  1  1  1  0                     8630.65220    8630.65349   -0.00129    0.00200   0.00000
    4:   3  1  3  2  1  2                    12904.34240   12904.33776    0.00464    0.00200   0.00000
    5:   3  0  3  2  0  2                    12922.76460   12922.76438    0.00022    0.00200   0.00000
    6:   3  1  2  2  1  1                    12945.96590   12945.96901   -0.00311    0.00200   0.00000
    7:   4  1  4  3  1  3                    17205.76530   17205.76272    0.00258    0.00200   0.00000
    8:   4  0  4  3  0  3                    17230.33030   17230.32985    0.00045    0.00200   0.00000
    9:   4  1  3  3  1  2                    17261.26780   17261.27105   -0.00325    0.00200   0.00000
   10:   5  1  5  4  1  4                    21507.16960   21507.16971   -0.00011    0.00200   0.00000
   11:   5  0  5  4  0  4                    21537.87720   21537.87590    0.00130    0.00200   0.00000
   12:   5  1  4  4  1  3                    21576.55420   21576.55512   -0.00092    0.00200   0.00000
   13:   6  1  6  5  1  5                    25808.54880   25808.55425   -0.00545    0.00200   0.00000
   14:   6  0  6  5  0  5                    25845.39630   25845.39767   -0.00137    0.00200   0.00000
   15:   6  1  5  5  1  4                    25891.81700   25891.81674    0.00026    0.00200   0.00000
   16:   7  1  7  6  1  6                    30109.91170   30109.91183   -0.00013    0.00200   0.00000
   17:   7  1  6  6  1  5                    30207.05540   30207.05140    0.00400    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   7.31086E-01    4   3.85405E-01    5   1.00000E+00    6   4.94535E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000             300000.00000082(  0)      -0.00000000
   2         20000                 2160.736206(188)         0.000000
   3         30000                 2146.859124(188)         0.000000
   4           200                    -0.18210(196)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                    0.397894(126)        -0.000000
   7         40100                -0.471096592(  0)E-24  0.000000000E-24
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000143 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002715 MHz, IR RMS =        0.00000
```

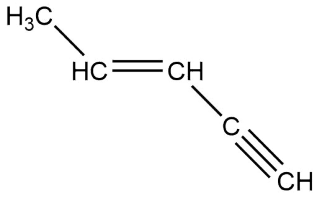
```
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.35746         1.35746
```

Molecule 66

IUPAC Name: (E)-3-penten-1-yne

Common name: propenyl acetylene (E)

SMILES: CC=CC#C



66_Estate: Line file

```
(E)-3-penten-1-yne, E state
  2  0  2  1  0  1                      8794.7095     0.002   /1-batch33
  3  0  3  2  0  2                     13191.5735     0.002   /1-batch33
  4  0  4  3  0  3                     17587.8340     0.002   /1-batch33
  5  0  5  4  0  4                     21983.2970     0.002   /1-batch33
  2  1  2  1  1  1                      8700.2628     0.002   \1-survey2212
  2  1  2  1  1  1                      8700.2868     0.002   \1-survey2212
  3  1  3  2  1  2                     13048.5814     0.002   \1-2357565
  4  1  4  3  1  3                     17396.8413     0.002   \1-2357565
  5  1  5  4  1  4                     21745.3190     0.002   \1-2358281
  6  1  6  5  1  5                     26093.6681     0.002   \1-2358283
  7  1  7  6  1  6                     30441.7233     0.002   \1-2358285
  8  1  8  7  1  7                     34789.4385     0.002   \1-2358288
  3  1  2  2  1  1                     13336.0552     0.002   \1-2357565
  4  1  3  3  1  2                     17782.1659     0.002   \1-2357565
  5  1  4  4  1  3                     22227.6250     0.002   \1-2358282
  6  1  5  5  1  4                     26672.6793     0.002   \1-2358284
  7  1  6  6  1  5                     31117.3505     0.002   \1-2358286
  8  1  7  7  1  6                     35561.6106     0.002   \1-2358289
```

66_Astate: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      8794.70870    8794.70495    0.00375    0.00200   0.00000
    2:   3  0  3  2  0  2                     13191.56260   13191.55991    0.00269    0.00200   0.00000
    3:   4  0  4  3  0  3                     17587.81990   17587.81793    0.00197    0.00200   0.00000
    4:   5  0  5  4  0  4                     21983.28060   21983.28021    0.00039    0.00200   0.00000
```

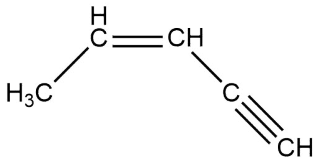
```
   5:   6  0  6  5  0  5                  26377.74510   26377.74819   -0.00309    0.00200   0.00000
   6:   7  0  7  6  0  6                  30771.01580   30771.02374   -0.00794    0.00200   0.00000
   7:   8  0  8  7  0  7                  35162.91550   35162.90941    0.00609    0.00200   0.00000
   8:   2  1  2  1  1  1                   8698.40780    8698.41359   -0.00579    0.00200   0.00000
   9:   2  1  2  1  1  1                   8698.42550    8698.41359    0.01191    0.00200   0.00000
  10:   4  1  4  3  1  3                  17396.40150   17396.39871    0.00279    0.00200   0.00000
  11:   5  1  5  4  1  4                  21745.09950   21745.09767    0.00183    0.00200   0.00000
  12:   6  1  6  5  1  5                  26093.52090   26093.53086   -0.00996    0.00200   0.00000
  13:   7  1  7  6  1  6                  30441.64720   30441.64650    0.00070    0.00200   0.00000
  14:   8  1  8  7  1  7                  34789.39630   34789.39352    0.00278    0.00200   0.00000
  15:   3  1  2  2  1  1                  13337.16040   13337.16100   -0.00060    0.00200   0.00000
  16:   4  1  3  3  1  2                  17782.62280   17782.62371   -0.00091    0.00200   0.00000
  17:   5  1  4  4  1  3                  22227.86500   22227.86491    0.00009    0.00200   0.00000
  18:   6  1  5  5  1  4                  26672.82830   26672.82833   -0.00003    0.00200   0.00000
  19:   7  1  6  6  1  5                  31117.45940   31117.45715    0.00225    0.00200   0.00000
  20:   8  1  7  7  1  6                  35561.69250   35561.69383   -0.00133    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.65646E-01    3   2.38223E-01    4   2.16917E-01    5   1.00000E+00    6   9.57094E-01
    7   9.99356E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A          38457.0(143)             -0.0
   2         20000          B       2247.00673( 32)          0.00000
   3         30000          C       2150.44628( 32)          0.00000
   4           200    Delta_J         -0.25644(199)E-03      0.00000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK         0.018815(224)        -0.000000
   7         40100     -del_J         -0.02993(141)E-03      0.00000E-03
   8         41000     -del_K     -0.400594727(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =        0.000381 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.004674 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        2.33718         2.33718
```

Molecule 67

IUPAC Name: (Z)-3-penten-1-yne

Common name: propenyl acetylene (Z)

SMILES: CC=CC#C



67_Estate: Line file

```
(Z)-3-penten-1-yne, E state
  2  1  2  1  1  1                    11404.8246    0.002  \1-2178097
  2  0  2  1  0  1                    12077.4390    0.002  \1-2178170
  2  1  1  1  0  0                    12837.5450    0.002  \1-2178161
  3  1  3  2  1  2                    17080.4869    0.002  \1-2178097
  3  0  3  2  0  2                    18007.4946    0.002  \1-2178115
  3  1  2  2  1  1                    19227.8380    0.002  \1-2178136
  4  1  4  3  1  3                    22726.4743    0.002  \1-2178122
  5  0  5  4  0  4                    29471.1949    0.002  \1-2177849
  6  0  6  5  0  5                    34981.4289    0.002  \1-2178093
```

67_Astate: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                    11405.16300   11405.15790    0.00510    0.00200   0.00000
    2:   2  0  2  1  0  1                    12076.70430   12076.70612   -0.00182    0.00200   0.00000
    4:   3  1  3  2  1  2                    17081.04240   17081.03971    0.00269    0.00200   0.00000
    5:   3  0  3  2  0  2                    18006.51170   18006.51257   -0.00087    0.00200   0.00000
    6:   3  1  2  2  1  1                    19226.16960   19226.17019   -0.00059    0.00200   0.00000
    7:   4  1  4  3  1  3                    22727.18050   22727.18401   -0.00351    0.00200   0.00000
    8:   4  2  3  3  2  2                    24208.53350   24208.53321    0.00029    0.00200   0.00000
    9:   4  0  4  3  0  3                    23812.18450   23812.18269    0.00181    0.00200   0.00000
   10:   5  1  5  4  1  4                    28337.32490   28337.33170   -0.00680    0.00200   0.00000
   11:   5  0  5  4  0  4                    29470.09330   29470.09006    0.00324    0.00200   0.00000
   12:   6  1  6  5  1  5                    33907.95120   33907.94640    0.00480    0.00200   0.00000
   13:   6  0  6  5  0  5                    34980.42930   34980.43190   -0.00260    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   5.60422E-01    3   4.19187E-01    4   2.40849E-01    5   1.00000E+00    6   9.46781E-01
```

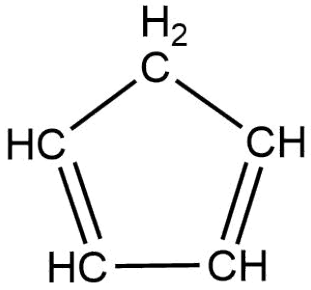
```
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       11784.8841(268)           0.0000
   2         20000          B       3387.94567( 48)         -0.00000
   3         30000          C       2672.34212( 38)          0.00000
   4           200    Delta_J          -1.7677( 56)E-03      -0.0000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK         0.060610( 94)        -0.000000
   7         40100     -del_J     -0.011993847(  0)E-21 -0.000000000E-21
   8         41000     -del_K     -0.012129138(  0)E-21  0.000000000E-21
 MICROWAVE AVG =        0.000145 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.003414 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.70712         1.70712
```

Molecule 68

IUPAC Name: 1,3-cyclopentadiene

Common name: cyclopentadiene

SMILES: C1C=CC=C1

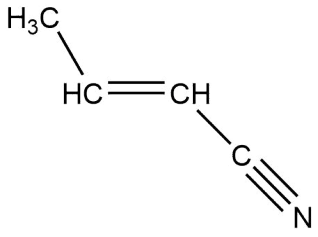


Molecule 69

IUPAC Name: (E)-2-butenenitrile

Common name: trans-crotonitrile

SMILES: CC=CC#N



69_Astate: Fit file

	EXP.FREQ.			CALC.FREQ.			DIFF.		EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	2	1	2	2	1	1	1	1			8881.76760	8881.77155	-0.00395	0.00200	0.00000
2:	2	1	2	3	1	1	1	2			8882.93100	8882.92861	0.00239	0.00200	0.00000
3:	2	0	2	2	1	0	1	2			8983.18200	8983.18090	0.00110	0.00200	0.00000
4:	2	0	2	1	1	0	1	0			8983.36710	8983.36708	0.00002	0.00200	0.00000
5:	2	0	2	3	1	0	1	2			8984.37830	8984.37711	0.00119	0.00200	0.00000
6:	2	0	2	1	1	0	1	1			8986.15920	8986.15830	0.00090	0.00200	0.00000
7:	2	1	1	2	1	1	0	1			9085.54710	9085.54777	-0.00067	0.00200	0.00000
8:	3	1	3	3	2	1	2	2			13323.66310	13323.66702	-0.00392	0.00200	0.00000
9:	3	1	3	4	2	1	2	3			13324.00080	13323.99981	0.00099	0.00200	0.00000
10:	3	0	3	3	2	0	2	3			13474.68870	13474.68893	-0.00023	0.00200	0.00000
11:	3	0	3	3	2	0	2	2			13475.88580	13475.88514	0.00066	0.00200	0.00000
12:	3	0	3	4	2	0	2	3			13475.93030	13475.92951	0.00079	0.00200	0.00000
13:	3	0	3	2	2	0	2	2			13477.55870	13477.56007	-0.00137	0.00200	0.00000
14:	3	1	2	3	2	1	1	2			13629.33010	13629.33106	-0.00096	0.00200	0.00000
15:	3	1	2	4	2	1	1	3			13629.66460	13629.66288	0.00172	0.00200	0.00000
16:	4	1	4	4	3	1	3	3			17764.82110	17764.82125	-0.00015	0.00200	0.00000
17:	4	1	4	3	3	1	3	2			17764.92210	17764.92005	0.00205	0.00200	0.00000
18:	4	1	4	5	3	1	3	4			17764.97070	17764.96961	0.00109	0.00200	0.00000
19:	4	0	4	4	3	0	3	4			17965.56000	17965.55945	0.00055	0.00200	0.00000
20:	4	0	4	3	3	0	3	2			17966.72000	17966.72035	-0.00035	0.00200	0.00000
21:	4	0	4	4	3	0	3	3			17966.80190	17966.80003	0.00187	0.00200	0.00000
22:	4	0	4	5	3	0	3	4			17966.82960	17966.82831	0.00129	0.00200	0.00000
23:	4	0	4	3	3	0	3	3			17968.39260	17968.39528	-0.00268	0.00200	0.00000
24:	4	1	3	4	3	1	2	3			18172.37180	18172.37196	-0.00016	0.00200	0.00000
25:	4	1	3	3	3	1	2	2			18172.47280	18172.47250	0.00030	0.00200	0.00000
26:	4	1	3	5	3	1	2	4			18172.51930	18172.51969	-0.00039	0.00200	0.00000

```
   27:   5  0  5  4  4  0  4  3              22456.77290   22456.77361   -0.00071    0.00200   0.00000
   28:   5  0  5  5  4  0  4  4              22456.81710   22456.81782   -0.00072    0.00200   0.00000
   29:   5  0  5  6  4  0  4  5              22456.83670   22456.83744   -0.00074    0.00200   0.00000
   30:   7  0  7  6  6  0  6  5              31433.26600   31433.24743    0.01857    0.00500   0.00000   31433.26404    0.00196
   31:   7  0  7  7  6  0  6  6              31433.26600   31433.26681   -0.00081    0.00500   0.00000   31433.26404    0.00196
   32:   7  0  7  8  6  0  6  7              31433.26600   31433.27789   -0.01189    0.00500   0.00000   31433.26404    0.00196
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   5.57555E-01    4   4.11800E-01    5   1.00000E+00    6   7.92337E-01
    7   1.00000E+00    8   1.00000E+00    9   9.99661E-01   10   9.85951E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A  38054.000000000(  1)     -0.000000000
   2         20000          B      2297.075046(224)        -0.000000
   3         30000          C      2195.186936(220)        -0.000000
   4           200    Delta_J          -0.2874( 35)E-03       0.0000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
   6          1100   Delta_JK         0.018772(114)        -0.000000
   7         40100     -del_J     -0.011993847(  0)E-21 -0.000000000E-21
   8         41000     -del_K     -0.012129138(  0)E-21 -0.000000000E-21
   9     110010000     chi_aa         -3.72162(190)          0.00000
  10     110020000     chi_bb            1.820( 48)           -0.000
 MICROWAVE AVG =        0.000062 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001551 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.75816         0.75816
```

69_Estate: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  2  1  0  1  2               8983.18200    8983.20728   -0.02528    0.00500   0.00000
    2:   2  0  2  1  1  0  1  0               8983.37290    8983.38720   -0.01430    0.00200   0.00000
    3:   2  0  2  3  1  0  1  2               8984.38610    8984.36935    0.01675    0.00200   0.00000
    4:   2  0  2  1  1  0  1  1               8986.15920    8986.10032    0.05888    0.00500   0.00000
    5:   3  0  3  3  2  0  2  3              13474.69830   13474.72789   -0.02959    0.00200   0.00000
    6:   3  0  3  3  2  0  2  2              13475.89640   13475.88995    0.00645    0.00200   0.00000
    7:   3  0  3  4  2  0  2  3              13475.93990   13475.93201    0.00789    0.00200   0.00000
    8:   3  0  3  2  2  0  2  2              13477.55870   13477.51566    0.04304    0.00500   0.00000
    9:   4  0  4  4  3  0  3  4              17965.57330   17965.61293   -0.03963    0.00200   0.00000
   10:   4  0  4  3  3  0  3  2              17966.73330   17966.73790   -0.00460    0.00200   0.00000
   11:   4  0  4  4  3  0  3  3              17966.81760   17966.81706    0.00054    0.00200   0.00000
   12:   4  0  4  5  3  0  3  4              17966.84410   17966.84306    0.00104    0.00200   0.00000
   13:   4  0  4  3  3  0  3  3              17968.40860   17968.36360    0.04500    0.00200   0.00000
   14:   3  1  3  3  2  1  2  2              13324.67280   13324.68805   -0.01525    0.00200   0.00000
   15:   3  1  3  4  2  1  2  3              13325.01740   13325.00238    0.01502    0.00200   0.00000
   16:   3  1  2  3  2  1  1  2              13628.30660   13628.30632    0.00028    0.00200   0.00000
   17:   3  1  2  4  2  1  1  3              13628.63700   13628.63756   -0.00056    0.00200   0.00000
   18:   4  1  4  4  3  1  3  3              17765.22820   17765.22858   -0.00038    0.00200   0.00000
   19:   4  1  4  3  3  1  3  2              17765.32970   17765.34028   -0.01058    0.00200   0.00000
   20:   4  1  4  5  3  1  3  4              17765.37790   17765.36676    0.01114    0.00200   0.00000
```

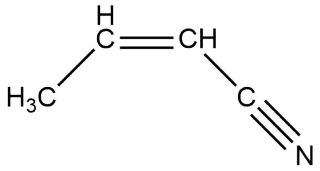
```
   21:   4  1  3  4  3  1  2  3              18171.94670   18171.95418   -0.00748    0.00200   0.00000
   22:   4  1  3  3  3  1  2  2              18172.05160   18172.03540    0.01620    0.00200   0.00000
   23:   4  1  3  5  3  1  2  4              18172.09460   18172.10311   -0.00851    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.18278E-01    3   1.38592E-01    4   1.17246E-01    5   1.00000E+00    6   9.79642E-01
    7   9.99913E-01    8   1.00000E+00    9   1.00000E+00   10   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            38399( 97)               1
   2         20000          B       2296.42533( 86)          0.00000
   3         30000          C       2195.83070( 85)          0.00000
   4           200    Delta_J          -0.2920(190)E-03      -0.0003E-03
   5          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK          0.01980( 51)          0.00001
   7         40100     -del_J           8.4936(140)E-03       0.0000E-03
   8         41000     -del_K     -0.012129138(  0)E-21 -0.000000000E-21
   9     110010000     chi_aa     -3.617489778(  0)     -0.000000000
  10     110020000     chi_bb      2.520000904(  0)     -0.000000000
 MICROWAVE AVG =        0.002873 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.022962 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        8.79813         8.79813
```

Molecule 70

IUPAC Name: (Z)-2-butenenitrile

Common name: cis-crotonitrile

SMILES: CC=CC#N



70_Estate: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  2  1  0  1  2              12517.91540   12517.91515    0.00025    0.00200   0.00000
    2:   2  0  2  1  1  0  1  0              12518.05490   12518.05497   -0.00007    0.00200   0.00000
    3:   2  0  2  2  1  0  1  1              12518.48640   12518.48708   -0.00068    0.00200   0.00000
    4:   2  0  2  3  1  0  1  2              12518.55720   12518.55654    0.00066    0.00200   0.00000
    5:   2  0  2  1  1  0  1  1              12519.48470   12519.48484   -0.00014    0.00200   0.00000
    6:   3  0  3  2  2  0  2  1              18653.23980   18653.23965    0.00015    0.00200   0.00000
    7:   3  0  3  3  2  0  2  2              18653.27990   18653.28047   -0.00057    0.00200   0.00000
    8:   3  0  3  4  2  0  2  3              18653.34830   18653.34790    0.00040    0.00200   0.00000
    9:   4  0  4  4  3  0  3  3              24646.78400   24646.78202    0.00198    0.00200   0.00000
   10:   4  0  4  3  3  0  3  2              24646.80460   24646.80768   -0.00308    0.00200   0.00000
   11:   4  0  4  5  3  0  3  4              24646.85590   24646.85479    0.00111    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   5.22329E-01    3   1.60240E-03    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   1.00000E+00   10   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A          11840.0( 49)              0.0
   2         20000          B         3524.565(104)            0.000
   3         30000          C         2759.868(105)           -0.000
   4           200    Delta_J     -0.270991860(  0)E-03 -0.000000000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
   6          1100   Delta_JK      0.018326742(  0)     -0.000000000
   7         40100     -del_J     -0.011993847(  0)E-21 -0.000000000E-21
   8         41000     -del_K     -0.012129138(  0)E-21 -0.000000000E-21
   9     110010000     chi_aa     -1.906479526(  0)      0.000000000
  10     110020000     chi_bb     -0.124551523(  0)      0.000000000
 MICROWAVE AVG =        0.000000 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001211 MHz, IR RMS =        0.00000
```

```
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.60563         0.60563
```

70_Astate: Fit file

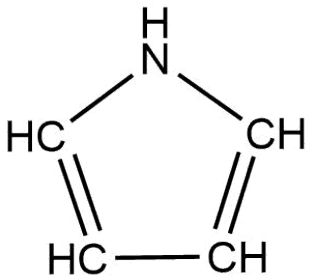
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  2  1  1  1  1              11803.81370   11803.81473   -0.00103    0.21040   0.00000
    2:   2  1  2  3  1  1  1  2              11804.42870   11804.42984   -0.00114    0.21040   0.00000
    3:   2  1  2  1  1  1  1  0              11804.74330   11804.74041    0.00289    0.21070   0.00000
    4:   2  1  2  2  1  1  1  1              11803.73410   11803.81473   -0.08063    9.00200   0.00000
    5:   2  1  2  3  1  1  1  2              11804.00000   11804.42984   -0.42984    9.10000   0.00000
    6:   2  1  1  2  1  1  0  1              13332.88380   13332.51789    0.36591    9.00200   0.00000
    7:   2  1  1  3  1  1  0  2              13333.45170   13333.08745    0.36425    9.00200   0.00000
    8:   2  0  2  2  1  0  1  2              12517.64440   12517.64383    0.00057    0.00200   0.00000
    9:   2  0  2  1  1  0  1  0              12517.78110   12517.78302   -0.00192    0.00200   0.00000
   10:   2  0  2  2  1  0  1  1              12518.21590   12518.21576    0.00014    0.00200   0.00000
   11:   2  0  2  3  1  0  1  2              12518.28670   12518.28481    0.00189    0.00200   0.00000
   12:   2  0  2  1  1  0  1  1              12519.21220   12519.21288   -0.00068    0.00200   0.00000
   13:   3  0  3  2  2  0  2  1              18652.87650   18652.87611    0.00039    0.00200   0.00000
   14:   3  0  3  3  2  0  2  2              18652.91640   18652.91770   -0.00130    0.00200   0.00000
   15:   3  0  3  4  2  0  2  3              18652.98540   18652.98450    0.00090    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.38310E-01    3   4.26875E-03    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   9.41549E-01   10   9.99731E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         11835.16(280)             0.00
   2         20000          B         3524.320( 61)            0.000
   3         30000          C         2759.969( 61)           -0.000
   4           200    Delta_J     -0.270991860(  0)E-03 -0.000000000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
   6          1100   Delta_JK      0.018326742(  0)     -0.000000000
   7         40100     -del_J     -0.011993847(  0)E-21 -0.000000000E-21
   8         41000     -del_K     -0.012129138(  0)E-21 -0.000000000E-21
   9     110010000     chi_aa          -1.9065( 33)           0.0000
  10     110020000     chi_bb           -0.110( 35)            0.000
 MICROWAVE AVG =        0.014693 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.174710 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.42319         0.42319
```

Molecule 71

IUPAC Name: 1H-pyrrole

Common name: pyrrole, azole

SMILES: C1=CNC=C1



71: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-			EST.ERR.	-AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	2	1	1	2	2	1	2	2				13406.71270		13406.71119		0.00151	0.00200	0.00000
2:	2	1	1	3	2	1	2	3				13407.99540		13407.99569		-0.00029	0.00200	0.00000
3:	2	1	1	1	2	1	2	1				13408.70680		13408.70934		-0.00254	0.00200	0.00000
4:	1	0	1	0	0	0	0	1				13532.76680		13532.76965		-0.00285	0.00200	0.00000
5:	1	0	1	2	0	0	0	1				13533.40110		13533.40178		-0.00068	0.00200	0.00000
6:	1	0	1	1	0	0	0	1				13533.81610		13533.82319		-0.00709	0.00200	0.00000
7:	1	0	1	1	0	0	0	1				13533.83380		13533.82319		0.01061	0.00200	0.00000
8:	2	2	1	2	2	0	2	2				13797.25920		13797.25247		0.00673	0.00200	0.00000
9:	2	2	1	3	2	0	2	3				13798.57100		13798.57224		-0.00124	0.00200	0.00000
10:	2	2	1	1	2	0	2	1				13799.31320		13799.30548		0.00772	0.00200	0.00000
11:	3	1	2	3	3	1	3	3				22656.35590		22656.35631		-0.00041	0.00200	0.00000
12:	3	1	2	4	3	1	3	4				22657.47700		22657.48098		-0.00398	0.00200	0.00000
13:	3	1	2	2	3	1	3	2				22657.87190		22657.87464		-0.00274	0.00200	0.00000
14:	2	1	2	1	1	1	1	1				22596.66720		22596.66580		0.00140	0.00200	0.00000
15:	2	1	2	3	1	1	1	2				22597.54540		22597.53674		0.00866	0.00200	0.00000
16:	2	1	2	1	1	1	1	0				22597.63920		22597.63760		0.00160	0.00200	0.00000
17:	2	1	2	2	1	1	1	1				22598.02280		22598.01604		0.00676	0.00200	0.00000
18:	2	1	2	2	1	1	1	2				22598.41110		22598.40476		0.00634	0.00200	0.00000
19:	2	0	2	1	1	0	1	1				22723.15450		22723.15819		-0.00369	0.00200	0.00000
20:	2	0	2	3	1	0	1	2				22724.05730		22724.06195		-0.00465	0.00200	0.00000
21:	2	0	2	1	1	0	1	0				22724.20300		22724.21172		-0.00872	0.00200	0.00000
22:	2	0	2	2	1	0	1	1				22724.50900		22724.50879		0.00021	0.00200	0.00000
23:	2	0	2	2	1	0	1	2				22724.92230		22724.93020		-0.00790	0.00200	0.00000

NORMALIZED DIAGONAL:

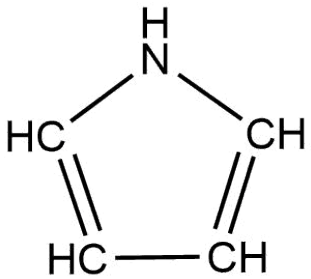
```
   1   1.00000E+00    2   9.20618E-01    3   1.87268E-01    4   9.76043E-01    5   2.83540E-01    6   1.00000E+00
   7   1.00000E+00    8   1.00000E+00    9   8.09521E-01   10   9.99577E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A       9130.64795(106)         -0.00000
  2         20000          B       9001.35664( 68)          0.00000
  3         30000          C       4532.11989( 72)         -0.00000
  4           200     -Del_J           -1.129( 93)E-03        0.000E-03
  5          1100    -Del_JK           -3.836(122)E-03        0.000E-03
  6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
  7         40100     -del_J     -0.010157300(  0)E-21 -0.000000000E-21
  8         41000     -del_K     -6.135949147(  0)E-24 -0.000000000E-24
  9     110010000     chi_aa          1.40475(181)         -0.00000
 10     110020000     chi_bb          1.29577(203)         -0.00000
 MICROWAVE AVG =        0.000207 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005315 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        2.65743         2.65743
```

Molecule 72

IUPAC Name: 1H-pyrrole (1v12)

Common name: pyrrole, azole (1v12)

SMILES: C1=CNC=C1



72: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0  0  1              13514.79540   13514.79530    0.00010    0.00200   0.00000
    2:   1  0  1  2  0  0  0  1              13515.43110   13515.43197   -0.00087    0.00200   0.00000
    3:   1  0  1  1  0  0  0  1              13515.84900   13515.85641   -0.00741    0.00200   0.00000
    4:   1  0  1  1  0  0  0  1              13515.86460   13515.85641    0.00819    0.00200   0.00000
    5:   2  0  2  1  1  0  1  1              22707.02010   22707.01997    0.00013    0.00200   0.00000
    6:   2  0  2  3  1  0  1  2              22707.92750   22707.92813   -0.00063    0.00200   0.00000
    7:   2  0  2  2  1  0  1  1              22708.37490   22708.37440    0.00050    0.00200   0.00000
    8:   3  0  3  4  2  0  2  3              31716.19700   31716.19464    0.00236    0.00200   0.00000
    9:   3  0  3  2  2  0  2  1              31716.28200   31716.28342   -0.00142    0.00200   0.00000
   10:   3  0  3  3  2  0  2  2              31716.45140   31716.45235   -0.00095    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.76566E-01    3   3.99782E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   8.42668E-01   10   9.97047E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       9108.48168(241)          0.00000
   2         20000          B       8981.40312(125)          0.00000
   3         30000          C       4534.10410( 49)         -0.00000
   4           200     -Del_J     -1.128615962(  0)E-03 -0.000000000E-03
   5          1100    -Del_JK     -3.890660879(  0)E-03  0.000000000E-03
   6          2000     -Del_K     -2.717900869(  0)E-24  0.000000000E-24
   7         40100     -del_J     -0.010157300(  0)E-21  0.000000000E-21
   8         41000     -del_K     -6.135949147(  0)E-24 -0.000000000E-24
   9     110010000     chi_aa          1.41486(303)         -0.00000
```

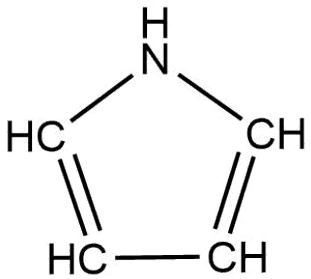
```
 10     110020000     chi_bb           1.2931( 62)           0.0000
MICROWAVE AVG =        0.000000 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.003632 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.81595         1.81595
```

Molecule 73

IUPAC Name: 1H-pyrrole (1v16)

Common name: pyrrole, azole (1v16)

SMILES: C1=CNC=C1



73: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  1  3  2  1  2  3              13370.54160   13370.53800    0.00360    0.00200   0.00000
    2:   1  0  1  0  0  0  0  1              13519.22630   13519.22963   -0.00333    0.00200   0.00000
    3:   1  0  1  2  0  0  0  1              13519.79460   13519.79490   -0.00030    0.00200   0.00000
    4:   1  0  1  1  0  0  0  1              13520.16670   13520.17174   -0.00504    0.00200   0.00000
    5:   1  0  1  1  0  0  0  1              13520.18040   13520.17174    0.00866    0.00200   0.00000
    6:   2  1  2  3  1  1  1  2              22582.81020   22582.80582    0.00438    0.00200   0.00000
    7:   2  1  2  1  1  1  1  0              22582.94750   22582.94628    0.00122    0.00200   0.00000
    8:   2  1  2  2  1  1  1  1              22583.23820   22583.23840   -0.00020    0.00200   0.00000
    9:   2  0  2  1  1  0  1  1              22701.52910   22701.52774    0.00136    0.00200   0.00000
   10:   2  0  2  3  1  0  1  2              22702.36820   22702.36853   -0.00033    0.00200   0.00000
   11:   2  0  2  2  1  0  1  1              22702.82580   22702.82682   -0.00102    0.00200   0.00000
   12:   2  1  1  3  1  1  0  2              31496.39450   31496.39452   -0.00002    0.00200   0.00000
   13:   2  1  1  2  1  1  0  1              31496.73720   31496.74258   -0.00538    0.00200   0.00000
   14:   3  0  3  4  2  0  2  3              31707.82620   31707.82407    0.00213    0.00200   0.00000
   15:   3  0  3  2  2  0  2  1              31707.90820   31707.90892   -0.00072    0.00200   0.00000
   16:   3  0  3  3  2  0  2  2              31708.07070   31708.07211   -0.00141    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.58874E-01    3   3.67492E-01    4   6.68439E-01    5   6.69652E-02    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   9.38132E-01   10   9.98190E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        9110.3669( 33)           0.0000
   2         20000          B        8988.30378( 44)         -0.00000
   3         30000          C        4531.55169( 48)         -0.00000
```

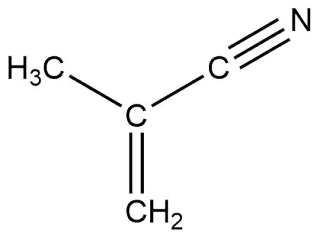
```
  4           200     -Del_J            0.558(117)E-03        0.000E-03
  5          1100    -Del_JK         -0.01309(121)         -0.00000
  6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
  7         40100     -del_J     -0.010157300(  0)E-21  0.000000000E-21
  8         41000     -del_K     -6.135949147(  0)E-24 -0.000000000E-24
  9     110010000     chi_aa          1.25617(238)          0.00000
 10     110020000     chi_bb           1.3439( 46)           0.0000
MICROWAVE AVG =        0.000225 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.003393 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.69662         1.69662
```

Molecule 74

IUPAC Name: 2-methyl-2-propenenitrile

Common name: methacrylonitrile, isopropene cyanide

SMILES: CC(=C)C#N

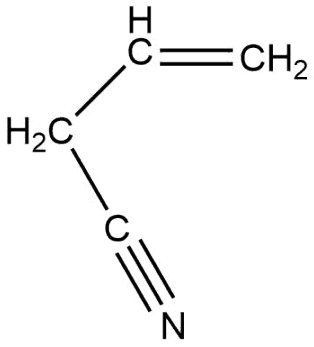


Molecule 75

IUPAC Name: 3-butenenitrile (cis)

Common name: allyl cyanide (cis)

SMILES: C=CCC#N



75: Fit file

	EXP.FREQ.		CALC.FREQ.			DIFF.			EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	2	1	2	2	1	1	1	1			12314.54660	12314.54692	-0.00032	0.00200	0.00096
2:	2	1	2	3	1	1	1	2			12315.10460	12315.10204	0.00256	0.00200	0.00076
3:	2	1	2	1	1	1	1	0			12315.31220	12315.31250	-0.00030	0.00200	0.00129
4:	2	0	2	2	1	0	1	2			13122.77360	13122.77433	-0.00073	0.00200	0.00085
5:	2	0	2	1	1	0	1	0			13122.92260	13122.92116	0.00144	0.00200	0.00079
6:	2	0	2	2	1	0	1	1			13123.29240	13123.28555	0.00685	0.05000	0.00050
7:	2	0	2	3	1	0	1	2			13123.36400	13123.36168	0.00232	0.00200	0.00051
8:	2	0	2	1	1	0	1	1			13124.19940	13124.19925	0.00015	0.00200	0.00117
9:	2	1	1	1	1	1	0	1			14075.89780	14075.89890	-0.00110	0.00200	0.00168
10:	2	1	1	2	1	1	0	1			14076.07080	14076.07173	-0.00093	0.00200	0.00089
11:	2	1	1	3	1	1	0	2			14076.57690	14076.57553	0.00137	0.00200	0.00067
12:	2	1	1	1	1	1	0	0			14077.43320	14077.43629	-0.00309	0.00200	0.00134
13:	3	1	3	3	2	1	2	2			18428.73000	18428.73127	-0.00127	0.00200	0.00073
14:	3	1	3	2	2	1	2	1			18428.83370	18428.83687	-0.00317	0.00200	0.00070
15:	3	1	3	4	2	1	2	3			18428.91210	18428.90982	0.00228	0.00200	0.00072
16:	3	0	3	2	2	0	2	1			19507.08580	19507.09113	-0.00533	0.00200	0.00062
17:	3	0	3	3	2	0	2	2			19507.10440	19507.10166	0.00274	0.00200	0.00059
18:	3	0	3	4	2	0	2	3			19507.18470	19507.18330	0.00140	0.00200	0.00060
19:	3	1	2	3	2	1	1	2			21067.16580	21067.16566	0.00014	0.00200	0.00097
20:	3	1	2	4	2	1	1	3			21067.31820	21067.31726	0.00094	0.00200	0.00096
21:	3	1	2	2	2	1	1	1			21067.39380	21067.39313	0.00067	0.00200	0.00098
22:	4	1	4	4	3	1	3	3			24495.38330	24495.38129	0.00201	0.00200	0.00109
23:	4	1	4	3	3	1	3	2			24495.41970	24495.42260	-0.00290	0.00200	0.00109

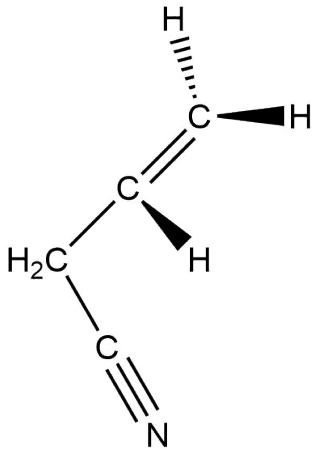
```
   24:   4  1  4  5  3  1  3  4              24495.47700   24495.47601    0.00099    0.00200   0.00109
   25:   4  0  4  4  3  0  3  3              25695.00430   25695.00428    0.00002    0.00200   0.00109
   26:   4  0  4  3  3  0  3  2              25695.05680   25695.05642    0.00038    0.00200   0.00107
   27:   4  0  4  5  3  0  3  4              25695.09490   25695.09518   -0.00028    0.00200   0.00107
   28:   4  2  3  4  3  2  2  3              26334.80620   26334.80865   -0.00245    0.00200   0.00117
   29:   4  2  3  5  3  2  2  4              26335.05180   26335.05085    0.00095    0.00200   0.00114
   30:   4  2  3  3  3  2  2  2              26335.11490   26335.11312    0.00178    0.00200   0.00115
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   5.69318E-01    3   3.15890E-01    4   1.77514E-01    5   9.80179E-01    6   1.00000E+00
    7   8.65720E-01    8   1.00000E+00    9   9.37741E-01   10   9.99998E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       11322.9760(311)           0.0000
   2         20000          B       3739.33690( 33)          -0.00000
   3         30000          C       2858.54169( 34)          -0.00000
   4           200     -Del_J          -2.9854(134)E-03       0.0000E-03
   5          1100    -Del_JK         0.018419( 92)         -0.000000
   6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
   7         40100     -del_J          -1.0247( 60)E-03       0.0000E-03
   8         41000     -del_K     -6.135949147(  0)E-24 -0.000000000E-24
   9     110010000     chi_aa          -1.70411(219)          -0.00000
  10     110020000     chi_bb           -0.3458( 35)           0.0000
 MICROWAVE AVG =        0.000238 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002272 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        0.95094         0.95094
```

Molecule 76

IUPAC Name: 3-butenenitrile (gauche)

Common name: allyl cyanide (gauche)

SMILES: C=CCC#N



76: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2	1	2	2	1	1	1	1			10111.95180		10111.95430		-0.00250	0.00200	0.00000
2:	2	1	2	3	1	1	1	2			10112.83190		10112.83039		0.00151	0.00200	0.00000
3:	2	1	2	1	1	1	1	0			10113.51310		10113.51366		-0.00056	0.00200	0.00000
4:	2	0	2	2	1	0	1	2			10233.15820		10233.15838		-0.00018	0.00200	0.00000
5:	2	0	2	1	1	0	1	0			10233.29750		10233.29945		-0.00195	0.00200	0.00000
6:	2	0	2	2	1	0	1	1			10233.98940		10233.98999		-0.00059	0.00200	0.00000
7:	2	0	2	3	1	0	1	2			10234.05200		10234.05097		0.00103	0.00200	0.00000
8:	2	0	2	1	1	0	1	1			10235.37890		10235.37858		0.00032	0.00200	0.00000
9:	2	1	1	3	1	1	0	2			10357.44540		10357.44435		0.00105	0.00200	0.00000
10:	3	1	3	2	2	1	2	1			15168.50000		15168.49816		0.00184	0.00200	0.00000
11:	3	1	3	4	2	1	2	3			15168.54660		15168.54586		0.00074	0.00200	0.00000
12:	3	0	3	2	2	0	2	1			15349.10440		15349.10210		0.00230	0.00200	0.00000
13:	3	0	3	3	2	0	2	2			15349.23750		15349.23767		-0.00017	0.00200	0.00000
14:	3	0	3	4	2	0	2	3			15349.27430		15349.27318		0.00112	0.00200	0.00000
15:	3	1	2	3	2	1	1	2			15535.22600		15535.22886		-0.00286	0.00200	0.00000
16:	3	1	2	4	2	1	1	3			15535.46800		15535.46865		-0.00065	0.00200	0.00000
17:	3	1	2	2	2	1	1	1			15535.50540		15535.50668		-0.00128	0.00200	0.00000
18:	4	1	4	4	3	1	3	3			20223.60290		20223.60353		-0.00063	0.00200	0.00000
19:	4	1	4	3	3	1	3	2			20223.66350		20223.66387		-0.00037	0.00200	0.00000
20:	4	1	4	5	3	1	3	4			20223.72010		20223.71983		0.00027	0.00200	0.00000

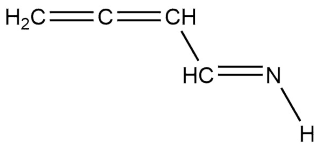
```
  21:   4  1  3  4  3  1  2  3              20712.80250   20712.80085    0.00165    0.00200   0.00000
  22:   4  1  3  3  3  1  2  2              20712.88960   20712.89090   -0.00130    0.00200   0.00000
  23:   4  1  3  5  3  1  2  4              20712.90860   20712.90668    0.00192    0.00200   0.00000
  24:   4  0  4  3  3  0  3  2              20462.33470   20462.33480   -0.00010    0.00200   0.00000
  25:   4  0  4  4  3  0  3  3              20462.39030   20462.39029    0.00001    0.00200   0.00000
  26:   4  0  4  5  3  0  3  4              20462.41500   20462.41472    0.00028    0.00200   0.00000
  27:   5  0  5  4  4  0  4  3              25572.72650   25572.72530    0.00120    0.00200   0.00000
  28:   5  0  5  5  4  0  4  4              25572.75040   25572.75349   -0.00309    0.00200   0.00000
  29:   5  0  5  6  4  0  4  5              25572.77470   25572.77237    0.00233    0.00200   0.00000
  30:   6  0  6  5  5  0  5  4              30679.62010   30679.62331   -0.00321    0.00200   0.00000
  31:   6  0  6  6  5  0  5  5              30679.63820   30679.63859   -0.00039    0.00200   0.00000
  32:   6  0  6  7  5  0  5  6              30679.65720   30679.65451    0.00269    0.00200   0.00000
  33:   2  1  2  1  1  0  1  0              27198.52320   27198.52306    0.00014    0.00200   0.00000
  34:   2  1  2  2  1  0  1  2              27198.72970   27198.73104   -0.00134    0.00200   0.00000
  35:   2  1  2  3  1  0  1  2              27199.39990   27199.39924    0.00066    0.00200   0.00000
  36:   2  1  2  2  1  0  1  1              27199.56070   27199.56265   -0.00195    0.00200   0.00000
  37:   2  1  2  1  1  0  1  1              27200.60000   27200.60219   -0.00219    0.00200   0.00000
  38:   1  1  1  0  0  0  0  1              22203.74070   22203.74071   -0.00001    0.00200   0.00000
  39:   1  1  1  2  0  0  0  1              22204.05310   22204.05264    0.00046    0.00200   0.00000
  40:   1  1  1  1  0  0  0  1              22204.26030   22204.26054   -0.00024    0.00200   0.00000
  41:   3  1  3  2  2  0  2  1              32133.72280   32133.72177    0.00103    0.00200   0.00000
  42:   3  1  3  3  2  0  2  2              32133.86200   32133.86226   -0.00026    0.00200   0.00000
  43:   3  1  3  4  2  0  2  3              32133.89540   32133.89413    0.00127    0.00200   0.00000
  44:   1  1  0  1  1  0  1  0              17208.20250   17208.20232    0.00018    0.00200   0.00000
  45:   1  1  0  2  1  0  1  2              17208.82860   17208.82620    0.00240    0.00200   0.00000
  46:   1  1  0  1  1  0  1  2              17209.44860   17209.44983   -0.00123    0.00200   0.00000
  47:   1  1  0  2  1  0  1  1              17209.65980   17209.65781    0.00199    0.00200   0.00000
  48:   1  1  0  1  1  0  1  1              17210.28020   17210.28144   -0.00124    0.00200   0.00000
  49:   2  1  1  3  2  0  2  3              17332.21990   17332.21958    0.00032    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99988E-01    3   2.84780E-01    4   4.01658E-01    5   6.74480E-01    6   1.00000E+00
    7   9.70140E-01    8   1.00000E+00    9   9.96197E-01   10   9.53119E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A      19706.42004( 69)         -0.00000
   2         20000          B       2619.84042( 32)         -0.00000
   3         30000          C      2497.512191(276)         0.000000
   4           200     -Del_J         -1.86221(264)E-03      0.00000E-03
   5          1100    -Del_JK         0.080855(103)        -0.000000
   6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
   7         40100     -del_J          -0.2001( 60)E-03       0.0000E-03
   8         41000     -del_K     -6.135949147(  0)E-24  0.000000000E-24
   9     110010000     chi_aa          -2.77216(175)          0.00000
  10     110020000     chi_bb           0.69329(219)         -0.00000
 MICROWAVE AVG =        0.000009 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001469 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.73446         0.73446
```

Molecule 77

IUPAC Name: 2,3-butadien-1-imine (anti)

Common name: 2,3-butadien-1-imine (anti)

SMILES: C=C=CC=N



77: Fit file

	EXP.FREQ.			CALC.FREQ.				DIFF.	EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	2	1	2	2	1	1	1	1			9103.71330	9103.66757	0.04573	9.06850	0.00000
2:	2	1	2	3	1	1	1	2			9104.39860	9104.39963	-0.00103	0.00200	0.00000
3:	2	0	2	2	1	0	1	2			9220.98250	9220.98175	0.00075	0.00200	0.00000
4:	2	0	2	1	1	0	1	0			9221.09600	9221.09688	-0.00088	0.00200	0.00000
5:	2	0	2	3	1	0	1	2			9221.70540	9221.70396	0.00144	0.00200	0.00000
6:	2	0	2	1	1	0	1	1			9222.78010	9222.77746	0.00264	0.00200	0.00000
7:	2	1	1	2	1	1	0	1			9339.42620	9339.42011	0.00609	0.00200	0.00000
8:	2	1	1	3	1	1	0	2			9340.07710	9340.08039	-0.00329	0.00200	0.00000
9:	3	1	3	3	2	1	2	2			13655.97520	13655.97749	-0.00229	0.00200	0.00000
10:	3	1	3	4	2	1	2	3			13656.19990	13656.19813	0.00177	0.00200	0.00000
11:	3	0	3	3	2	0	2	3			13830.92300	13830.92335	-0.00035	0.00200	0.00000
12:	3	0	3	2	2	0	2	1			13831.53750	13831.53734	0.00016	0.00200	0.00000
13:	3	0	3	3	2	0	2	2			13831.64490	13831.64555	-0.00065	0.00200	0.00000
14:	3	0	3	4	2	0	2	3			13831.67510	13831.67538	-0.00028	0.00200	0.00000
15:	3	0	3	2	2	0	2	2			13832.66170	13832.66085	0.00085	0.00200	0.00000
16:	3	1	2	3	2	1	1	2			14009.60340	14009.60099	0.00241	0.00200	0.00000
17:	3	1	2	4	2	1	1	3			14009.78060	14009.78176	-0.00116	0.00200	0.00000
18:	4	1	4	4	3	1	3	3			18207.68740	18207.68423	0.00317	0.00200	0.00000
19:	4	1	4	5	3	1	3	4			18207.78590	18207.78705	-0.00115	0.00200	0.00000
20:	4	0	4	3	3	0	3	2			18440.59270	18440.59182	0.00088	0.00200	0.00000
21:	4	0	4	4	3	0	3	3			18440.63430	18440.63490	-0.00060	0.00200	0.00000
22:	4	0	4	5	3	0	3	4			18440.65560	18440.65619	-0.00059	0.00200	0.00000
23:	4	1	3	4	3	1	2	3			18679.16970	18679.17066	-0.00096	0.00200	0.00000
24:	4	1	3	5	3	1	2	4			18679.24680	18679.24811	-0.00131	0.00200	0.00000
25:	4	1	3	3	3	1	2	2			18679.26500	18679.26779	-0.00279	0.00200	0.00000
26:	5	1	5	5	4	1	4	4			22758.97980	22758.97986	-0.00006	0.00200	0.00000
27:	5	1	5	6	4	1	4	5			22759.03790	22759.03874	-0.00084	0.00200	0.00000
28:	5	0	5	4	4	0	4	3			23048.26750	23048.26778	-0.00028	0.00200	0.00000
29:	5	0	5	5	4	0	4	4			23048.28620	23048.28839	-0.00219	0.00200	0.00000

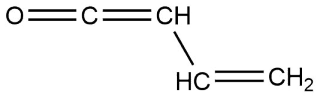
```
   30:   5  0  5  6  4  0  4  5              23048.30580   23048.30560    0.00020    0.00200   0.00000
   31:   5  1  4  5  4  1  3  4              23348.31440   23348.31590   -0.00150    0.00200   0.00000
   32:   5  1  4  6  4  1  3  5              23348.36090   23348.35722    0.00368    0.00200   0.00000
   33:   6  0  6  5  5  0  5  4              27654.26070   27654.26335   -0.00265    0.00200   0.00000
   34:   6  0  6  6  5  0  5  5              27654.27640   27654.27312    0.00328    0.00200   0.00000
   35:   6  0  6  7  5  0  5  6              27654.28760   27654.28836   -0.00076    0.00200   0.00000
   36:   7  0  7  6  6  0  6  5              32258.25510   32258.25408    0.00102    0.00500   0.00000   32258.25578   -0.00068
   37:   7  0  7  7  6  0  6  6              32258.25510   32258.25748   -0.00238    0.00500   0.00000   32258.25578   -0.00068
   38:   7  0  7  8  6  0  6  7              32258.27810   32258.27183    0.00627    0.00500   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.84479E-01    3   3.40185E-01    4   1.31546E-01    5   1.00000E+00    6   9.90683E-01
    7   9.97434E-01    8   1.00000E+00    9   9.99997E-01   10   9.75592E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A          34376.5(174)              0.0
   2         20000          B       2364.43698( 45)          -0.00000
   3         30000          C       2246.55939( 44)           0.00000
   4           200    Delta_J          -0.3848( 66)E-03       -0.0000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK         0.030881(236)          0.000000
   7         40100     -del_J          -0.0401( 53)E-03        0.0000E-03
   8         41000     -del_K     -0.012129138(  0)E-21  0.000000000E-21
   9     110010000     chi_aa         -2.24078(226)           0.00000
  10     110020000     chi_bb           -0.556( 52)             0.000
 MICROWAVE AVG =        0.001433 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.007833 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.99172         0.99172
```

Molecule 78

IUPAC Name: 1,3-butadien-1-one (anti)

Common name: vinylketene (anti)

SMILES: C=CC=C=O



78: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                     9161.06610    9161.06880   -0.00270    0.00200   0.00000
    2:   2  0  2  1  0  1                     9297.47450    9297.47516   -0.00066    0.00200   0.00000
    3:   2  1  1  1  1  0                     9434.91690    9434.91262    0.00428    0.00200   0.00000
    4:   3  1  3  2  1  2                    13741.34160   13741.34409   -0.00249    0.00200   0.00000
    5:   3  0  3  2  0  2                    13945.24360   13945.24378   -0.00018    0.00200   0.00000
    6:   3  1  2  2  1  1                    14152.11150   14152.10814    0.00336    0.00200   0.00000
    7:   4  1  4  3  1  3                    18321.31120   18321.31076    0.00044    0.00200   0.00000
    8:   4  0  4  3  0  3                    18591.84980   18591.84980   -0.00000    0.00200   0.00000
    9:   4  1  3  3  1  2                    18868.98930   18868.98837    0.00093    0.00200   0.00000
   10:   5  1  5  4  1  4                    22900.87210   22900.86984    0.00226    0.00200   0.00000
   11:   5  0  5  4  0  4                    23236.90570   23236.90622   -0.00052    0.00200   0.00000
   12:   5  1  4  4  1  3                    23585.44150   23585.44432   -0.00282    0.00200   0.00000
   13:   6  1  6  5  1  5                    27479.92560   27479.92563   -0.00003    0.00200   0.00000
   14:   6  0  6  5  0  5                    27880.02770   27880.02693    0.00077    0.00200   0.00000
   15:   6  1  5  5  1  4                    28301.35900   28301.36359   -0.00459    0.00200   0.00000
   16:   7  0  7  6  0  6                    32520.82830   32520.82752    0.00078    0.00200   0.00000
   17:   7  1  6  6  1  5                    33016.63230   33016.62955    0.00275    0.00200   0.00000
   18:   8  0  8  7  0  7                    37158.92580   37158.92650   -0.00070    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.17017E-01    3   3.41804E-01    4   1.38003E-01    5   1.00000E+00    6   9.10322E-01
    7   1.00000E+00    8   9.99816E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    39506.2(120)             -0.0
   2         20000                 2392.927431(291)         0.000000
   3         30000                 2256.005524(284)        -0.000000
   4           200                     -0.3934( 43)E-03       0.0000E-03
   5          2000                -1.944804792(  0)E-27 -0.000000000E-27
   6          1100                    0.034347(260)        -0.000000
   7         40100                -2.651610039(  0)E-24 -0.000000000E-24
```

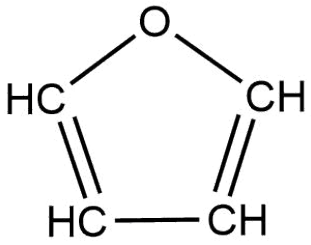
```
  8         50000                       3.068(167)E-03        0.000E-03
MICROWAVE AVG =        0.000049 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002215 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.10738         1.10738
```

Molecule 79

IUPAC Name: 1,4-epoxybuta-1,3-diene

Common name: furan, oxole

SMILES: C1=COC=C1



79: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	7 6 1	7 6 2								11319.10210		11319.10063		0.00147		0.00200		0.00000
2:	6 5 1	6 5 2								11977.70630		11977.70766		-0.00136		0.00200		0.00000
3:	5 4 1	5 4 2								12552.71580		12552.71599		-0.00019		0.00200		0.00000
4:	4 3 1	4 3 2								13038.53430		13038.53442		-0.00012		0.00200		0.00000
5:	3 2 1	3 2 2								13431.13330		13431.13353		-0.00023		0.00200		0.00000
6:	2 1 1	2 1 2								13727.69740		13727.69752		-0.00012		0.00200		0.00000
7:	1 0 1	0 0 0								13917.56640		13917.56350		0.00290		0.00200		0.00000
8:	2 2 1	2 0 2								14335.26590		14335.26748		-0.00158		0.00200		0.00000
9:	3 3 1	3 1 2								14665.40500		14665.39944		0.00556		0.00200		0.00000
10:	4 4 1	4 2 2								15137.46920		15137.47271		-0.00351		0.00200		0.00000
11:	5 5 1	5 3 2								15777.52550		15777.51928		0.00622		0.00200		0.00000
12:	6 6 1	6 4 2								16615.66000		16615.66212		-0.00212		0.00200		0.00000
13:	14 12 2	14 12 3								17681.02860		17681.02913		-0.00053		0.00200		0.00000
14:	7 7 1	7 5 2								17683.61470		17683.61525		-0.00055		0.00200		0.00000
15:	13 11 2	13 11 3								18778.01960		18778.01922		0.00038		0.00200		0.00000
16:	8 8 1	8 6 2								19011.46490		19011.46837		-0.00347		0.00200		0.00000
17:	12 10 2	12 10 3								19767.91750		19767.91697		0.00053		0.00200		0.00000
18:	9 9 1	9 7 2								20624.38920		20624.38695		0.00225		0.00200		0.00000
19:	6 4 2	6 4 3								23055.93080		23055.93272		-0.00192		0.00200		0.00000
20:	5 3 2	5 3 3								23213.61680		23213.61740		-0.00060		0.00200		0.00000
21:	2 1 2	1 1 1								23259.19230		23259.19220		0.00010		0.00200		0.00000
22:	4 2 2	4 2 3								23305.52230		23305.52271		-0.00041		0.00200		0.00000
23:	3 1 2	3 1 3								23352.19480		23352.19485		-0.00005		0.00200		0.00000
24:	3 2 2	3 0 3								23384.45770		23384.45772		-0.00002		0.00200		0.00000
25:	4 3 2	4 1 3								23402.51620		23402.51575		0.00045		0.00200		0.00000

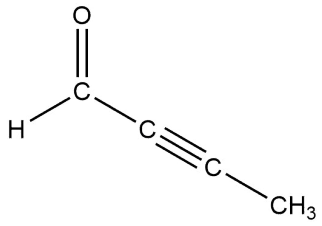
```
   26:   2  0  2  1  0  1                    23453.13590   23453.13553    0.00037    0.00500   0.00000
   27:   6  5  2  6  3  3                    23507.72380   23507.72337    0.00043    0.00200   0.00000
   28:   7  6  2  7  4  3                    23619.07070   23619.07032    0.00038    0.00200   0.00000
   29:   2  1  1  1  1  0                    32410.97690   32410.97938   -0.00248    0.00200   0.00000
   30:   3  1  3  2  1  2                    32697.03130   32697.03095    0.00035    0.00200   0.00000
   31:   3  0  3  2  0  2                    32703.33760   32703.33737    0.00023    0.00200   0.00000
   32:   4  1  3  4  1  4                    32720.06720   32720.06644    0.00076    0.00200   0.00000
   33:   4  2  3  4  0  4                    32720.97210   32720.97232   -0.00022    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.46121E-01    3   9.86643E-01    4   4.14913E-01    5   6.03626E-01    6   3.35422E-01
    7   1.23068E-01    8   1.87901E-01    9   1.00000E+00   10   1.00000E+00   11   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1          1000  C-(A+B)/2     -4676.108049(280)         0.000000
   2           100    (A+B)/2       9346.93308( 58)         -0.00000
   3         40000    (B-A)/4      -50.0948350(205)        0.0000000
   4          2000        -DK          -2.2826(141)E-03      -0.0000E-03
   5          1100       -DJK           5.2630( 54)E-03       0.0000E-03
   6           200        -DJ           -3.344( 37)E-03        0.000E-03
   7         40100         d1          0.05087( 32)E-03     -0.00000E-03
   8         50000         d2         0.043423(281)E-03     0.000000E-03
   9          2100        HKJ      0.946021710( 10)E-27  0.000000000E-27
  10          1200        HJK     -2.470199128( 10)E-27 -0.000000000E-27
  11         40200         h1     -0.076536185( 10)E-27 -0.000000000E-27
 MICROWAVE AVG =        0.000088 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001995 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.99700         0.99700
```

Molecule 80

IUPAC Name: 2-butynal

Common name: 2-butynal

SMILES: CC#CC=O



80: Fit file

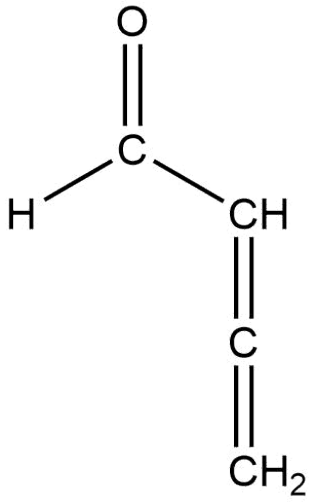
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      8304.68730    8304.68924   -0.00194    0.00200   0.00000
    2:   3  0  3  2  0  2                     12456.82690   12456.82863   -0.00173    0.00200   0.00000
    3:   4  0  4  3  0  3                     16608.72290   16608.72175    0.00115    0.00200   0.00000
    4:   5  0  5  4  0  4                     20760.28810   20760.28652    0.00158    0.00200   0.00000
    5:   6  0  6  5  0  5                     24911.44110   24911.44090    0.00020    0.00200   0.00000
    6:   7  0  7  6  0  6                     29062.10260   29062.10290   -0.00030    0.00200   0.00000
    7:   8  0  8  7  0  7                     33212.19020   33212.19062   -0.00042    0.00200   0.00000
    8:   9  0  9  8  0  8                     37361.62240   37361.62231    0.00009    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.88320E-02    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A  43000.000000447(  0)      0.000000000
   2         20000          B        2109.6569( 64)          -0.0000
   3         30000          C        2042.7288( 62)           0.0000
   4           200    Delta_J     -5.630753973(  0)E-24  0.000000000E-24
   5          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
   6          1100   Delta_JK      0.041377332(  0)E-21  0.000000000E-21
   7         40100     -del_J     -1.158454703(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
 MICROWAVE AVG =       -0.000170 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001166 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.58317         0.58317
```

Molecule 81

IUPAC Name: 2,3-butadienal (anti)

Common name: 2,3-butadienal (anti)

SMILES: C=C=CC=O



81: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                     9268.39080    9268.39245   -0.00165    0.00200   0.00000
    2:   2  0  2  1  0  1                     9388.06950    9388.06939    0.00011    0.00200   0.00000
    3:   2  1  1  1  1  0                     9508.75150    9508.74459    0.00691    0.00200   0.00000
    4:   3  1  3  2  1  2                    13902.35410   13902.35540   -0.00130    0.00200   0.00000
    5:   3  0  3  2  0  2                    14081.24470   14081.24422    0.00048    0.00200   0.00000
    6:   3  1  2  2  1  1                    14262.88100   14262.88303   -0.00203    0.00200   0.00000
    7:   4  1  4  3  1  3                    18536.03950   18536.03923    0.00027    0.00200   0.00000
    8:   4  0  4  3  0  3                    18773.38800   18773.38737    0.00063    0.00200   0.00000
    9:   4  1  3  3  1  2                    19016.73810   19016.74003   -0.00193    0.00200   0.00000
   10:   5  1  5  4  1  4                    23169.35350   23169.35227    0.00123    0.00200   0.00000
   11:   5  0  5  4  0  4                    23464.15580   23464.15531    0.00049    0.00200   0.00000
   12:   6  0  6  5  0  5                    28153.20250   28153.20519   -0.00269    0.00200   0.00000
   13:   7  0  7  6  0  6                    32840.19670   32840.19534    0.00136    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.49569E-01    3   3.76397E-01    4   9.51040E-02    5   1.00000E+00    6   9.97715E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
```

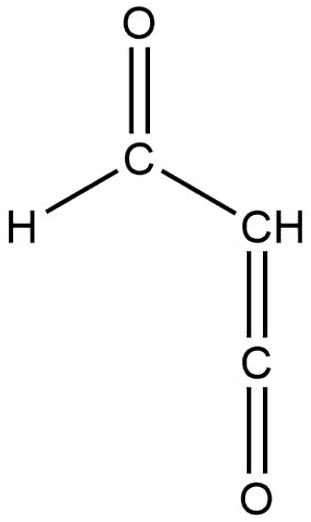
```
  1         10000                    34773.7(281)             -0.0
  2         20000                  2407.19220( 32)          0.00000
  3         30000                  2287.01613( 34)         -0.00000
  4           200                     -0.4133(115)E-03       0.0000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                     0.04128( 36)          0.00000
  7         40100                -2.651610039(  0)E-24 -0.000000000E-24
  8         50000                -0.212827842(  0)E-21  0.000000000E-21
MICROWAVE AVG =        0.000143 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002346 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.17277         1.17277
```

Molecule 82

IUPAC Name: 3-oxoprop-2-enal (anti)

Common name: formylketene (anti)

SMILES: O=CC=C=O



82: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 0 2 1 0 1						9667.72020	9667.72191		-0.00171		0.00200	0.00000
2:	3 0 3 2 0 2						14500.60150	14500.60193		-0.00043		0.00200	0.00000
3:	4 0 4 3 0 3						19332.30500	19332.30512		-0.00012		0.00200	0.00000
4:	5 0 5 4 0 4						24162.44040	24162.43988		0.00052		0.00200	0.00000
5:	6 0 6 5 0 5						28990.61590	28990.61551		0.00039		0.00200	0.00000
6:	7 0 7 6 0 6						33816.44410	33816.44284		0.00126		0.00200	0.00000
7:	8 0 8 7 0 7						38639.53410	38639.53518		-0.00108		0.00200	0.00000
8:	2 1 2 1 1 1						9527.35870	9527.35861		0.00009		0.00200	0.00000
9:	2 1 1 1 1 0						9809.30560	9809.30633		-0.00073		0.00200	0.00000
10:	3 1 3 2 1 2						14290.77250	14290.77257		-0.00007		0.00200	0.00000
11:	3 1 2 2 1 1						14713.68450	14713.68389		0.00061		0.00200	0.00000
12:	4 1 4 3 1 3						19053.86860	19053.86907		-0.00047		0.00200	0.00000
13:	4 1 3 3 1 2						19617.73000	19617.72987		0.00013		0.00200	0.00000
14:	5 1 5 4 1 4						23816.54440	23816.54384		0.00056		0.00200	0.00000
15:	5 1 4 4 1 3						24521.33220	24521.33233		-0.00013		0.00200	0.00000
16:	6 1 6 5 1 5						28578.69380	28578.69395		-0.00015		0.00200	0.00000
17:	6 1 5 5 1 4						29424.37810	29424.37814		-0.00004		0.00200	0.00000

NORMALIZED DIAGONAL:

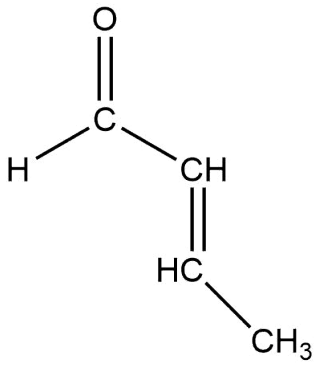
```
   1   1.00000E+00    2   2.25175E-01    3   3.02494E-01    4   1.35787E-01    5   9.93766E-01    6   1.00000E+00
   7   9.91409E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A          41749.4(136)              0.0
  2         20000          B       2487.51792( 44)          0.00000
  3         30000          C       2346.54148( 42)         -0.00000
  4           200    Delta_J          -0.5606( 48)E-03       0.0000E-03
  5          1100   Delta_JK         0.057901(267)        -0.000000
  6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
  7         40100     -del_J          -0.0803( 36)E-03      -0.0000E-03
  8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000080 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000678 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.33918         0.33918
```

Molecule 83

IUPAC Name: (E)-2-butenal (anti)

Common name: crotonaldehyde (anti-trans)

SMILES: CC=CC=O



83_Astate: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      8513.01650    8513.01662   -0.00012    0.00200   0.00000
    2:   3  1  3  2  1  2                     12604.68700   12604.68845   -0.00145    0.00200   0.00000
    3:   3  0  3  2  0  2                     12768.77020   12768.76931    0.00089    0.00200   0.00000
    4:   3  1  2  2  1  1                     12934.88850   12934.88913   -0.00063    0.00200   0.00000
    5:   4  1  4  3  1  3                     16805.88570   16805.88430    0.00140    0.00200   0.00000
    6:   4  0  4  3  0  3                     17023.61580   17023.61534    0.00046    0.00200   0.00000
    7:   4  1  3  3  1  2                     17246.14790   17246.14951   -0.00161    0.00200   0.00000
    8:   5  1  5  4  1  4                     21006.76750   21006.76710    0.00040    0.00200   0.00000
    9:   5  0  5  4  0  4                     21277.25320   21277.25278    0.00042    0.00200   0.00000
   10:   5  1  4  4  1  3                     21557.09090   21557.09182   -0.00092    0.00200   0.00000
   11:   6  0  6  5  0  5                     25529.38020   25529.38020    0.00000    0.00200   0.00000
   12:   2  1  2  3  0  3                     17574.93780   17574.93891   -0.00111    0.00200   0.00000
   13:   1  1  0  1  0  1                     30563.53410   30563.53495   -0.00085    0.00200   0.00000
   14:   2  1  1  2  0  2                     30673.90740   30673.90940   -0.00200    0.00200   0.00000
   15:   3  1  2  3  0  3                     30840.03300   30840.02922    0.00378    0.00200   0.00000
   16:   4  1  3  4  0  4                     31062.56450   31062.56339    0.00111    0.00200   0.00000
   17:   5  1  4  5  0  5                     31342.40150   31342.40243   -0.00093    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.33018E-01    3   4.87114E-01    4   9.99446E-01    5   1.00000E+00    6   6.48652E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
```

```
  1         10000                 32636.82673(141)          0.00000
  2         20000                 2183.363617(260)         0.000000
  3         30000                 2073.296558(234)         0.000000
  4           200                     -0.1847( 40)E-03       0.0000E-03
  5          2000                -7.148762971(  0)E-27 -0.000000000E-27
  6          1100                       2.392( 98)E-03       -0.000E-03
  7         40100                -0.047468413(  0)E-24 -0.000000000E-24
  8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =       -0.000069 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001364 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.68206         0.68206
```

83_Estate: Line file

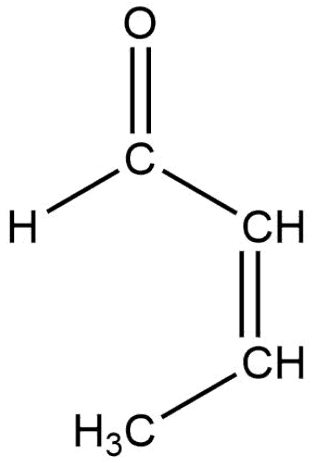
```
(E)-but-2-enal (anti), E state
  2  0  2  1  0  1                      8512.9889     0.002   \1-2219654
  3  0  3  2  0  2                     12768.7432     0.002   \1-2219652
  4  1  4  3  1  3                     16806.2929     0.002   \1-2437847
  4  0  4  3  0  3                     17023.5804     0.002   \1-2219653
  4  1  3  3  1  2                     17245.6870     0.002   \1-2437849
  5  1  5  4  1  4                     21006.9680     0.002   \1-2437844
  5  0  5  4  0  4                     21277.2181     0.002   \1-2219664
  5  1  4  4  1  3                     21556.8266     0.002   \1-2437846
  6  0  6  5  0  5                     25529.3389     0.002   \1-2219665
```

Molecule 84

IUPAC Name: (Z)-2-butenal (anti)

Common name: crotonaldehyde (anti-cis)

SMILES: CC=CC=O



84_Estate: Line file

```
(Z)-but-2-enal (anti), E state
  2  1  2  1  1  1                      9813.6785     0.002  \1-2170724
  2  1  2  1  1  1                      9813.6785     0.002  \1-2170724
  3  1  3  2  1  2                     14716.2337     0.002  \1-2170790
  4  1  4  3  1  3                     19613.4612     0.002  \1-2170848
  2  1  1  1  1  0                     10520.8232     0.002  \1-2170915
  3  1  2  2  1  1                     15779.3501     0.002  \1-2170813
  4  1  3  3  1  2                     21031.3211     0.002  \1-2170882
  2  0  2  1  0  1                     10161.2188     0.002  \1-2170507
  3  0  3  2  0  2                     15224.6494     0.002  \1-2170548
  4  0  4  3  0  3                     20267.5672     0.002  \1-2170600
  5  0  5  4  0  4                     25283.4572     0.002  \1-2170620
  6  0  6  5  0  5                     30266.3705     0.002  \1-2170901
  7  0  7  6  0  6                     35211.3816     0.002  \1-2170904
```

84_Astate: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                    14716.34690   14716.34628    0.00062    0.00200   0.00000
```

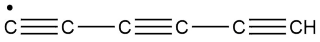
```
    2:   4  1  4  3  1  3                    19613.76880   19613.76928   -0.00048    0.00200   0.00000
    3:   2  1  1  1  1  0                    10523.54520   10523.54554   -0.00034    0.00200   0.00000
    4:   3  1  2  2  1  1                    15780.93890   15780.93907   -0.00017    0.00200   0.00000
    5:   4  1  3  3  1  2                    21032.96000   21032.95972    0.00028    0.00200   0.00000
    6:   2  0  2  1  0  1                    10161.72170   10161.71653    0.00517    0.00200   0.00000
    7:   3  0  3  2  0  2                    15225.38250   15225.38263   -0.00013    0.00200   0.00000
    8:   4  0  4  3  0  3                    20268.50570   20268.51156   -0.00586    0.00200   0.00000
    9:   5  0  5  4  0  4                    25284.56800   25284.56527    0.00273    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.80613E-01    3   1.88678E-01    4   1.16630E-01    5   1.00000E+00    6   9.89505E-01
    7   9.58261E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         16334.04(137)             0.00
   2         20000          B       2719.57962(107)          0.00000
   3         30000          C       2364.72601( 99)         -0.00000
   4           200    Delta_J          -1.4883(247)E-03      -0.0000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK          0.02783( 64)          0.00000
   7         40100     -del_J           0.5303(178)E-03      -0.0000E-03
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =        0.000202 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002777 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.38846         1.38846
```

Molecule 85

IUPAC Name: 1,3,5-hexatriynyl radical

Common name: hexatriynyl radical

SMILES: [C]#CC#CC#C

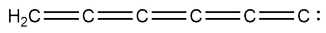


Molecule 86

IUPAC Name: hexapentaenylidene

Common name: hexapentaenylidene

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



Molecule 87

IUPAC Name: isocyanobuta-1,3-diyne

Common name: isocyanodiacetylene

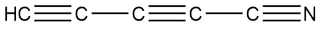
SMILES: C#CC#C[N+]#[C-]

Molecule 88

IUPAC Name: 2,4-pentadiynenitrile

Common name: cyanobutadiyne, cyanodiacetylene

SMILES: C#CC#CC#N

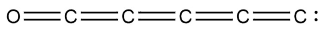


Molecule 89

IUPAC Name: 5-oxo-1,2,3,4-pentatetraenylidene

Common name: pentacarbonmonoxide

SMILES: [C]=C=C=C=C=O

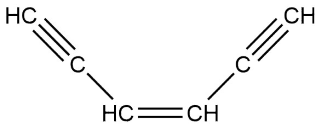


Molecule 90

IUPAC Name: (Z)-3-hexene-1,5-diyne

Common name: 3-hexene-1,5-diyne (cis)

SMILES: C#CC=CC#C

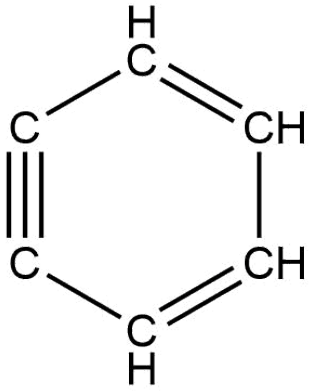


Molecule 91

IUPAC Name: ortho-benzyne, o-benzyne

Common name: ortho-benzyne, o-benzyne

SMILES: C1=CC#CC=C1

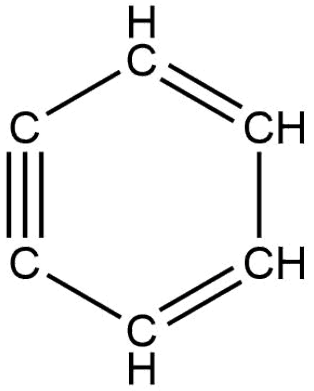


Molecule 92

IUPAC Name: ortho-benzyne, o-benzyne (1v15)

Common name: ortho-benzyne, o-benzyne (1v15)

SMILES: C1=CC#CC=C1



92: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  1  1  0  0  0                    10125.51760   10125.51837   -0.00077    0.00200   0.00000
    2:   2  0  2  1  1  1                    14752.25130   14752.25117    0.00013    0.00200   0.00000
    3:   3  1  3  2  0  2                    22216.27210   22216.27076    0.00134    0.00200   0.00000
    4:   2  1  2  1  0  1                    16408.23230   16408.23314   -0.00084    0.00200   0.00000
    5:   4  0  4  3  1  3                    28231.93160   28231.93244   -0.00084    0.00200   0.00000
    6:   2  2  1  1  1  0                    24093.78890   24093.78866    0.00024    0.00200   0.00000
    7:   4  1  4  3  0  3                    28315.06280   28315.06201    0.00079    0.00200   0.00000
    8:   5  0  5  4  1  4                    34546.88020   34546.88062   -0.00042    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99972E-01    3   6.46300E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 6984.15884( 65)          0.00000
   2         20000                 5702.20695(148)          0.00000
   3         30000                3141.361377(207)        -0.000000
   4           200               -0.694002097(  0)E-03 -0.000000000E-03
   5          1100               -0.375443583(  0)E-03  0.000000000E-03
   6          2000               -1.461683189(  0)E-03  0.000000000E-03
   7         40100               -0.277466708(  0)E-03  0.000000000E-03
   8         41000               -1.016380664(  0)E-03  0.000000000E-03
```

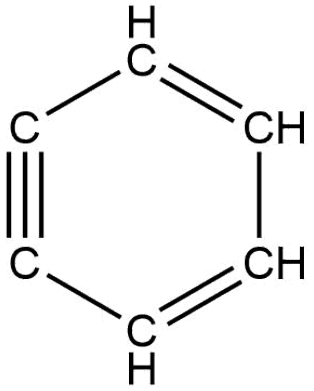
```
  9           300                       0.288(100)E-18       -0.000E-18
MICROWAVE AVG =       -0.000046 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000766 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.38304         0.38304
```

Molecule 93

IUPAC Name: ortho-benzyne, o-benzyne (1v16)

Common name: ortho-benzyne, o-benzyne (1v16)

SMILES: C1=CC#CC=C1



93: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  1  1  0  0  0                     10123.71180   10123.71186   -0.00006    0.00200   0.00026
    2:   2  0  2  1  1  1                     14762.36130   14762.36261   -0.00131    0.00200   0.00068
    3:   2  1  2  1  0  1                     16410.74350   16410.74461   -0.00111    0.00200   0.00039
    4:   3  1  3  2  0  2                     22224.48870   22224.48875   -0.00005    0.00200   0.00058
    5:   3  0  3  2  1  2                     21781.86090   21781.86090   -0.00000    0.00200   0.00058
    6:   2  2  1  1  1  0                     24084.05550   24084.05115    0.00435    0.00200   0.00077
    7:   2  2  0  1  1  1                     28298.35990   28298.35995   -0.00005    0.00200   0.00134
    8:   4  1  4  3  0  3                     28328.75110   28328.75073    0.00037    0.00200   0.00079
    9:   3  2  2  2  1  1                     30371.04190   30371.04457   -0.00267    0.00200   0.00077
   10:   4  1  3  3  2  2                     33487.55550   33487.55523    0.00027    0.00200   0.00156
   11:   5  0  5  4  1  4                     34565.40820   34565.40737    0.00083    0.00200   0.00102
   12:   5  1  5  4  0  4                     34578.19740   34578.19623    0.00117    0.00200   0.00102
   13:   4  2  3  3  1  2                     35647.48900   35647.49107   -0.00207    0.00200   0.00080
   14:   3  3  1  2  2  0                     38517.56330   38517.56325    0.00005    0.00200   0.00137
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.95662E-01    3   8.57587E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 6980.193344(266)         0.000000
   2         20000                  5703.34345( 44)         -0.00000
```

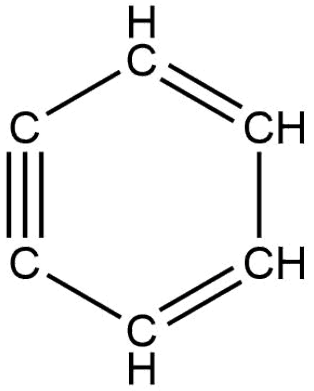
```
  3         30000                 3143.520367(127)         0.000000
  4           200                -0.694002097(  0)E-03 -0.000000000E-03
  5          1100                -0.375443583(  0)E-03 -0.000000000E-03
  6          2000                -1.461683189(  0)E-03  0.000000000E-03
  7         40100                -0.277466708(  0)E-03 -0.000000000E-03
  8         41000                -1.016380664(  0)E-03 -0.000000000E-03
  9           300                       0.288(100)E-18        0.000E-18
MICROWAVE AVG =       -0.000020 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001594 MHz, IR RMS =        0.00000
END OF ITERATION  2 OLD, NEW RMS ERROR=        0.79720         0.79720
```

Molecule 94

IUPAC Name: ortho-benzyne, o-benzyne (2v16)

Common name: ortho-benzyne, o-benzyne (2v16)

SMILES: C1=CC#CC=C1



94: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  1  1  0  0  0                    10117.34530   10117.34541   -0.00011    0.00200   0.00000
    2:   2  0  2  1  1  1                    14770.69420   14770.69453   -0.00033    0.00200   0.00000
    3:   3  1  3  2  0  2                    22232.54970   22232.55071   -0.00101    0.00200   0.00000
    4:   2  1  2  1  0  1                    16410.62340   16410.62021    0.00319    0.00200   0.00000
    5:   3  0  3  2  1  2                    21792.89280   21792.89365   -0.00085    0.00200   0.00000
    6:   2  2  1  1  1  0                    24058.71040   24058.70974    0.00066    0.00200   0.00000
    7:   3  1  2  2  2  1                    24861.31900   24861.32084   -0.00184    0.00200   0.00000
    8:   4  0  4  3  1  3                    28262.58580   28262.58569    0.00011    0.00200   0.00000
    9:   2  2  0  1  1  1                    28263.63330   28263.63241    0.00089    0.00200   0.00000
   10:   4  1  4  3  0  3                    28344.18150   28344.18168   -0.00018    0.00200   0.00000
   11:   3  2  2  2  1  1                    30351.94370   30351.94522   -0.00152    0.00200   0.00000
   12:   4  1  3  3  2  2                    33492.37850   33492.37611    0.00239    0.00200   0.00000
   13:   5  0  5  4  1  4                    34587.51470   34587.51350    0.00120    0.00200   0.00000
   14:   4  2  3  3  1  2                    35638.13830   35638.14037   -0.00207    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.88296E-01    3   8.35836E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  6970.70586( 35)         -0.00000
   2         20000                 5699.927775(308)         0.000000
```

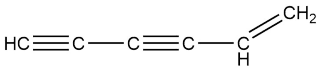
```
  3         30000                 3146.641394(136)         0.000000
  4           200                -0.694002097(  0)E-03  0.000000000E-03
  5          1100                -0.375443583(  0)E-03 -0.000000000E-03
  6          2000                -1.461683189(  0)E-03  0.000000000E-03
  7         40100                -0.277466708(  0)E-03 -0.000000000E-03
  8         41000                -1.016380664(  0)E-03 -0.000000000E-03
  9           300                       0.288(100)E-18        0.000E-18
MICROWAVE AVG =        0.000037 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001475 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.73755         0.73755
```

Molecule 95

IUPAC Name: 1-hexene-3,5-diyne

Common name: vinyldiacetylene

SMILES: C=CC#CC#C

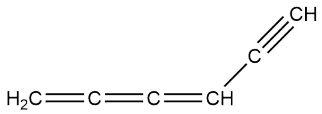


Molecule 96

IUPAC Name: 1,2,3-hexatrien-5-yne

Common name: ethynylbutatriene

SMILES: C#CC=C=C=C



96: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                      8683.02330    8683.02233    0.00097    0.00200   0.00000
    2:   3  0  3  2  0  2                      8854.84480    8854.84600   -0.00120    0.00200   0.00000
    3:   3  1  2  2  1  1                      9031.10740    9031.10526    0.00214    0.00200   0.00000
    4:   4  1  4  3  1  3                     11576.66180   11576.66120    0.00060    0.00200   0.00000
    5:   4  0  4  3  0  3                     11803.73420   11803.73667   -0.00247    0.00200   0.00000
    6:   4  1  3  3  1  2                     12040.74330   12040.74079    0.00251    0.00200   0.00000
    7:   5  1  5  4  1  4                     14469.70420   14469.70397    0.00023    0.00200   0.00000
    8:   5  0  5  4  0  4                     14750.29240   14750.29495   -0.00255    0.00200   0.00000
    9:   5  2  4  4  2  3                     14762.36290   14762.36440   -0.00150    0.00200   0.00000
   10:   5  1  4  4  1  3                     15049.74490   15049.74305    0.00185    0.00200   0.00000
   11:   6  1  6  5  1  5                     17362.00980   17362.00853    0.00127    0.00200   0.00000
   12:   6  0  6  5  0  5                     17693.94060   17693.94352   -0.00292    0.00200   0.00000
   13:   6  1  5  5  1  4                     18057.94740   18057.94735    0.00005    0.00200   0.00000
   14:   7  1  7  6  1  6                     20253.43740   20253.43730    0.00010    0.00200   0.00000
   15:   7  0  7  6  0  6                     20634.10960   20634.11207   -0.00247    0.00200   0.00000
   16:   7  1  6  6  1  5                     21065.18320   21065.18472   -0.00152    0.00200   0.00000
   17:   8  1  8  7  1  7                     23143.85840   23143.85812    0.00028    0.00200   0.00000
   18:   8  0  8  7  0  7                     23570.24050   23570.24166   -0.00116    0.00200   0.00000
   19:   9  1  9  8  1  8                     26033.14490   26033.14507   -0.00017    0.00200   0.00000
   20:   9  0  9  8  0  8                     26501.79270   26501.79077    0.00193    0.00200   0.00000
   21:  10  0 10  9  0  9                     29428.24760   29428.24288    0.00472    0.00200   0.00000
   22:  11  0 11 10  0 10                     32349.12050   32349.11581    0.00469    0.00200   0.00000
   23:  12  0 12 11  0 11                     35263.96670   35263.97246   -0.00576    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.68422E-01    3   2.19035E-01    4   1.04761E-01    5   9.94060E-01    6   1.00000E+00
    7   7.51095E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    19071.01( 94)             0.00
```

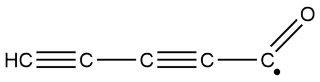
```
  2         20000                  1534.21570( 33)         -0.00000
  3         30000                 1418.180170(245)         0.000000
  4           200     -Del_J         -0.42858(170)E-03      0.00000E-03
  5          1100    -Del_JK         0.046858( 59)         0.000000
  6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
  7         40100     -del_J         -0.10131(164)E-03      0.00000E-03
  8         41000     -del_K     -3.860510216(  0)E-21  0.000000000E-21
MICROWAVE AVG =       -0.000016 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002407 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.20330         1.20330
```

Molecule 97

IUPAC Name: 2,4-pentadiyn-1-on-1-yl

Common name: 2,4-pentadiyn-1-on-1-yl

SMILES: C#CC#C[C]=O

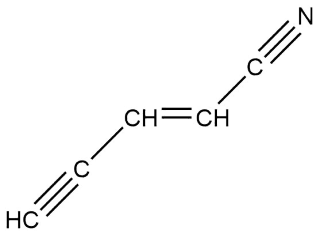


Molecule 98

IUPAC Name: (E)-2-penten-4-ynenitrile

Common name: cyanovinylacetylene (trans)

SMILES: C#CC=CC#N



98: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG.	CALC.FREQ.	-	DIFF.	-	WT.			
1:	3 1 3	0	3 2 1	2 0 2								8626.16310		8626.16245		0.00065	0.00200	0.00000	
2:	3 1 3	0	2 2 1	2 0 1								8626.49610		8626.49650		-0.00040	0.00200	0.00000	
3:	3 1 3	0	4 2 1	2 0 3								8626.51270		8626.51199		0.00071	0.00200	0.00000	
4:	3 0 3	0	2 2 0	2 0 1								8694.86040		8694.86018		0.00022	0.00200	0.00000	
5:	3 0 3	0	3 2 0	2 0 2								8695.05620		8695.05500		0.00120	0.00200	0.00000	
6:	3 0 3	0	4 2 0	2 0 3								8695.10260		8695.10148		0.00112	0.00200	0.00000	
7:	3 1 2	0	3 2 1	1 0 2								8763.87600		8763.87667		-0.00067	0.00200	0.00000	
8:	3 1 2	0	4 2 1	1 0 3								8764.22170		8764.22302		-0.00132	0.00200	0.00000	8764.22339 -0.0016
9:	3 1 2	0	2 2 1	1 0 1								8764.22170		8764.22417		-0.00247	0.00200	0.00000	8764.22339 -0.0016
10:	4 1 4	0	4 3 1	3 0 3								11501.72760		11501.72626		0.00134	0.00200	0.00000	
11:	4 1 4	0	3 3 1	3 0 2								11501.82910		11501.82771		0.00139	0.00200	0.00000	
12:	4 1 4	0	5 3 1	3 0 4								11501.88190		11501.88229		-0.00039	0.00200	0.00000	
13:	4 0 4	0	3 3 0	3 0 2								11593.14750		11593.14783		-0.00033	0.00200	0.00000	
14:	4 0 4	0	4 3 0	3 0 3								11593.23150		11593.23126		0.00024	0.00200	0.00000	
15:	4 0 4	0	5 3 0	3 0 4								11593.26130		11593.26089		0.00041	0.00200	0.00000	
16:	4 1 3	0	4 3 1	2 0 3								11685.34380		11685.34356		0.00024	0.00200	0.00000	
17:	4 1 3	0	3 3 1	2 0 2								11685.45220		11685.45078		0.00142	0.00200	0.00000	
18:	4 1 3	0	5 3 1	2 0 4								11685.49860		11685.49756		0.00104	0.00200	0.00000	
19:	5 1 5	0	5 4 1	4 0 4								14377.14800		14377.14904		-0.00104	0.00200	0.00000	
20:	5 1 5	0	4 4 1	4 0 3								14377.19000		14377.18919		0.00081	0.00200	0.00000	
21:	5 1 5	0	6 4 1	4 0 5								14377.23590		14377.23459		0.00131	0.00200	0.00000	
22:	5 0 5	0	4 4 0	4 0 3								14491.21200		14491.21090		0.00110	0.00200	0.00000	
23:	5 0 5	0	5 4 0	4 0 4								14491.25790		14491.25718		0.00072	0.00200	0.00000	
24:	5 0 5	0	6 4 0	4 0 5								14491.27740		14491.27774		-0.00034	0.00200	0.00000	
25:	5 1 4	0	5 4 1	3 0 4								14606.66800		14606.66789		0.00011	0.00200	0.00000	
26:	5 1 4	0	4 4 1	3 0 3								14606.71200		14606.71124		0.00076	0.00200	0.00000	

27:	5	1	4	0	6	4	1	3	0	5	14606.75390	14606.75204	0.00186	0.00200	0.00000			
28:	6	1	6	0	6	5	1	5	0	5	17252.48830	17252.48952	-0.00122	0.00200	0.00000			
29:	6	1	6	0	5	5	1	5	0	4	17252.50780	17252.50750	0.00030	0.00200	0.00000			
30:	6	1	6	0	7	5	1	5	0	6	17252.54200	17252.54253	-0.00053	0.00200	0.00000			
31:	6	0	6	0	5	5	0	5	0	4	17389.06550	17389.06582	-0.00032	0.00200	0.00000			
32:	6	0	6	0	6	5	0	5	0	5	17389.09380	17389.09519	-0.00139	0.00200	0.00000			
33:	6	0	6	0	7	5	0	5	0	6	17389.11140	17389.11033	0.00107	0.00200	0.00000			
34:	6	1	5	0	6	5	1	4	0	5	17527.90730	17527.90788	-0.00058	0.00200	0.00000			
35:	6	1	5	0	5	5	1	4	0	4	17527.92780	17527.92789	-0.00009	0.00200	0.00000			
36:	6	1	5	0	7	5	1	4	0	6	17527.96000	17527.95986	0.00014	0.00200	0.00000			
37:	7	1	7	0	7	6	1	6	0	6	20127.75200	20127.75430	-0.00230	0.00200	0.00000			
38:	7	1	7	0	6	6	1	6	0	5	20127.76370	20127.76276	0.00094	0.00200	0.00000			
39:	7	1	7	0	8	6	1	6	0	7	20127.78710	20127.78995	-0.00285	0.00200	0.00000			
40:	7	0	7	0	6	6	0	6	0	5	20286.69050	20286.68750	0.00300	0.00200	0.00000			
41:	7	0	7	0	7	6	0	6	0	6	20286.70710	20286.70776	-0.00066	0.00200	0.00000			
42:	7	0	7	0	8	6	0	6	0	7	20286.72270	20286.71940	0.00330	0.00200	0.00000			
43:	7	1	6	0	7	6	1	5	0	6	20449.06640	20449.06953	-0.00313	0.00200	0.00000			
44:	7	1	6	0	6	6	1	5	0	5	20449.08010	20449.07939	0.00071	0.00200	0.00000			
45:	7	1	6	0	8	6	1	5	0	7	20449.10260	20449.10439	-0.00179	0.00200	0.00000			
46:	8	1	8	0	8	7	1	7	0	7	23002.93850	23002.93845	0.00005	0.00200	0.00000	23002.94027	-0.00177	
47:	8	1	8	0	7	7	1	7	0	6	23002.93850	23002.94235	-0.00385	0.00200	0.00000	23002.94027	-0.00177	
48:	8	1	8	0	9	7	1	7	0	8	23002.96290	23002.96386	-0.00096	0.00200	0.00000			
49:	8	0	8	0	7	7	0	7	0	6	23184.04100	23184.04257	-0.00157	0.00200	0.00000			
50:	8	0	8	0	8	7	0	7	0	7	23184.05660	23184.05735	-0.00075	0.00200	0.00000			
51:	8	0	8	0	9	7	0	7	0	8	23184.06840	23184.06660	0.00180	0.00200	0.00000			
52:	8	1	7	0	8	7	1	6	0	7	23370.14650	23370.14721	-0.00071	0.00300	0.00000	23370.14952	-0.00302	
53:	8	1	7	0	7	7	1	6	0	6	23370.14650	23370.15215	-0.00565	0.00300	0.00000	23370.14952	-0.00302	
54:	8	1	7	0	9	7	1	6	0	8	23370.17000	23370.17200	-0.00200	0.00200	0.00000			
55:	10	0	10	0	9	9	0	9	0	8	28977.80370	28977.80894	-0.00524	0.00400	0.00000			
56:	10	0	10	0	10	9	0	9	0	9	28977.81740	28977.81773	-0.00033	0.00400	0.00000			
57:	10	0	10	0	11	9	0	9	0	10	28977.82620	28977.82403	0.00217	0.00400	0.00000			
58:	12	0	12	0	11	11	0	11	0	10	34770.06840	34770.07140	-0.00300	0.00400	0.00000			
59:	12	0	12	0	12	11	0	11	0	11	34770.08400	34770.07714	0.00686	0.00400	0.00000	34770.07956	0.00444	
60:	12	0	12	0	13	11	0	11	0	12	34770.08400	34770.08178	0.00222	0.00400	0.00000	34770.07956	0.00444	
61:	13	0	13	0	12	12	0	12	0	11	37665.54880	37665.54613	0.00267	0.00400	0.00000	37665.55087	-0.00207	
62:	13	0	13	0	13	12	0	12	0	12	37665.54880	37665.55087	-0.00207	0.00400	0.00000	37665.55087	-0.00207	
63:	13	0	13	0	14	12	0	12	0	13	37665.54880	37665.55493	-0.00613	0.00400	0.00000	37665.55087	-0.00207	
64:	10	1	10	1	10	9	1	9	1	9	28753.09000	28753.03612	0.05388	0.03000	0.00000			
65:	10	2	9	1	10	9	2	8	1	9	28984.05000	28983.93566	0.11434	0.03000	0.00000			
66:	10	3	8	1	10	9	3	7	1	9	28987.21000	28987.09682	0.11318	0.03000	0.00000	28987.10355	0.10645	
67:	10	3	7	1	10	9	3	6	1	9	28987.21000	28987.11027	0.09973	0.03000	0.00000	28987.10355	0.10645	
68:	10	4	6	1	10	9	4	5	1	9	28988.88000	28988.83318	0.04682	0.03000	0.00000	28988.83318	0.04682	
69:	10	4	7	1	10	9	4	6	1	9	28988.88000	28988.83317	0.04683	0.03000	0.00000	28988.83318	0.04682	
70:	10	2	8	1	10	9	2	7	1	9	28989.77000	28989.76150	0.00850	0.03000	0.00000			
71:	10	5	5	1	10	9	5	4	1	9	28991.37000	28991.35128	0.01872	0.03000	0.00000	28991.35128	0.01872	
72:	10	5	6	1	10	9	5	5	1	9	28991.37000	28991.35128	0.01872	0.03000	0.00000	28991.35128	0.01872	
73:	10	6	4	1	10	9	6	3	1	9	28994.57000	28994.53172	0.03828	0.03000	0.00000	28994.53172	0.03828	
74:	10	6	5	1	10	9	6	4	1	9	28994.57000	28994.53172	0.03828	0.03000	0.00000	28994.53172	0.03828	
75:	10	7	3	1	10	9	7	2	1	9	28998.39000	28998.33597	0.05403	0.03000	0.00000	28998.33597	0.05403	

```
  76:  10  7  4  1 10  9  7  3  1  9        28998.39000   28998.33597    0.05403    0.03000   0.00000   28998.33597    0.05403
  77:  10  1  9  1 10  9  1  8  1  9        29212.11000   29212.01857    0.09143    0.03000   0.00000
  78:  11  1 11  1 11 10  1 10  1 10        31628.01000   31627.92268    0.08732    0.03000   0.00000
  79:  11  0 11  1 11 10  0 10  1 10        31874.20000   31874.15389    0.04611    0.03000   0.00000
  80:  11  2 10  1 11 10  2  9  1 10        31882.12000   31882.01536    0.10464    0.03000   0.00000
  81:  11  3  9  1 11 10  3  8  1 10        31885.96000   31885.88555    0.07445    0.03000   0.00000   31885.89647    0.06353
  82:  11  3  8  1 11 10  3  7  1 10        31885.96000   31885.90740    0.05260    0.03000   0.00000   31885.89647    0.06353
  83:  11  4  7  1 11 10  4  6  1 10        31887.77000   31887.71979    0.05021    0.03000   0.00000   31887.71978    0.05022
  84:  11  4  8  1 11 10  4  7  1 10        31887.77000   31887.71976    0.05024    0.03000   0.00000   31887.71978    0.05022
  85:  11  2  9  1 11 10  2  8  1 10        31889.85000   31889.78225    0.06775    0.03000   0.00000
  86:  11  5  6  1 11 10  5  5  1 10        31890.46000   31890.45571    0.00429    0.03000   0.00000   31890.45571    0.00429
  87:  11  5  7  1 11 10  5  6  1 10        31890.46000   31890.45571    0.00429    0.03000   0.00000   31890.45571    0.00429
  88:  11  6  5  1 11 10  6  4  1 10        31893.96000   31893.93640    0.02360    0.03000   0.00000   31893.93640    0.02360
  89:  11  6  6  1 11 10  6  5  1 10        31893.96000   31893.93640    0.02360    0.03000   0.00000   31893.93640    0.02360
  90:  11  7  4  1 11 10  7  3  1 10        31898.13000   31898.11055    0.01945    0.03000   0.00000   31898.11055    0.01945
  91:  11  7  5  1 11 10  7  4  1 10        31898.13000   31898.11055    0.01945    0.03000   0.00000   31898.11055    0.01945
  92:  11  1 10  1 11 10  1  9  1 10        32132.81000   32132.78321    0.02679    0.03000   0.00000
  93:  12  1 12  1 12 11  1 11  1 11        34502.75000   34502.69097    0.05903    0.03000   0.00000
  94:  12  2 11  1 12 11  2 10  1 11        34780.05000   34780.00542    0.04458    0.03000   0.00000
  95:  12  3 10  1 12 11  3  9  1 11        34784.75000   34784.69598    0.05402    0.03000   0.00000   34784.71297    0.03703
  96:  12  3  9  1 12 11  3  8  1 11        34784.75000   34784.72997    0.02003    0.03000   0.00000   34784.71297    0.03703
  97:  12  4  9  1 12 11  4  8  1 11        34786.62000   34786.60728    0.01272    0.03000   0.00000   34786.60730    0.01270
  98:  12  4  8  1 12 11  4  7  1 11        34786.62000   34786.60732    0.01268    0.03000   0.00000   34786.60730    0.01270
  99:  12  5  7  1 12 11  5  6  1 11        34789.49000   34789.55135   -0.06135    0.03000   0.00000   34789.55135   -0.06135
 100:  12  5  8  1 12 11  5  7  1 11        34789.49000   34789.55135   -0.06135    0.03000   0.00000   34789.55135   -0.06135
 101:  12  2 10  1 12 11  2  9  1 11        34790.04000   34790.10092   -0.06092    0.03000   0.00000
 102:  12  6  6  1 12 11  6  5  1 11        34793.29000   34793.32721   -0.03721    0.03000   0.00000   34793.32721   -0.03721
 103:  12  6  7  1 12 11  6  6  1 11        34793.29000   34793.32721   -0.03721    0.03000   0.00000   34793.32721   -0.03721
 104:  12  7  5  1 12 11  7  4  1 11        34797.83000   34797.86827   -0.03827    0.03000   0.00000   34797.86827   -0.03827
 105:  12  7  6  1 12 11  7  5  1 11        34797.83000   34797.86827   -0.03827    0.03000   0.00000   34797.86827   -0.03827
 106:  12  8  4  1 12 11  8  3  1 11        34803.16000   34803.14831    0.01169    0.03000   0.00000   34803.14831    0.01169
 107:  12  8  5  1 12 11  8  4  1 11        34803.16000   34803.14831    0.01169    0.03000   0.00000   34803.14831    0.01169
 108:  12  9  3  1 12 11  9  2  1 11        34809.10000   34809.15522   -0.05522    0.03000   0.00000   34809.15522   -0.05522
 109:  12  9  4  1 12 11  9  3  1 11        34809.10000   34809.15522   -0.05522    0.03000   0.00000   34809.15522   -0.05522
 110:  12  1 11  1 12 11  1 10  1 11        35053.50000   35053.42211    0.07789    0.03000   0.00000
NORMALIZED DIAGONAL:
   1   1.00000E+00    2   7.01747E-01    3   2.49250E-01    4   2.59923E-01    5   9.99549E-01    6   1.00000E+00
   7   9.94205E-01    8   1.00000E+00    9   9.84506E-01   10   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10099          A          46194.3(191)              0.0
   2         20099          B       1472.153720(179)          0.000000
   3         30099          C       1426.248460(173)          0.000000
   4           299     -Del_J          -0.09451( 73)E-03     -0.00000E-03
   5          1199    -Del_JK         0.0148069( 95)         0.0000000
   6          2099     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
   7         40199     -del_J             -7.09( 93)E-06          0.00E-06
   8         41099     -del_K     -3.860510216(  0)E-21 -0.000000000E-21
   9     110010000     chi_aa           -3.8966(162)           -0.0000
```

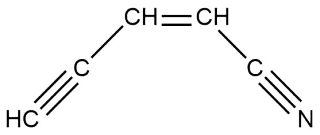
```
 10     110020000     chi_bb            1.814( 32)            0.000
MICROWAVE AVG =        0.011612 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.034397 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.27852         1.27852
```

Molecule 99

IUPAC Name: (Z)-2-penten-4-ynenitrile

Common name: cyanovinylacetylene (cis)

SMILES: C#CC=CC#N

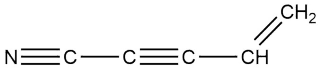


Molecule 100

IUPAC Name: 4-penten-2-ynenitrile

Common name: vinylcyanoacetylene

SMILES: C=CC#CC#N



100: Fit file

											EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG.	CALC.FREQ.	-	DIFF.	-	WT.			
1:	3	1	3	0	3	2	1	2	0	2	8048.69580		8048.69443		0.00137		0.00200		0.00000									
2:	3	1	3	0	2	2	1	2	0	1	8049.05080		8049.05037		0.00043		0.00200		0.00000									
3:	3	1	3	0	4	2	1	2	0	3	8049.06450		8049.06346		0.00104		0.00200		0.00000									
4:	3	0	3	0	2	2	0	2	0	1	8118.75200		8118.75272		-0.00072		0.00200		0.00000									
5:	3	0	3	0	3	2	0	2	0	2	8118.95730		8118.95880		-0.00150		0.00200		0.00000									
6:	3	0	3	0	4	2	0	2	0	3	8119.00740		8119.00794		-0.00054		0.00200		0.00000									
7:	3	1	2	0	3	2	1	1	0	2	8189.35210		8189.35088		0.00122		0.00200		0.00000									
8:	3	1	2	0	2	2	1	1	0	1	8189.71830		8189.71568		0.00262		0.00200		0.00000		8189.71713		0.00117					
9:	3	1	2	0	4	2	1	1	0	3	8189.71830		8189.71781		0.00049		0.00200		0.00000		8189.71713		0.00117					
10:	4	1	4	0	4	3	1	3	0	3	10731.77390		10731.77295		0.00095		0.00200		0.00000									
11:	4	1	4	0	3	3	1	3	0	2	10731.88040		10731.88138		-0.00098		0.00200		0.00000									
12:	4	1	4	0	5	3	1	3	0	4	10731.93750		10731.93756		-0.00006		0.00200		0.00000									
13:	4	0	4	0	3	3	0	3	0	2	10824.97760		10824.97875		-0.00115		0.00200		0.00000									
14:	4	0	4	0	4	3	0	3	0	3	10825.06690		10825.06702		-0.00012		0.00200		0.00000									
15:	4	0	4	0	5	3	0	3	0	4	10825.09820		10825.09833		-0.00013		0.00200		0.00000									
16:	4	1	3	0	4	3	1	2	0	3	10919.31150		10919.31134		0.00016		0.00200		0.00000									
17:	4	1	3	0	3	3	1	2	0	2	10919.42390		10919.42356		0.00034		0.00200		0.00000									
18:	4	1	3	0	5	3	1	2	0	4	10919.47510		10919.47461		0.00049		0.00200		0.00000									
19:	5	1	5	0	5	4	1	4	0	4	13414.69730		13414.69712		0.00018		0.00200		0.00000									
20:	5	1	5	0	4	4	1	4	0	3	13414.74120		13414.74021		0.00099		0.00200		0.00000									
21:	5	1	5	0	6	4	1	4	0	5	13414.78760		13414.78731		0.00029		0.00200		0.00000									
22:	5	0	5	0	4	4	0	4	0	3	13530.94340		13530.94510		-0.00170		0.00200		0.00000									
23:	5	0	5	0	5	4	0	4	0	4	13530.99270		13530.99409		-0.00139		0.00200		0.00000									
24:	5	0	5	0	6	4	0	4	0	5	13531.01570		13531.01581		-0.00011		0.00200		0.00000									
25:	5	1	4	0	5	4	1	3	0	4	13649.11480		13649.11424		0.00056		0.00200		0.00000									
26:	5	1	4	0	4	4	1	3	0	3	13649.15870		13649.15944		-0.00074		0.00200		0.00000									
27:	5	1	4	0	6	4	1	3	0	5	13649.20360		13649.20351		0.00009		0.00200		0.00000									
28:	6	1	6	0	6	5	1	5	0	5	16097.52840		16097.52777		0.00063		0.00200		0.00000									
29:	6	1	6	0	5	5	1	5	0	4	16097.54890		16097.54718		0.00172		0.00200		0.00000									
30:	6	1	6	0	7	5	1	5	0	6	16097.58400		16097.58362		0.00038		0.00200		0.00000									
31:	6	0	6	0	5	5	0	5	0	4	16236.65990		16236.66365		-0.00375		0.00200		0.00000									

32:	6	0	6	0	6	5	0	5	0	5	16236.69540	16236.69476	0.00064	0.00200	0.00000		
33:	6	0	6	0	7	5	0	5	0	6	16236.71000	16236.71073	-0.00073	0.00200	0.00000		
34:	6	1	5	0	6	5	1	4	0	5	16378.82080	16378.81946	0.00134	0.00200	0.00000		
35:	6	1	5	0	5	5	1	4	0	4	16378.84140	16378.84021	0.00119	0.00200	0.00000		
36:	6	1	5	0	7	5	1	4	0	6	16378.87500	16378.87463	0.00037	0.00200	0.00000		
37:	7	1	7	0	7	6	1	6	0	6	18780.27150	18780.27063	0.00087	0.00200	0.00000		
38:	7	1	7	0	6	6	1	6	0	5	18780.27830	18780.27983	-0.00153	0.00200	0.00000		
39:	7	1	7	0	8	6	1	6	0	7	18780.30760	18780.30816	-0.00056	0.00200	0.00000		
40:	7	0	7	0	6	6	0	6	0	5	18942.10060	18942.10235	-0.00175	0.00200	0.00000		
41:	7	0	7	0	7	6	0	6	0	6	18942.12410	18942.12383	0.00027	0.00200	0.00000		
42:	7	0	7	0	8	6	0	6	0	7	18942.13580	18942.13609	-0.00029	0.00200	0.00000		
43:	7	1	6	0	7	6	1	5	0	6	19108.43360	19108.43160	0.00200	0.00200	0.00000		
44:	7	1	6	0	6	6	1	5	0	5	19108.44050	19108.44174	-0.00124	0.00200	0.00000		
45:	7	1	6	0	8	6	1	5	0	7	19108.46880	19108.46861	0.00019	0.00200	0.00000		
46:	8	1	8	0	8	7	1	7	0	7	21462.91900	21462.91924	-0.00024	0.00200	0.00000		
47:	8	1	8	0	7	7	1	7	0	6	21462.92480	21462.92355	0.00125	0.00200	0.00000		
48:	8	1	8	0	9	7	1	7	0	8	21462.94730	21462.94598	0.00132	0.00200	0.00000		
49:	8	0	8	0	7	7	0	7	0	6	21647.21880	21647.22046	-0.00166	0.00200	0.00000		
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52:	8	1	7	0	8	7	1	6	0	7	21837.94240	21837.94298	-0.00058	0.00200	0.00000		
53:	8	1	7	0	7	7	1	6	0	6	21837.94920	21837.94797	0.00123	0.00200	0.00000		
54:	8	1	7	0	9	7	1	6	0	8	21837.96970	21837.96930	0.00040	0.00200	0.00000		
55:	9	1	9	0	9	8	1	8	0	8	24145.46390	24145.46356	0.00034	0.00200	0.00000	24145.46441	-0.00051
56:	9	1	9	0	8	8	1	8	0	7	24145.46390	24145.46536	-0.00146	0.00200	0.00000	24145.46441	-0.00051
57:	9	1	9	0	10	8	1	8	0	9	24145.48340	24145.48346	-0.00006	0.00200	0.00000		
58:	9	0	9	0	8	8	0	8	0	7	24351.97270	24351.97469	-0.00199	0.00200	0.00000		
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60:	9	0	9	0	10	8	0	8	0	9	24351.99610	24351.99456	0.00154	0.00200	0.00000		
61:	9	1	8	0	9	8	1	7	0	8	24567.34380	24567.34211	0.00169	0.00200	0.00000	24567.34321	0.00059
62:	9	1	8	0	8	8	1	7	0	7	24567.34380	24567.34443	-0.00063	0.00200	0.00000	24567.34321	0.00059
63:	9	1	8	0	10	8	1	7	0	9	24567.36230	24567.36169	0.00061	0.00200	0.00000		
64:	10	1	10	0	10	9	1	9	0	9	26827.89260	26827.89230	0.00030	0.00400	0.00000	26827.89252	0.00008
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66:	10	1	10	0	11	9	1	9	0	10	26827.91120	26827.90764	0.00356	0.00400	0.00000		
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68:	10	0	10	0	10	9	0	9	0	9	27056.32910	27056.33030	-0.00120	0.00400	0.00000		
69:	10	0	10	0	11	9	0	9	0	10	27056.33890	27056.33689	0.00201	0.00400	0.00000		
70:	10	2	9	1	10	9	2	8	1	9	27064.71400	27064.66057	0.05343	0.03000	0.00000		
71:	10	3	8	1	10	9	3	7	1	9	27069.62000	27069.64412	-0.02412	0.03000	0.00000	27069.65376	-0.03376
72:	10	3	7	1	10	9	3	6	1	9	27069.62000	27069.66340	-0.04340	0.03000	0.00000	27069.65376	-0.03376
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74:	10	4	6	1	10	9	4	5	1	9	27073.38500	27073.37066	0.01434	0.03000	0.00000	27073.37065	0.01435
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76:	10	5	5	1	10	9	5	4	1	9	27078.47400	27078.50560	-0.03160	0.03000	0.00000	27078.50560	-0.03160
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78:	10	6	4	1	10	9	6	3	1	9	27084.92000	27084.90599	0.01401	0.03000	0.00000	27084.90599	0.01401
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80:	10	7	3	1	10	9	7	2	1	9	27092.51500	27092.52520	-0.01020	0.03000	0.00000	27092.52520	-0.01020

81:	10	7	4	1	10	9	7	3	1	9	27092.51500	27092.52520	-0.01020	0.03000	0.00000	27092.52520	-0.01020
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87:	11	0	11	0	11	10	0	10	0	10	29760.23050	29760.22229	0.00821	0.00400	0.00000	29760.22521	0.00529
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89:	11	2	10	1	11	10	2	9	1	10	29770.77000	29770.75444	0.01556	0.03000	0.00000		
90:	11	3	9	1	11	10	3	8	1	10	29776.74000	29776.71081	0.02919	0.03000	0.00000	29776.72647	0.01353
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94:	11	5	6	1	11	10	5	5	1	10	29786.35000	29786.32647	0.02353	0.03000	0.00000	29786.32647	0.02353
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96:	11	6	5	1	11	10	6	4	1	10	29793.34500	29793.34537	-0.00037	0.03000	0.00000	29793.34537	-0.00037
97:	11	6	6	1	11	10	6	5	1	10	29793.34500	29793.34537	-0.00037	0.03000	0.00000	29793.34537	-0.00037
98:	11	7	4	1	11	10	7	3	1	10	29801.69500	29801.71378	-0.01878	0.03000	0.00000	29801.71378	-0.01878
99:	11	7	5	1	11	10	7	4	1	10	29801.69500	29801.71378	-0.01878	0.03000	0.00000	29801.71378	-0.01878
100:	11	1	10	0	11	10	1	9	0	10	30025.74900	30025.75145	-0.00245	0.00400	0.00000	30025.75147	-0.00247
101:	11	1	10	0	10	10	1	9	0	9	30025.74900	30025.75149	-0.00249	0.00400	0.00000	30025.75147	-0.00247
102:	11	1	10	0	12	10	1	9	0	11	30025.76470	30025.76336	0.00134	0.00400	0.00000		
103:	12	1	12	0	11	11	1	11	0	10	32192.35450	32192.35537	-0.00087	0.00400	0.00000	32192.35573	-0.00123
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106:	12	0	12	0	11	11	0	11	0	10	32463.60940	32463.61175	-0.00235	0.00400	0.00000		
107:	12	0	12	0	12	11	0	11	0	11	32463.62500	32463.61791	0.00709	0.00400	0.00000	32463.62042	0.00458
108:	12	0	12	0	13	11	0	11	0	12	32463.62500	32463.62273	0.00227	0.00400	0.00000	32463.62042	0.00458
109:	12	2	11	1	12	11	2	10	1	11	32476.75500	32476.74203	0.01297	0.03000	0.00000		
110:	12	3	10	1	12	11	3	9	1	11	32483.83000	32483.80545	0.02455	0.03000	0.00000	32483.82981	0.00019
111:	12	3	9	1	12	11	3	8	1	11	32483.83000	32483.85417	-0.02417	0.03000	0.00000	32483.82981	0.00019
112:	12	5	7	1	12	11	5	6	1	11	32494.14500	32494.13885	0.00615	0.03000	0.00000	32494.13885	0.00615
113:	12	5	8	1	12	11	5	7	1	11	32494.14500	32494.13885	0.00615	0.03000	0.00000	32494.13885	0.00615
114:	12	6	6	1	12	11	6	5	1	11	32501.81000	32501.77011	0.03989	0.03000	0.00000	32501.77011	0.03989
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116:	12	7	5	1	12	11	7	4	1	11	32510.86500	32510.88409	-0.01909	0.03000	0.00000	32510.88409	-0.01909
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118:	12	8	4	1	12	11	8	3	1	11	32521.42500	32521.44904	-0.02404	0.03000	0.00000	32521.44904	-0.02404
119:	12	8	5	1	12	11	8	4	1	11	32521.42500	32521.44904	-0.02404	0.03000	0.00000	32521.44904	-0.02404
120:	12	1	11	0	11	11	1	10	0	10	32754.73240	32754.73375	-0.00135	0.00400	0.00000	32754.73397	-0.00157
121:	12	1	11	0	12	11	1	10	0	11	32754.73240	32754.73417	-0.00177	0.00400	0.00000	32754.73397	-0.00157
122:	12	1	11	0	13	11	1	10	0	12	32754.74710	32754.74381	0.00329	0.00400	0.00000		
123:	13	1	13	0	12	12	1	12	0	11	34874.36330	34874.36650	-0.00320	0.00400	0.00000	34874.36697	-0.00367
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126:	13	0	13	0	12	12	0	12	0	11	35166.46880	35166.46757	0.00123	0.00400	0.00000		
127:	13	0	13	0	13	12	0	12	0	12	35166.48050	35166.47269	0.00781	0.00400	0.00000	35166.47487	0.00563
128:	13	0	13	0	14	12	0	12	0	13	35166.48050	35166.47689	0.00361	0.00400	0.00000	35166.47487	0.00563
129:	13	2	12	1	13	12	2	11	1	12	35182.62500	35182.61374	0.01126	0.03000	0.00000		

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  130:  13  3 11  1 13 12  3 10  1 12        35190.96800   35190.92999    0.03801    0.03000   0.00000
  131:  13  4 10  1 13 12  4  9  1 12        35195.45500   35195.42602    0.02898    0.03000   0.00000   35195.42608    0.02892
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  136:  13  7  6  1 13 12  7  5  1 12        35220.00000   35220.03445   -0.03445    0.03000   0.00000   35220.03445   -0.03445
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  138:  13  1 12  0 12 12  1 11  0 11        35483.54490   35483.54945   -0.00455    0.00400   0.00000   35483.54980   -0.00490
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  140:  13  1 12  0 14 12  1 11  0 13        35483.55860   35483.55808    0.00052    0.00400   0.00000
  141:  14  1 14  0 13 13  1 13  0 12        37556.21490   37556.21503   -0.00013    0.00400   0.00000   37556.21816   -0.00326
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  143:  14  1 14  0 15 13  1 13  0 14        37556.21490   37556.22285   -0.00795    0.00400   0.00000   37556.21816   -0.00326
  144:  14  0 14  0 13 13  0 13  0 12        37868.74420   37868.73810    0.00610    0.00400   0.00000   37868.74240    0.00180
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  147:  14  2 13  1 14 13  2 12  1 13        37888.36000   37888.35994    0.00006    0.03000   0.00000
  148:  14  3 12  1 14 13  3 11  1 13        37898.14000   37898.08625    0.05375    0.03000   0.00000   37898.13938    0.00062
  149:  14  3 11  1 14 13  3 10  1 13        37898.14000   37898.19250   -0.05250    0.03000   0.00000   37898.13938    0.00062
  150:  14  4 11  1 14 13  4 10  1 13        37902.81400   37902.78500    0.02900    0.03000   0.00000   37902.78511    0.02889
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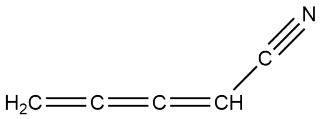
  153:  14  1 13  0 13 13  1 12  0 12        38212.18560   38212.18413    0.00147    0.00400   0.00000   38212.18707   -0.00147
  154:  14  1 13  0 14 13  1 12  0 13        38212.18560   38212.18494    0.00066    0.00400   0.00000   38212.18707   -0.00147
  155:  14  1 13  0 15 13  1 12  0 14        38212.18560   38212.19161   -0.00601    0.00400   0.00000   38212.18707   -0.00147
  156:  15  1 15  0 14 14  1 14  0 13        40237.88870   40237.88929   -0.00059    0.00400   0.00000   40237.88984   -0.00114
  157:  15  1 15  0 15 14  1 14  0 14        40237.88870   40237.89034   -0.00164    0.00400   0.00000   40237.88984   -0.00114
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   6.55033E-01    3   3.69050E-01    4   4.28013E-01    5   9.95015E-01    6   9.95483E-01
    7   9.84345E-01    8   9.99996E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A          39919.7( 57)              0.0
   2         20000          B       1376.633518( 89)         -0.000000
   3         30000          C       1329.746918( 85)          0.000000
   4           200     -Del_J        -0.106251(207)E-03     0.000000E-03
   5          1100    -Del_JK         0.0295166( 92)        -0.0000000
   6         40100     -del_J        -0.015363(202)E-03     0.000000E-03
   7     110010000     chi_aa          -4.1211(161)           -0.0000
   8     110020000     chi_bb           1.9720(314)           -0.0000
 MICROWAVE AVG =        0.000947 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.012001 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.67607         0.67607
```

Molecule 101

IUPAC Name: 2,3,4-pentatrienenitrile

Common name: cyanobutatriene

SMILES: C=C=C=CC#N



101: Fit file

	EXP.FREQ.			CALC.FREQ.				DIFF.	EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	2	1	2	2	1	1	1	1			5873.10900	5873.10577	0.00323	0.00400	0.00000
2:	2	1	2	3	1	1	1	2			5873.72700	5873.72646	0.00054	0.00200	0.00000
3:	2	1	2	1	1	1	1	0			5874.03400	5874.03502	-0.00102	0.00400	0.00000
4:	3	1	3	3	2	1	2	2			8809.86200	8809.86212	-0.00012	0.00200	0.00000
5:	3	1	3	2	2	1	2	1			8809.97800	8809.97687	0.00113	0.00200	0.00000
6:	3	1	3	4	2	1	2	3			8810.04800	8810.04752	0.00048	0.00200	0.00000
7:	4	1	4	4	3	1	3	4			11745.01100	11745.01252	-0.00152	0.00200	0.00000
8:	4	1	4	4	3	1	3	3			11745.85800	11745.85719	0.00081	0.00200	0.00000
9:	4	1	4	3	3	1	3	2			11745.88800	11745.88676	0.00124	0.00200	0.00000
10:	4	1	4	5	3	1	3	4			11745.94300	11745.94311	-0.00011	0.00200	0.00000
11:	4	1	4	3	3	1	3	3			11747.02500	11747.02711	-0.00211	0.00200	0.00000
12:	5	1	5	5	4	1	4	5			14680.24600	14680.24731	-0.00131	0.00200	0.00000
13:	5	1	5	5	4	1	4	4			14681.17700	14681.17790	-0.00090	0.00200	0.00000
14:	5	1	5	4	4	1	4	3			14681.18800	14681.18730	0.00070	0.00200	0.00000
15:	5	1	5	6	4	1	4	5			14681.22800	14681.22703	0.00097	0.00200	0.00000
16:	5	1	5	4	4	1	4	4			14682.35600	14682.35722	-0.00122	0.00200	0.00000
17:	2	1	1	2	1	1	0	1			6111.11300	6111.11252	0.00048	0.00200	0.00000
18:	2	1	1	3	1	1	0	2			6111.68500	6111.68656	-0.00156	0.00200	0.00000
19:	2	1	1	1	1	1	0	0			6112.58800	6112.58677	0.00123	0.00200	0.00000
20:	4	1	3	4	3	1	2	3			12221.81800	12221.81769	0.00031	0.00200	0.00000
21:	4	1	3	5	3	1	2	4			12221.88800	12221.88713	0.00087	0.00200	0.00000
22:	4	1	3	3	3	1	2	2			12221.89700	12221.89398	0.00302	0.00200	0.00000
23:	2	0	2	2	1	0	1	1			5991.79400	5991.79445	-0.00045	0.00200	0.00000
24:	2	0	2	3	1	0	1	2			5991.83800	5991.83802	-0.00002	0.00200	0.00000
25:	3	0	3	2	2	0	2	1			8986.06760	8986.06776	-0.00016	0.00200	0.00000
26:	3	0	3	3	2	0	2	2			8986.15780	8986.15934	-0.00154	0.00200	0.00000
27:	3	0	3	4	2	0	2	3			8986.18630	8986.18598	0.00032	0.00200	0.00000
28:	4	0	4	3	3	0	3	2			11978.65300	11978.65120	0.00180	0.00200	0.00000
29:	4	0	4	4	3	0	3	3			11978.68600	11978.68653	-0.00053	0.00200	0.00000

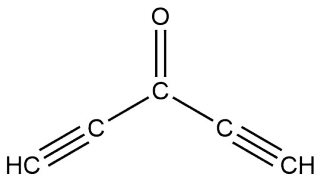
```
  30:   4  0  4  5  3  0  3  4              11978.70700   11978.70623    0.00077    0.00200   0.00000
  31:   5  0  5  4  4  0  4  3              14968.75000   14968.75057   -0.00057    0.00200   0.00000
  32:   5  0  5  5  4  0  4  4              14968.76600   14968.76625   -0.00025    0.00200   0.00000
  33:   5  0  5  6  4  0  4  5              14968.78300   14968.78283    0.00017    0.00200   0.00000
  34:   6  0  6  5  5  0  5  4              17955.78300   17955.78695   -0.00395    0.00200   0.00000
  35:   6  0  6  6  5  0  5  5              17955.79300   17955.79296    0.00004    0.00200   0.00000
  36:   6  0  6  7  5  0  5  6              17955.80900   17955.80821    0.00079    0.00200   0.00000
  37:   7  0  7  6  6  0  6  5              20939.16900   20939.16860    0.00040    0.00400   0.00000   20939.16869    0.00031
  38:   7  0  7  7  6  0  6  6              20939.16900   20939.16878    0.00022    0.00400   0.00000   20939.16869    0.00031
  39:   7  0  7  8  6  0  6  7              20939.18500   20939.18364    0.00136    0.00200   0.00000
  40:   8  0  8  8  7  0  7  7              23918.30900   23918.30832    0.00068    0.00400   0.00000   23918.31023   -0.00123
  41:   8  0  8  7  7  0  7  6              23918.30900   23918.31215   -0.00315    0.00400   0.00000   23918.31023   -0.00123
  42:   8  0  8  9  7  0  7  8              23918.32600   23918.32332    0.00268    0.00200   0.00000
  43:  11  0 11 11 10  0 10 10              32824.79100   32824.79266   -0.00166    0.00200   0.00000
  44:  11  0 11 10 10  0 10  9              32824.81300   32824.80404    0.00896    0.00400   0.00000   32824.80677    0.00623
  45:  11  0 11 12 10  0 10 11              32824.81300   32824.80950    0.00350    0.00400   0.00000   32824.80677    0.00623
  46:  10  0 10 10  9  0  9  9              29861.63000   29861.64049   -0.01049    0.00400   0.00000
  47:  10  0 10  9  9  0  9  8              29861.66000   29861.64981    0.01019    0.00400   0.00000   29861.65320    0.00680
  48:  10  0 10 11  9  0  9 10              29861.66000   29861.65659    0.00341    0.00400   0.00000   29861.65320    0.00680
  49:   3  1  2  3  2  1  1  2               9166.85250    9166.85737   -0.00487    0.00200   0.00000
  50:   3  1  2  4  2  1  1  3               9167.01650    9167.01686   -0.00036    0.00200   0.00000
  51:   5  1  4  5  4  1  3  4              15276.06480   15276.06379    0.00101    0.00200   0.00000
  52:   5  1  4  4  4  1  3  3              15276.10140   15276.09918    0.00222    0.00200   0.00000   15276.10036    0.00104
  53:   5  1  4  6  4  1  3  5              15276.10140   15276.10154   -0.00014    0.00200   0.00000   15276.10036    0.00104
  54:   6  1  6  6  5  1  5  5              17615.71240   17615.70936    0.00304    0.00200   0.00000   17615.71097    0.00143
  55:   6  1  6  5  5  1  5  4              17615.71240   17615.71257   -0.00017    0.00200   0.00000   17615.71097    0.00143
  56:   6  1  6  7  5  1  5  6              17615.74140   17615.74134    0.00006    0.00200   0.00000
  57:   6  1  5  5  5  1  4  4              18329.47640   18329.47640    0.00000    0.00200   0.00000   18329.47833   -0.00193
  58:   6  1  5  7  5  1  4  6              18329.47640   18329.48027   -0.00387    0.00200   0.00000   18329.47833   -0.00193
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.33407E-01    3   4.08513E-01    4   7.67830E-02    5   9.94298E-01    6   1.00000E+00
    7   7.16833E-01    8   1.00000E+00    9   9.99999E-01   10   3.93442E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         19145.84(246)            -0.00
   2         20000          B      1557.606704(282)         0.000000
   3         30000          C      1438.599829(214)        -0.000000
   4           200     -Del_J          -0.4667( 34)E-03       0.0000E-03
   5          1100    -Del_JK         0.047906(148)        -0.000000
   6          2000     -Del_K     -2.717900869(  0)E-24 -0.000000000E-24
   7         40100     -del_J         -0.10851(241)E-03     -0.00000E-03
   8         41000     -del_K     -3.860510216(  0)E-21 -0.000000000E-21
   9     110010000     chi_aa          -1.9228( 43)          -0.0000
  10     110020000     chi_bb          -0.1283( 62)           0.0000
 MICROWAVE AVG =        0.000038 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002448 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.85584         0.85584
```

Molecule 102

IUPAC Name: 1,4-pentadiyn-3-one

Common name: diethynyl ketone

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



102: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	3	1	2	3	0	3		7334.13500		7334.13462		0.00038	0.00200	0.00000
2:	3	2	1	3	1	2		10573.80320		10573.80324		-0.00004	0.00200	0.00000
3:	3	0	3	2	1	2		11070.03560		11070.03571		-0.00011	0.00200	0.00000
4:	2	1	2	1	0	1		12548.92160		12548.92175		-0.00015	0.00200	0.00000
5:	2	2	1	2	1	2		13745.79180		13745.79198		-0.00018	0.00200	0.00000
6:	1	1	1	0	0	0		8565.48040		8565.47932		0.00108	0.00200	0.00000
7:	2	2	0	2	1	1		11263.61860		11263.61909		-0.00049	9.00200	0.00000
8:	4	0	4	3	1	3		16111.51740		16111.51772		-0.00032	0.00200	0.00000
9:	3	2	2	3	1	3		15135.11610		15135.11639		-0.00029	0.00200	0.00000
10:	3	1	3	2	0	2		16152.93420		16152.93459		-0.00039	0.00200	0.00000
11:	4	1	4	3	0	3		19552.06790		19552.06770		0.00020	0.00200	0.00000
12:	5	0	5	4	1	4		20864.91200		20864.91255		-0.00055	0.00200	0.00000
13:	2	2	1	1	1	0		21712.64650		21712.64621		0.00029	0.00200	0.00000
14:	2	2	0	1	1	1		22722.37760		22722.37706		0.00054	0.00200	0.00000
15:	3	2	2	2	1	1		25696.21710		25696.21836		-0.00126	0.00200	0.00000
16:	3	2	1	2	1	2		28977.97390		28977.97358		0.00032	0.00200	0.00000
17:	3	3	1	2	2	0		35238.06300		35238.06490		-0.00190	0.00200	0.00000
18:	3	3	0	2	2	1		35388.39910		35388.39918		-0.00008	0.00200	0.00000
19:	4	1	3	4	0	4		9966.14680		9966.14625		0.00055	0.00200	0.00000
20:	4	2	2	4	1	3		10241.49410		10241.49499		-0.00089	0.00200	0.00000
21:	5	2	3	5	1	4		10578.63190		10578.63210		-0.00020	0.00200	0.00000
22:	4	1	3	3	2	2		10942.54750		10942.54758		-0.00008	0.00200	0.00000
23:	5	1	4	5	0	5		13489.00350		13489.00255		0.00095	0.00200	0.00000
24:	4	2	3	4	1	4		17011.65200		17011.65209		-0.00009	0.00200	0.00000
25:	5	1	4	4	2	3		17342.26300		17342.26300		-0.00000	0.00200	0.00000
26:	4	3	1	4	2	2		19378.73940		19378.73808		0.00132	0.00200	0.00000
27:	3	3	0	3	2	1		20156.21650		20156.21759		-0.00109	0.00200	0.00000
28:	3	3	1	3	2	2		20805.46700		20805.46563		0.00137	0.00200	0.00000

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   29:   5  1  5  4  0  4                    22955.25130   22955.24669    0.00461    0.00200   0.00000
   30:   6  0  6  5  1  5                    25335.39210   25335.39263   -0.00053    0.00200   0.00000
   31:   6  1  6  5  0  5                    26498.25130   26498.25196   -0.00066    0.00200   0.00000
   32:   4  2  3  3  1  2                    29229.58570   29229.58517    0.00053    0.00200   0.00000
   33:   7  1  7  6  0  6                    30203.47850   30203.47855   -0.00005    0.00200   0.00000
   34:   5  2  4  4  1  3                    32354.62740   32354.62891   -0.00151    0.00200   0.00000
   35:   4  2  2  3  1  3                    36319.15820   36319.15897   -0.00077    0.00200   0.00000
   36:   4  3  2  3  2  1                    39806.19240   39806.19132    0.00108    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.58303E-01    3   9.99495E-01    4   1.60488E-01    5   3.13954E-01    6   4.03761E-01
    7   4.50464E-01    8   3.47555E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       6573.79655( 42)          0.00000
   2         20000          B       2864.69845( 32)         -0.00000
   3         30000          C      1991.704026(189)        -0.000000
   4           200    Delta_J          -1.5646( 57)E-03       0.0000E-03
   5          1100   Delta_JK        0.0128020(264)        0.0000000
   6          2000    Delta_K        -0.045604( 32)        -0.000000
   7         40100     -del_J         -0.70681(279)E-03      0.00000E-03
   8         41000     -del_K           -1.088( 52)E-03       -0.000E-03
 MICROWAVE AVG =        0.000044 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001069 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.53294         0.53294
```
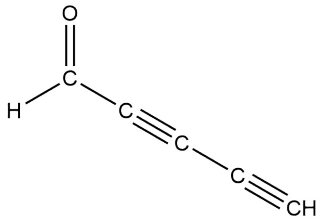

Molecule 103

IUPAC Name: 2,4-pentadiynal

Common name: 2,4-pentadiynal

SMILES: C#CC#CC=O

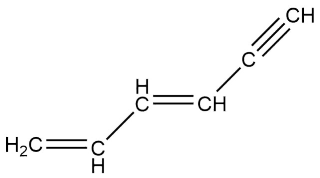


Molecule 104

IUPAC Name: (3E)-1,3-hexadien-5-yne (anti)

Common name: 1,3-hexadien-5-yne (anti-(3E))

SMILES: C=CC=CC#C



104: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-	AVG. CALC.FREQ.	- DIFF.	- WT.	
1:	1 1 1 2 0 2						19706.00200	19706.00222	-0.00022	0.02000	0.00000
2:	1 0 1 0 0 0						2775.82360	2775.82301	0.00059	0.05000	0.00000
3:	2 1 2 1 1 1						5479.33510	5479.33548	-0.00038	0.00200	0.00000
4:	2 0 2 1 0 1						5551.48770	5551.48808	-0.00038	0.00200	0.00000
5:	2 1 1 1 1 0						5624.07830	5624.07801	0.00029	0.00200	0.00000
6:	3 1 3 2 1 2						8218.90040	8218.90070	-0.00030	0.00200	0.00000
7:	3 0 3 2 0 2						8326.83630	8326.83729	-0.00099	0.00200	0.00000
8:	3 2 2 2 2 1						8327.83940	8327.83868	0.00072	0.00200	0.00000
9:	3 2 1 2 2 0						8328.46460	8328.45988	0.00472	0.00200	0.00000
10:	3 1 2 2 1 1						8436.01130	8436.01224	-0.00094	0.00200	0.00000
11:	4 1 4 3 1 3						10958.34290	10958.34321	-0.00031	0.00200	0.00000
12:	4 0 4 3 0 3						11101.71270	11101.71276	-0.00006	0.00200	0.00000
13:	4 2 3 3 2 2						11103.65150	11103.65183	-0.00033	0.00200	0.00000
14:	4 2 2 3 2 1						11105.20530	11105.20475	0.00055	0.00200	0.00000
15:	4 1 3 3 1 2						11247.81970	11247.82044	-0.00074	0.00200	0.00000
16:	5 1 5 4 1 4						13697.62200	13697.62259	-0.00059	0.00200	0.00000
17:	5 0 5 4 0 4						13875.95720	13875.95674	0.00046	0.00200	0.00000
18:	5 2 4 4 2 3						13879.35020	13879.35092	-0.00072	0.00200	0.00000
19:	5 2 3 4 2 2						13882.45680	13882.45653	0.00027	0.00200	0.00000
20:	5 1 4 4 1 3						14059.45990	14059.46013	-0.00023	0.00200	0.00000
21:	6 1 6 5 1 5						16436.69870	16436.69886	-0.00016	0.00200	0.00000
22:	6 0 6 5 0 5						16649.41280	16649.41167	0.00113	0.00200	0.00000
23:	6 1 5 5 1 4						16870.88840	16870.88844	-0.00004	0.00200	0.00000
24:	7 1 7 6 1 6						19175.53180	19175.53258	-0.00078	0.00200	0.00000
25:	7 0 7 6 0 6						19421.92160	19421.92036	0.00124	0.00200	0.00000
26:	7 1 6 6 1 5						19682.06110	19682.06196	-0.00086	0.00200	0.00000
27:	8 1 8 7 1 7						21914.08300	21914.08492	-0.00192	0.00200	0.00000
28:	8 0 8 7 0 7						22193.32700	22193.32626	0.00074	0.00200	0.00000

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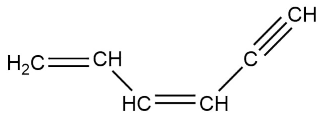
   29:   8  1  7  7  1  6                    22492.93550   22492.93669   -0.00119    0.00200   0.00000
   30:   9  1  9  8  1  8                    24652.31740   24652.31782   -0.00042    0.00200   0.00000
   31:   9  0  9  8  0  8                    24963.47650   24963.47370    0.00280    0.00200   0.00000
   32:   9  1  8  8  1  7                    25303.46720   25303.46789   -0.00069    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.45021E-01    3   2.56457E-01    4   8.77180E-01    5   1.00000E+00    6   9.99975E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 26681.5562(200)           0.0000
   2         20000                1424.097631(237)         0.000000
   3         30000                1351.725815(232)         0.000000
   4           200                   -0.10976( 73)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                   0.015842( 32)        -0.000000
   7         40100                   -0.01716( 91)E-03     -0.00000E-03
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000039 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001200 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.59738         0.59738
```

Molecule 105

IUPAC Name: (3Z)-1,3-hexadien-5-yne (anti)

Common name: 1,3-hexadien-5-yne (anti-(3Z))

SMILES: C=CC=CC#C



105: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	2	1	2	1	1	1		6943.91370		6943.91369		0.00001	0.00200	0.00000
2:	2	0	2	1	0	1		7275.82470		7275.82442		0.00028	0.00200	0.00000
3:	2	1	1	1	1	0		7630.51520		7630.51481		0.00039	0.00200	0.00000
4:	3	1	3	2	1	2		10408.86410		10408.86338		0.00072	0.00200	0.00000
5:	3	0	3	2	0	2		10885.41940		10885.41977		-0.00037	0.00200	0.00000
6:	3	2	2	2	2	1		10930.99050		10930.98880		0.00170	0.00200	0.00000
7:	3	2	1	2	2	0		10976.27450		10976.27530		-0.00080	0.00200	0.00000
8:	3	1	2	2	1	1		11438.50610		11438.50513		0.00097	0.00200	0.00000
9:	4	1	4	3	1	3		13865.73040		13865.73000		0.00040	0.00200	0.00000
10:	4	0	4	3	0	3		14461.51760		14461.51756		0.00004	0.00200	0.00000
11:	4	2	3	3	2	2		14565.74450		14565.74501		-0.00051	0.00200	0.00000
12:	4	2	2	3	2	1		14678.41380		14678.41544		-0.00164	0.00200	0.00000
13:	4	1	3	3	1	2		15237.44510		15237.44535		-0.00025	0.00200	0.00000
14:	5	1	5	4	1	4		17312.35210		17312.34991		0.00219	0.00200	0.00000
15:	5	0	5	4	0	4		17994.45350		17994.45376		-0.00026	0.00200	0.00000
16:	5	2	4	4	2	3		18192.87900		18192.87825		0.00075	0.00200	0.00000
17:	5	2	3	4	2	2		18415.99660		18415.99896		-0.00236	0.00200	0.00000
18:	5	1	4	4	1	3		19023.76230		19023.76383		-0.00153	0.00200	0.00000
19:	6	1	6	5	1	5		20746.99280		20746.98782		0.00498	0.00200	0.00000
20:	6	0	6	5	0	5		21477.05400		21477.05377		0.00023	0.00200	0.00000
21:	6	1	5	5	1	4		22793.40360		22793.40769		-0.00409	0.00200	0.00000
22:	2	1	1	2	0	2		8316.31640		8316.31398		0.00242	0.00200	0.00000
23:	3	1	2	3	0	3		8869.39350		8869.39933		-0.00583	0.00200	0.00000
24:	4	1	3	4	0	4		9645.32700		9645.32712		-0.00012	0.00200	0.00000
25:	5	1	4	5	0	5		10674.63300		10674.63719		-0.00419	0.00200	0.00000
26:	1	1	1	0	0	0		11261.91200		11261.91039		0.00161	0.00200	0.00000
27:	6	1	5	6	0	6		11990.99790		11990.99111		0.00679	0.00200	0.00000
28:	2	1	2	1	0	1		14562.23260		14562.23161		0.00099	0.00200	0.00000
29:	3	1	3	2	0	2		17695.26910		17695.27057		-0.00147	0.00200	0.00000

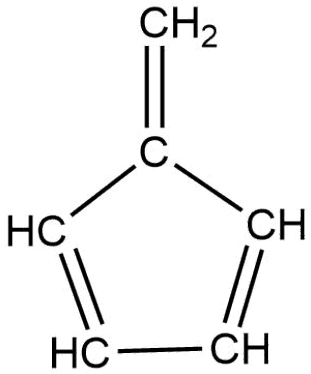
```
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.70420E-01    3   3.67481E-01    4   9.99226E-01    5   1.00000E+00    6   6.61385E-01
    7   8.92883E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  9611.74493( 86)         -0.00000
   2         20000                 1993.451408(287)         0.000000
   3         30000                 1650.144032(185)         0.000000
   4           200                    -0.74123(271)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                    0.011772( 37)        -0.000000
   7         40100                    -0.21305(205)E-03     -0.00000E-03
   8         50000                 -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000036 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002441 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.22061         1.22061
```

Molecule 106

IUPAC Name: 5-methylene-1,3-cyclopentadiene

Common name: fulvene

SMILES: C=C1C=CC=C1



106: Fit file

	EXP.FREQ.			CALC.FREQ.			DIFF.	EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	2	1	2	1	1	1				11592.05320	11592.05116	0.00204	0.00200	0.00000
2:	2	0	2	1	0	1				12581.84690	12581.84708	-0.00018	0.00200	0.00000
3:	2	1	1	1	1	0				14004.65210	14004.65262	-0.00052	0.00200	0.00000
4:	3	1	3	2	1	2				17263.01640	17263.01645	-0.00005	0.00200	0.00000
5:	3	0	3	2	0	2				18373.96170	18373.96179	-0.00009	0.00200	0.00000
6:	3	2	2	2	2	1				19197.48160	19197.48606	-0.00446	0.00200	0.00000
7:	3	2	1	2	2	0				20021.04530	20021.04283	0.00247	0.00200	0.00000
8:	3	1	2	2	1	1				20857.14350	20857.14395	-0.00045	0.00200	0.00000
9:	4	1	4	3	1	3				22815.37960	22815.38011	-0.00051	0.00200	0.00000
10:	4	0	4	3	0	3				23752.95440	23752.95156	0.00284	0.00200	0.00000
11:	4	2	3	3	2	2				25426.88310	25426.88360	-0.00050	0.00200	0.00000
12:	4	3	2	3	3	1				25965.24400	25965.24559	-0.00159	0.00200	0.00000
13:	4	3	1	3	3	0				26110.56360	26110.55988	0.00372	0.00200	0.00000
14:	4	2	2	3	2	1				27268.24870	27268.24935	-0.00065	0.00200	0.00000
15:	4	1	3	3	1	2				27495.23360	27495.23344	0.00016	0.00200	0.00000
16:	5	1	5	4	1	4				28252.35060	28252.35101	-0.00041	0.00200	0.00000
17:	5	0	5	4	0	4				28884.00590	28884.00586	0.00004	0.00200	0.00000
18:	5	2	4	4	2	3				31515.96290	31515.96345	-0.00055	0.00200	0.00000
19:	5	3	3	4	3	2				32517.49890	32517.49517	0.00373	0.00200	0.00000
20:	5	3	2	4	3	1				33001.84620	33001.85256	-0.00636	0.00200	0.00000
21:	6	1	6	5	1	5				33595.19470	33595.19684	-0.00214	0.00200	0.00000
22:	5	1	4	4	1	3				33799.22090	33799.22004	0.00086	0.00200	0.00000

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   23:   6  0  6  5  0  5                    33957.29670   33957.29658    0.00012    0.00200   0.00000
   24:   5  2  3  4  2  2                    34609.25890   34609.25690    0.00200    0.00200   0.00000
   25:   7  1  7  6  1  6                    38872.00990   38872.00726    0.00264    0.00200   0.00000
   26:   6  3  4  5  3  3                    39026.95020   39026.94884    0.00136    0.00200   0.00000
   27:   7  0  7  6  0  6                    39058.90610   39058.90747   -0.00137    0.00200   0.00000
   28:   6  1  5  5  1  4                    39654.59970   39654.60138   -0.00168    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99954E-01    3   2.24687E-01    4   1.01523E-01    5   4.99632E-01    6   8.16103E-01
    7   2.71172E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        8186.1763( 52)          -0.0000
   2         20000          B       3802.74581( 48)          0.00000
   3         30000          C       2596.43749( 33)         -0.00000
   4           200     -Del_J          -0.2900( 66)E-03      -0.0000E-03
   5          1100    -Del_JK          -1.3548(312)E-03       0.0000E-03
   6         40100     -del_J         -0.09194(306)E-03     -0.00000E-03
   7         41000     -del_K           -1.161( 94)E-03       -0.000E-03
 MICROWAVE AVG =        0.000015 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002186 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.09289         1.09289
```
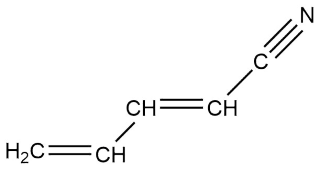

Molecule 107

IUPAC Name: (2E)-2,4-pentadienenitrile (anti)

Common name: 1-cyano-1,3-butadiene (anti-(2E))

SMILES: C=CC=CC#N



107: Fit file

	EXP.FREQ.								EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.		
1:	3	0	3	2	2	0	2	1			8434.35250	8434.35241	0.00009	0.00200	0.00000
2:	3	0	3	3	2	0	2	2			8434.51880	8434.51773	0.00107	0.00200	0.00000
3:	3	0	3	4	2	0	2	3			8434.55700	8434.55782	-0.00082	0.00200	0.00000
4:	4	1	4	4	3	1	3	3			11095.62950	11095.62992	-0.00042	0.00200	0.00000
5:	4	1	4	3	3	1	3	2			11095.71120	11095.71107	0.00013	0.00200	0.00000
6:	4	1	4	5	3	1	3	4			11095.76250	11095.76492	-0.00242	0.00200	0.00000
7:	4	0	4	3	3	0	3	2			11245.13720	11245.13655	0.00065	0.00200	0.00000
8:	4	0	4	4	3	0	3	3			11245.20330	11245.20680	-0.00350	0.00200	0.00000
9:	4	0	4	5	3	0	3	4			11245.23420	11245.23274	0.00146	0.00200	0.00000
10:	4	1	3	4	3	1	2	3			11397.62580	11397.62578	0.00002	0.00200	0.00000
11:	4	1	3	3	3	1	2	2			11397.72290	11397.72278	0.00012	0.00200	0.00000
12:	4	1	3	5	3	1	2	4			11397.75390	11397.75518	-0.00128	0.00200	0.00000
13:	5	0	5	4	4	0	4	3			14055.15890	14055.15752	0.00138	0.00200	0.00000
14:	5	0	5	5	4	0	4	4			14055.19680	14055.19595	0.00085	0.00200	0.00000
15:	5	0	5	6	4	0	4	5			14055.21580	14055.21436	0.00144	0.00200	0.00000
16:	5	1	4	5	4	1	3	4			14246.74590	14246.74501	0.00089	0.00200	0.00000
17:	5	1	4	4	4	1	3	3			14246.78380	14246.78523	-0.00143	0.00200	0.00000
18:	5	1	4	6	4	1	3	5			14246.81560	14246.81557	0.00003	0.00200	0.00000
19:	6	1	6	6	5	1	5	5			16642.64030	16642.64094	-0.00064	0.00200	0.00000
20:	6	1	6	5	5	1	5	4			16642.65460	16642.65461	-0.00001	0.00200	0.00000
21:	6	1	6	7	5	1	5	6			16642.68730	16642.68734	-0.00004	0.00200	0.00000
22:	6	0	6	5	5	0	5	4			16864.28440	16864.28672	-0.00232	0.00200	0.00000
23:	6	0	6	6	5	0	5	5			16864.31010	16864.31057	-0.00047	0.00200	0.00000
24:	6	0	6	7	5	0	5	6			16864.32550	16864.32454	0.00096	0.00200	0.00000
25:	6	1	5	6	5	1	4	5			17095.60440	17095.60627	-0.00187	0.00200	0.00000
26:	6	1	5	5	5	1	4	4			17095.62490	17095.62555	-0.00065	0.00200	0.00000
27:	6	1	5	7	5	1	4	6			17095.64950	17095.64983	-0.00033	0.00200	0.00000
28:	8	1	8	8	7	1	7	7			22188.53330	22188.53215	0.00115	0.00200	0.00000	22188.53343	-0.00013

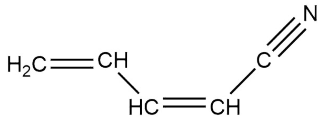
```
  29:   8  1  8  7  7  1  7  6              22188.53330   22188.53487   -0.00157    0.00200   0.00000   22188.53343   -0.00013
  30:   8  1  8  9  7  1  7  8              22188.55740   22188.55474    0.00266    0.00200   0.00000
  31:   8  1  7  8  7  1  6  7              22792.41060   22792.41079   -0.00019    0.00200   0.00000
  32:   8  0  8  7  7  0  7  6              22479.20630   22479.20939   -0.00309    0.00200   0.00000
  33:   8  0  8  8  7  0  7  7              22479.22000   22479.22044   -0.00044    0.00200   0.00000
  34:   8  0  8  9  7  0  7  8              22479.23260   22479.22977    0.00283    0.00200   0.00000
  35:   8  1  7  7  7  1  6  6              22792.41890   22792.41637    0.00253    0.00200   0.00000
  36:   8  1  7  9  7  1  6  8              22792.43450   22792.43168    0.00282    0.00200   0.00000
  37:  10  0 10  9  9  0  9  8              28088.54950   28088.54928    0.00022    0.00200   0.00000   28088.55221   -0.00271
  38:  10  0 10 10  9  0  9  9              28088.54950   28088.55485   -0.00535    0.00200   0.00000   28088.55221   -0.00271
  39:  10  0 10 11  9  0  9 10              28088.56490   28088.56204    0.00286    0.00200   0.00000
  40:  12  1 11 12 11  1 10 11              34181.01440   34181.01264    0.00176    0.00200   0.00000   34181.01577   -0.00137
  41:  12  1 11 11 11  1 10 10              34181.01440   34181.01339    0.00101    0.00200   0.00000   34181.01577   -0.00137
  42:  12  1 11 13 11  1 10 12              34181.01440   34181.02067   -0.00627    0.00200   0.00000   34181.01577   -0.00137
  43:  13  0 13 13 12  0 12 12              36489.15660   36489.15438    0.00222    0.00200   0.00000   36489.15598    0.00062
  44:  13  0 13 12 12  0 12 11              36489.15660   36489.15279    0.00381    0.00200   0.00000   36489.15598    0.00062
  45:  13  0 13 14 12  0 12 13              36489.15660   36489.16020   -0.00360    0.00200   0.00000   36489.15598    0.00062
  46:  14  1 14 14 13  1 13 13              38816.41520   38816.41366    0.00154    0.00200   0.00000   38816.41578   -0.00058
  47:  14  1 14 13 13  1 13 12              38816.41520   38816.41316    0.00204    0.00200   0.00000   38816.41578   -0.00058
  48:  14  1 14 15 13  1 13 14              38816.41520   38816.42002   -0.00482    0.00200   0.00000   38816.41578   -0.00058
  49:   2  1  2  3  3  0  3  4              16288.41390   16288.41389    0.00001    0.00200   0.00000
  50:   2  1  2  2  3  0  3  3              16288.86990   16288.86882    0.00108    0.00200   0.00000
  51:   1  1  1  2  0  0  0  1              27610.00450   27610.00451   -0.00001    0.00200   0.00000
  52:   1  1  1  1  0  0  0  1              27610.39010   27610.39119   -0.00109    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.45067E-01    3   2.95075E-04    4   7.16710E-01    5   1.00000E+00    6   9.82704E-01
    7   9.99995E-01    8   5.35173E-01    9   9.97269E-01   10   8.54030E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 26241.91858(127)          0.00000
   2         20000                    1443.611(145)           -0.001
   3         30000                    1368.129(145)            0.001
   4           200                      -0.118( 55)E-03        0.000E-03
   5          2000                 0.011600000(  0)E-18 -0.000000000E-18
   6          1100                     0.01580( 34)         -0.00000
   7         40100     -del_J         -0.01761(158)E-03      0.00001E-03
   8         41000     -del_K               5( 72)E-03            0E-03
   9     110010000     chi_aa          -3.3190(263)          -0.0000
  10     110020000     chi_bb           1.2895( 64)          -0.0000
 MICROWAVE AVG =       -0.000030 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001527 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.76364         0.76364
```

Molecule 108

IUPAC Name: (2Z)-2,4-pentadienenitrile (anti)

Common name: 1-cyano-1,3-butadiene (anti-(2Z))

SMILES: C=CC=CC#N



108: Fit file

EXP.FREQ.	-								CALC.FREQ.	-	DIFF.	- EXP.ERR.	- EST.ERR.	-AVG. CALC.FREQ.	- DIFF. - WT.
1:	2	0	2	1	1	0	1	0	7439.77480	7439.76864	0.00616	0.00200	0.00000		
2:	2	0	2	3	1	0	1	2	7439.85320	7439.85338	-0.00018	0.00200	0.00000		
3:	3	1	3	2	2	1	2	1	10639.96870	10639.96487	0.00383	0.00200	0.00000		
4:	3	1	3	3	2	1	2	2	10640.00510	10640.01298	-0.00788	0.00200	0.00000		
5:	3	1	3	4	2	1	2	3	10640.08010	10640.07563	0.00447	0.00200	0.00000		
6:	3	0	3	3	2	0	2	2	11130.10850	11130.10881	-0.00031	0.00200	0.00000		
7:	3	0	3	2	2	0	2	1	11130.13780	11130.14111	-0.00331	0.00200	0.00000		
8:	3	0	3	4	2	0	2	3	11130.15390	11130.15462	-0.00072	0.00200	0.00000		
9:	3	1	2	3	2	1	1	2	11700.23620	11700.24061	-0.00441	0.00200	0.00000		
10:	3	1	2	4	2	1	1	3	11700.26450	11700.26024	0.00426	0.00200	0.00000		
11:	3	1	2	2	2	1	1	1	11700.37660	11700.37561	0.00099	0.00200	0.00000		
12:	4	1	4	3	3	1	3	2	14173.35140	14173.35429	-0.00289	0.00200	0.00000		
13:	4	1	4	4	3	1	3	3	14173.36760	14173.36843	-0.00083	0.00200	0.00000		
14:	4	1	4	5	3	1	3	4	14173.41160	14173.40949	0.00211	0.00200	0.00000		
15:	4	0	4	4	3	0	3	3	14785.37460	14785.37515	-0.00055	0.00200	0.00000		
16:	4	0	4	3	3	0	3	2	14785.43470	14785.43142	0.00328	0.00200	0.00000	14785.43267	0.00203
17:	4	0	4	5	3	0	3	4	14785.43470	14785.43391	0.00079	0.00200	0.00000	14785.43267	0.00203
18:	4	1	3	4	3	1	2	3	15585.78530	15585.78963	-0.00433	0.00200	0.00000		
19:	4	1	3	5	3	1	2	4	15585.80840	15585.80444	0.00396	0.00200	0.00000		
20:	4	1	3	3	3	1	2	2	15585.85290	15585.85544	-0.00254	0.00200	0.00000		
21:	5	1	5	4	4	1	4	3	17696.01280	17696.01351	-0.00071	0.00200	0.00000	17696.01331	-0.00051
22:	5	1	5	5	4	1	4	4	17696.01280	17696.01310	-0.00030	0.00200	0.00000	17696.01331	-0.00051
23:	5	1	5	6	4	1	4	5	17696.04940	17696.04671	0.00269	0.00200	0.00000		
24:	5	0	5	5	4	0	4	4	18395.56310	18395.56352	-0.00042	0.00200	0.00000		
25:	5	0	5	4	4	0	4	3	18395.63280	18395.63569	-0.00289	0.00200	0.00000	18395.63509	-0.00229
26:	5	0	5	6	4	0	4	5	18395.63280	18395.63449	-0.00169	0.00200	0.00000	18395.63509	-0.00229
27:	5	1	4	5	4	1	3	4	19458.09940	19458.10102	-0.00162	0.00200	0.00000		
28:	5	1	4	6	4	1	3	5	19458.12010	19458.11860	0.00150	0.00200	0.00000		
29:	5	1	4	4	4	1	3	3	19458.15120	19458.14854	0.00266	0.00200	0.00000		

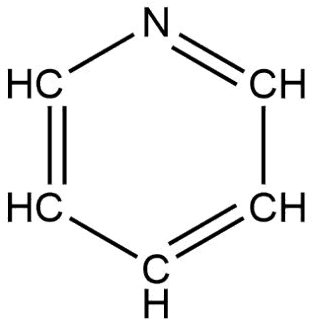
```
   30:   6  1  6  6  5  1  5  5              21206.15270   21206.15476   -0.00206    0.00200   0.00000
   31:   6  1  6  5  5  1  5  4              21206.16420   21206.16342    0.00078    0.00200   0.00000
   32:   6  1  6  7  5  1  5  6              21206.18580   21206.18553    0.00027    0.00200   0.00000
   33:   6  0  6  6  5  0  5  5              21953.29650   21953.29482    0.00168    0.00200   0.00000
   34:   6  0  6  5  5  0  5  4              21953.37690   21953.37830   -0.00140    0.00200   0.00000   21953.37704   -0.00014
   35:   6  0  6  7  5  0  5  6              21953.37690   21953.37578    0.00112    0.00200   0.00000   21953.37704   -0.00014
   36:   6  1  5  6  5  1  4  5              23312.92140   23312.92024    0.00116    0.00200   0.00000
   37:   6  1  5  7  5  1  4  6              23312.94220   23312.94270   -0.00050    0.00200   0.00000
   38:   6  1  5  5  5  1  4  4              23312.96180   23312.96309   -0.00129    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.50042E-01    3   2.17032E-01    4   1.96740E-01    5   1.00000E+00    6   8.98999E-01
    7   9.65799E-01    8   1.00000E+00    9   9.97971E-01   10   9.86713E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         9759.111( 91)            0.000
   2         20000          B       2039.68760( 34)         -0.00000
   3         30000          C      1686.177884(307)         0.000000
   4           200    Delta_J          -0.8215( 35)E-03       0.0000E-03
   5          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK         0.011264(234)         0.000000
   7         40100     -del_J         -0.24140(235)E-03      0.00000E-03
   8         41000     -del_K      0.138257511(  0)E-21  0.000000000E-21
   9     110010000     chi_aa           -0.3657( 76)          -0.0000
  10     110020000     chi_bb           -1.6425(207)          -0.0000
 MICROWAVE AVG =        0.000052 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002868 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.43389         1.43389
```

Molecule 109

IUPAC Name: azinine

Common name: pyridene, azabenzene

SMILES: C1=CC=NC=C1



109: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	3	2	1	3	3	2	2	3	8194.34790		8194.34854		-0.00064	0.00200	0.00000
2:	3	2	1	4	3	2	2	4	8194.51010		8194.50892		0.00118	0.00200	0.00000
3:	3	2	1	2	3	2	2	2	8194.56300		8194.56504		-0.00204	0.00200	0.00000
4:	2	1	1	2	2	1	2	3	8536.46230		8536.46557		-0.00327	0.00200	0.00000
5:	2	1	1	1	2	1	2	1	8536.55810		8536.55924		-0.00114	0.00200	0.00000
6:	2	1	1	3	2	1	2	3	8536.92710		8536.92544		0.00166	0.00200	0.00000
7:	2	1	1	2	2	1	2	2	8537.58340		8537.58454		-0.00114	0.00200	0.00000
8:	2	1	1	3	2	1	2	2	8538.04720		8538.04441		0.00279	0.00200	0.00000
9:	2	1	1	1	2	1	2	2	8538.29730		8538.30017		-0.00287	0.00200	0.00000
10:	1	0	1	1	0	0	0	1	8762.88880		8762.88877		0.00003	0.00200	0.00000
11:	1	0	1	2	0	0	0	1	8764.36610		8764.36238		0.00372	0.00200	0.00000
12:	1	0	1	0	0	0	0	1	8766.57120		8766.57296		-0.00176	0.00200	0.00000
13:	2	2	1	1	2	0	2	1	9251.81670		9251.81778		-0.00108	0.00200	0.00000
14:	2	2	1	3	2	0	2	3	9253.35800		9253.35988		-0.00188	0.00200	0.00000
15:	2	2	1	1	2	0	2	2	9253.67760		9253.67966		-0.00206	0.00200	0.00000
16:	2	2	1	2	2	0	2	1	9254.27690		9254.27376		0.00314	0.00200	0.00000
17:	2	2	1	3	2	0	2	2	9254.55840		9254.55677		0.00163	0.00200	0.00000
18:	2	2	1	2	2	0	2	3	9254.93530		9254.93876		-0.00346	0.00200	0.00000
19:	2	2	1	2	2	0	2	2	9256.13590		9256.13564		0.00026	0.00200	0.00000
20:	4	2	2	3	4	2	3	3	14654.30000		14654.30063		-0.00063	0.00200	0.00000
21:	4	2	2	5	4	2	3	5	14654.46010		14654.45742		0.00268	0.00200	0.00000
22:	4	2	2	4	4	2	3	4	14655.06690		14655.06683		0.00007	0.00200	0.00000
23:	2	1	2	2	1	1	1	1	14681.30210		14681.30179		0.00031	0.00200	0.00000

24:	2	1	2	2	1	1	1	2	14681.72980	14681.73094	-0.00114	0.00200	0.00000
25:	2	1	2	3	1	1	1	2	14682.85020	14682.84991	0.00029	0.00200	0.00000
26:	2	1	2	1	1	1	1	1	14683.04270	14683.04272	-0.00002	0.00200	0.00000
27:	2	1	2	1	1	1	1	0	14684.11550	14684.11565	-0.00015	0.00200	0.00000
28:	3	1	2	2	3	1	3	2	14752.84100	14752.84226	-0.00126	0.00200	0.00000
29:	3	1	2	4	3	1	3	4	14753.29140	14753.28852	0.00288	0.00200	0.00000
30:	3	1	2	3	3	1	3	3	14754.56320	14754.56326	-0.00006	0.00200	0.00000
31:	3	2	2	2	3	0	3	2	14822.34250	14822.34332	-0.00082	0.00200	0.00000
32:	3	2	2	4	3	0	3	4	14822.86270	14822.86025	0.00245	0.00200	0.00000
33:	3	2	2	3	3	0	3	3	14824.33740	14824.33725	0.00015	0.00200	0.00000
34:	4	3	2	3	4	1	3	3	14862.81210	14862.81353	-0.00143	0.00200	0.00000
35:	4	3	2	5	4	1	3	5	14863.06750	14863.06540	0.00210	0.00200	0.00000
36:	4	3	2	4	4	1	3	4	14864.04490	14864.04488	0.00002	0.00200	0.00000
37:	2	0	2	1	1	0	1	0	14901.45850	14901.45830	0.00020	0.00200	0.00000
38:	2	0	2	2	1	0	1	2	14901.80610	14901.80700	-0.00090	0.00200	0.00000
39:	2	0	2	3	1	0	1	2	14903.00460	14903.00388	0.00072	0.00200	0.00000
40:	2	0	2	2	1	0	1	1	14903.28150	14903.28061	0.00089	0.00200	0.00000
41:	2	0	2	1	1	0	1	1	14905.14180	14905.14249	-0.00069	0.00200	0.00000
42:	2	1	1	2	1	1	0	1	20372.67850	20372.67785	0.00065	0.00200	0.00000
43:	2	1	1	1	1	1	0	1	20373.39110	20373.39348	-0.00238	0.00200	0.00000
44:	2	1	1	2	1	1	0	2	20373.72010	20373.72216	-0.00206	0.00200	0.00000
45:	2	1	1	3	1	1	0	2	20374.18370	20374.18203	0.00167	0.00200	0.00000
46:	2	1	1	1	1	1	0	0	20376.00380	20376.00433	-0.00053	0.00200	0.00000
47:	5	2	3	4	5	2	4	4	20689.45910	20689.46040	-0.00130	0.00200	0.00000
48:	5	2	3	6	5	2	4	6	20689.62100	20689.61907	0.00193	0.00200	0.00000
49:	5	2	3	5	5	2	4	5	20690.39820	20690.39789	0.00031	0.00200	0.00000
50:	3	1	3	3	2	1	2	3	20708.31380	20708.31470	-0.00090	0.00200	0.00000
51:	3	1	3	3	2	1	2	2	20709.43410	20709.43367	0.00043	0.00200	0.00000
52:	3	1	3	2	2	1	2	1	20709.68460	20709.68382	0.00078	0.00200	0.00000
53:	3	1	3	4	2	1	2	3	20709.78940	20709.78944	-0.00004	0.00200	0.00000
54:	3	1	3	2	2	1	2	2	20711.42320	20711.42475	-0.00155	0.00200	0.00000
55:	4	1	3	3	4	1	4	3	20711.80480	20711.80660	-0.00180	0.00200	0.00000
56:	4	1	3	5	4	1	4	5	20712.11620	20712.11400	0.00220	0.00200	0.00000
57:	4	1	3	4	4	1	4	4	20713.30940	20713.30943	-0.00003	0.00200	0.00000
58:	3	2	2	3	2	2	1	2	26291.06440	26291.06439	0.00001	0.00200	0.00000
59:	3	2	2	4	2	2	1	3	26292.64750	26292.64324	0.00426	0.00200	0.00000
60:	3	2	2	2	2	2	1	1	26293.51970	26293.52053	-0.00083	0.00200	0.00000
61:	6	3	4	7	6	1	5	7	26624.26050	26624.25932	0.00118	0.00200	0.00000
62:	6	2	4	6	6	2	5	6	26624.28880	26624.28988	-0.00108	0.00200	0.00000
63:	6	3	4	6	6	1	5	6	26625.00540	26625.00721	-0.00181	0.00200	0.00000
64:	4	1	4	4	3	1	3	4	26632.52590	26632.52616	-0.00026	0.00200	0.00000
65:	4	0	4	4	3	0	3	4	26633.02440	26633.02511	-0.00071	0.00200	0.00000
66:	4	1	4	4	3	1	3	3	26634.00090	26634.00091	-0.00001	0.00200	0.00000
67:	4	1	4	3	3	1	3	2	26634.12300	26634.12302	-0.00002	0.00200	0.00000
68:	4	1	4	5	3	1	3	4	26634.20710	26634.20701	0.00009	0.00200	0.00000
69:	4	0	4	4	3	0	3	3	26634.50180	26634.50208	-0.00028	0.00200	0.00000
70:	4	0	4	3	3	0	3	2	26634.62140	26634.62126	0.00014	0.00200	0.00000
71:	4	0	4	5	3	0	3	4	26634.70650	26634.70600	0.00050	0.00200	0.00000

NORMALIZED DIAGONAL:

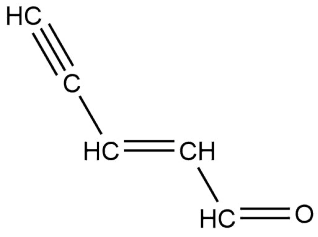
```
   1   1.00000E+00    2   8.32752E-01    3   3.03107E-01    4   9.82485E-01    5   2.14776E-01    6   4.60717E-01
   7   6.57098E-02    8   5.94649E-01    9   6.98610E-01   10   9.99675E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A       6039.24716( 45)         -0.00000
  2         20000          B       5804.91011( 38)          0.00000
  3         30000          C      2959.209676(172)        -0.000000
  4           200     -Del_J          -0.7644(200)E-03      -0.0000E-03
  5          1100    -Del_JK            0.649( 48)E-03        0.000E-03
  6          2000     -Del_K           -1.219( 47)E-03        0.000E-03
  7         40100     -del_J          -0.3261(107)E-03      -0.0000E-03
  8         41000     -del_K          -0.4922(118)E-03      -0.0000E-03
  9     110010000     chi_aa         -4.91224(147)         -0.00000
 10     110020000     chi_bb          1.43083(151)          0.00000
 MICROWAVE AVG =       -0.000038 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001592 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.79576         0.79576
```

Molecule 111

IUPAC Name: (E)-2-penten-4-ynal (anti)

Common name: 2-penten-4-ynal (anti-(E))

SMILES: C#CC=CC=O



111: Fit file

	EXP.FREQ.		CALC.FREQ.		DIFF.		EXP.ERR.-	EST.ERR.-AVG.	CALC.FREQ.	DIFF.	WT.	
1:	3	1	3	2	1	2		8215.50970	8215.51003	-0.00033	0.00200	0.00000
2:	3	0	3	2	0	2		8303.35360	8303.35400	-0.00040	0.00200	0.00000
3:	3	1	2	2	1	1		8391.96380	8391.96389	-0.00009	0.00200	0.00000
4:	4	1	4	3	1	3		10953.90680	10953.90710	-0.00030	0.00200	0.00000
5:	4	0	4	3	0	3		11070.74020	11070.74039	-0.00019	0.00200	0.00000
6:	4	1	3	3	1	2		11189.17560	11189.17588	-0.00028	0.00200	0.00000
7:	5	1	5	4	1	4		13692.21270	13692.21331	-0.00061	0.00200	0.00000
8:	5	0	5	4	0	4		13837.78540	13837.78544	-0.00004	0.00200	0.00000
9:	5	1	4	4	1	3		13986.29400	13986.29398	0.00002	0.00200	0.00000
10:	6	1	6	5	1	5		16430.40580	16430.40622	-0.00042	0.00200	0.00000
11:	6	0	6	5	0	5		16604.40380	16604.40393	-0.00013	0.00200	0.00000
12:	6	1	5	5	1	4		16783.29490	16783.29443	0.00047	0.00200	0.00000
13:	7	1	7	6	1	6		19168.46390	19168.46359	0.00031	0.00200	0.00000
14:	7	0	7	6	0	6		19370.51050	19370.51072	-0.00022	0.00200	0.00000
15:	7	1	6	6	1	5		19580.15350	19580.15333	0.00017	0.00200	0.00000
16:	8	1	8	7	1	7		21906.36350	21906.36341	0.00009	0.00200	0.00000
17:	8	0	8	7	0	7		22136.02160	22136.02082	0.00078	0.00200	0.00000
18:	8	1	7	7	1	6		22376.84890	22376.84655	0.00235	0.00200	0.00000
19:	9	1	8	8	1	7		25173.34840	25173.34970	-0.00130	0.00200	0.00000
20:	9	0	9	8	0	8		24900.84900	24900.84948	-0.00048	0.00200	0.00000
21:	10	0	10	9	0	9		27664.91210	27664.91231	-0.00021	0.00200	0.00000
22:	3	1	3	4	0	4		20012.26420	20012.26459	-0.00039	0.00200	0.00000
23:	6	1	6	7	0	7		11276.09130	11276.09113	0.00017	0.00200	0.00000
24:	5	1	5	6	0	6		14216.19580	14216.19562	0.00018	0.00200	0.00000
25:	4	1	4	5	0	5		17128.38620	17128.38625	-0.00005	0.00200	0.00000
26:	1	1	0	1	0	1		31288.33620	31288.33461	0.00159	0.00200	0.00000

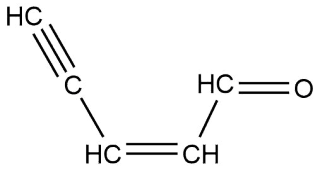
```
  27:   2  1  1  2  0  2                    31347.30470   31347.30461    0.00009    0.00200   0.00000
  28:   3  1  2  3  0  3                    31435.91440   31435.91450   -0.00010    0.00200   0.00000
  29:   4  1  3  4  0  4                    31554.35010   31554.35000    0.00010    0.00200   0.00000
  30:   5  1  4  5  0  5                    31702.85610   31702.85853   -0.00243    0.00200   0.00000
  31:   6  1  5  6  0  6                    31881.75240   31881.74903    0.00337    0.00200   0.00000
  32:   7  1  6  7  0  7                    32091.39000   32091.39165   -0.00165    0.00200   0.00000
  33:   1  1  1  0  0  0                    33997.41230   33997.41433   -0.00203    0.00200   0.00000
  34:   2  1  2  1  0  1                    36706.56170   36706.56054    0.00116    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.98026E-01    3   9.41604E-01    4   4.09082E-01    5   1.00000E+00    6   6.34404E-01
    7   5.00015E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                32642.84039( 89)          0.00000
   2         20000                1413.358852( 95)        -0.000000
   3         30000                1354.540010(123)        -0.000000
   4           200                   -0.09778( 65)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                   0.0171356(299)       -0.0000000
   7         40100                   -0.01200( 64)E-03     -0.00000E-03
   8         50000                -0.328707538(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000024 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001054 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.52709         0.52709
```

Molecule 112

IUPAC Name: (E)-2-penten-4-ynal (syn)

Common name: 2-penten-4-ynal (syn-(E))

SMILES: C#CC=CC=O



112: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	2	1	2	3	0	3				10500.92850		10500.92937		-0.00087		0.00200		0.00121
2:	1	1	1	2	0	2				13705.19520		13705.19506		0.00014		0.00200		0.00094
3:	1	1	0	1	0	1				20005.73350		20005.73298		0.00052		0.00200		0.00088
4:	2	1	1	2	0	2				20117.49320		20117.49329		-0.00009		0.00200		0.00077
5:	3	1	2	3	0	3				20286.00460		20286.00498		-0.00038		0.00200		0.00075
6:	4	1	3	4	0	4				20512.31290		20512.31147		0.00143		0.00200		0.00088
7:	5	1	4	5	0	5				20797.80070		20797.80003		0.00067		0.00200		0.00102
8:	6	1	5	6	0	6				21144.19340		21144.19740		-0.00400		0.00200		0.00105
9:	7	1	6	7	0	7				21553.56590		21553.56306		0.00284		0.00200		0.00105
10:	8	1	7	8	0	8				22028.27930		22028.27936		-0.00006		0.00200		0.00173
11:	1	1	1	0	0	0				22989.30550		22989.30571		-0.00021		0.00200		0.00107
12:	3	1	3	2	1	2				9117.35730		9117.35775		-0.00045		0.00200		0.00082
13:	3	0	3	2	0	2				9282.70300		9282.70310		-0.00010		0.00200		0.00069
14:	3	1	2	2	1	1				9451.21500		9451.21479		0.00021		0.00200		0.00065
15:	4	1	4	3	1	3				12155.92070		12155.92176		-0.00106		0.00200		0.00094
16:	4	0	4	3	0	3				12374.74880		12374.74834		0.00046		0.00200		0.00074
17:	4	1	3	3	1	2				12601.05570		12601.05483		0.00087		0.00200		0.00069
18:	5	1	5	4	1	4				15194.01550		15194.01352		0.00198		0.00200		0.00105
19:	5	0	5	4	0	4				15464.91870		15464.91848		0.00022		0.00200		0.00069
20:	5	1	4	4	1	3				15750.40460		15750.40704		-0.00244		0.00200		0.00064
21:	6	1	6	5	1	5				18231.51930		18231.51954		-0.00024		0.00200		0.00137
22:	6	1	5	5	1	4				18899.14430		18899.14492		-0.00062		0.00200		0.00072
23:	7	1	6	6	1	5				22047.13830		22047.13889		-0.00059		0.00200		0.00127
24:	6	0	6	5	0	5				18552.74780		18552.74755		0.00025		0.00200		0.00074
25:	7	0	7	6	0	6				21637.77420		21637.77323		0.00097		0.00200		0.00123

NORMALIZED DIAGONAL:

1 1.00000E+00 2 3.27858E-01 3 2.65678E-01 4 9.99886E-01 5 2.57259E-01 6 1.00000E+00
7 8.50946E-01 8 1.00000E+00

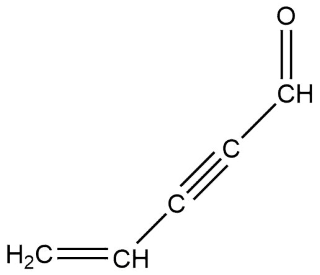
```
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A      21497.51569(103)         -0.00000
   2         20000          B      1603.073960(219)         0.000000
   3         30000          C      1491.786596(212)        -0.000000
   4           200    Delta_J         -0.15080(199)E-03      0.00000E-03
   5          1100   Delta_JK            1.980( 70)E-03       -0.000E-03
   6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   7         40100     -del_J         -0.01773(110)E-03      0.00000E-03
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000022 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001294 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        0.64706         0.64706
```

Molecule 113

IUPAC Name: (Z)-2-penten-4-ynal (anti)

Common name: 2-penten-4-ynal (anti-(Z))

SMILES: C=CC#CC=O



113: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 1 2 1 1 1									7045.89260		7045.89254		0.00006	0.00200	0.00000
2:	2 0 2 1 0 1									7380.91400		7380.91387		0.00013	0.00200	0.00000
3:	2 1 1 1 1 0									7738.63870		7738.64014		-0.00144	0.00200	0.00000
4:	3 1 3 2 1 2									10561.85290		10561.85323		-0.00033	0.00200	0.00000
5:	3 0 3 2 0 2									11043.14530		11043.14532		-0.00002	0.00200	0.00000
6:	3 1 2 2 1 1									11600.71680		11600.71689		-0.00009	0.00200	0.00000
7:	4 1 4 3 1 3									14069.75240		14069.75179		0.00061	0.00200	0.00000
8:	4 0 4 3 0 3									14671.97630		14671.97608		0.00022	0.00200	0.00000
9:	4 2 3 3 2 2									14775.87900		14775.87818		0.00082	0.00200	0.00000
10:	4 2 2 3 2 1									14888.18890		14888.18982		-0.00092	0.00200	0.00000
11:	4 1 3 3 1 2									15453.77770		15453.77726		0.00044	0.00200	0.00000
12:	5 1 5 4 1 4									17567.42330		17567.42374		-0.00044	0.00200	0.00000
13:	5 0 5 4 0 4									18257.73550		18257.73542		0.00008	0.00200	0.00000
14:	5 2 4 4 2 3									18455.58980		18455.58867		0.00113	0.00200	0.00000
15:	5 2 3 4 2 2									18678.04790		18678.04981		-0.00191	0.00200	0.00000
16:	5 1 4 4 1 3									19294.27470		19294.26967		0.00503	0.00200	0.00000
17:	6 1 6 5 1 5									21053.12670		21053.12694		-0.00024	0.00200	0.00000
18:	6 0 6 5 0 5									21793.18260		21793.18208		0.00052	0.00200	0.00000
19:	6 1 5 5 1 4									23118.16390		23118.16882		-0.00492	0.00200	0.00000
20:	7 1 7 6 1 6									24525.61080		24525.60985		0.00095	0.00200	0.00000
21:	7 0 7 6 0 6									25275.02990		25275.03086		-0.00096	0.00200	0.00000
22:	7 1 6 6 1 5									26920.86650		26920.86428		0.00222	0.00200	0.00000
23:	8 0 8 7 0 7									28705.11440		28705.11669		-0.00229	0.00200	0.00000
24:	9 0 9 8 0 8									32090.41580		32090.41587		-0.00007	0.00200	0.00000
25:	10 0 10 9 0 9									35441.56560		35441.56473		0.00087	0.00200	0.00000

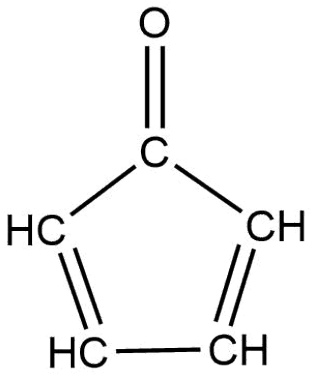
```
   26:   2  1  1  2  0  2                    8487.61710    8487.61799   -0.00089    0.00200   0.00000
   27:   1  1  1  0  0  0                   11479.63180   11479.63101    0.00079    0.00200   0.00000
   28:   3  1  3  2  0  2                   18010.34400   18010.34441   -0.00041    0.00200   0.00000
   29:   5  1  5  4  0  4                   23932.39910   23932.39854    0.00056    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   3.52195E-01    4   2.32614E-01    5   1.00000E+00    6   6.57428E-01
    7   9.78904E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 9804.73909(116)         -0.00000
   2         20000                2021.251266(250)         0.000000
   3         30000                1674.870266(145)         0.000000
   4           200                   -0.75973(139)E-03      0.00000E-03
   5          2000                -0.057532920(  0)E-24 -0.000000000E-24
   6          1100                    0.011897( 36)        -0.000000
   7         40100                   -0.22502(123)E-03     -0.00000E-03
   8         50000                 0.042658247(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000018 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001597 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.79843         0.79843
```

Molecule 114

IUPAC Name: 2,4-cyclopentadien-1-one

Common name: cyclopentadienone

SMILES: C1=CC(=O)C=C1



114: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	3 1 2 3 1 3									7670.99970		7670.99798		0.00172	0.00200	0.00000
2:	2 1 2 1 1 1									11906.93600		11906.93512		0.00088	0.00200	0.00000
3:	4 1 3 4 1 4									12622.06650		12622.06679		-0.00029	0.00200	0.00000
4:	2 0 2 1 0 1									12939.33170		12939.33151		0.00019	0.00200	0.00000
5:	2 1 1 1 1 0									14474.43060		14474.43048		0.00012	0.00200	0.00000
6:	3 1 3 2 1 2									17716.10570		17716.10576		-0.00006	0.00200	0.00000
7:	3 0 3 2 0 2									18838.35720		18838.35732		-0.00012	0.00200	0.00000
8:	3 2 2 2 2 1									19785.98110		19785.98145		-0.00035	0.00200	0.00000
9:	3 2 2 3 0 3									20616.87860		20616.87853		0.00007	0.00200	0.00000
10:	3 2 1 2 2 0									20733.63710		20733.63713		-0.00003	0.00200	0.00000
11:	3 1 2 2 1 1									21535.85870		21535.85837		0.00033	0.00200	0.00000
12:	4 2 3 4 0 4									22507.35370		22507.35387		-0.00017	0.00200	0.00000
13:	4 1 4 3 1 3									23391.66070		23391.66053		0.00017	0.00200	0.00000
14:	4 0 4 3 0 3									24293.44800		24293.44727		0.00073	0.00200	0.00000
15:	5 2 4 5 0 5									25412.58650		25412.58674		-0.00024	0.00200	0.00000
16:	4 2 3 3 2 2									26183.92240		26183.92262		-0.00022	0.00200	0.00000
17:	4 3 2 3 3 1									26803.38730		26803.38769		-0.00039	0.00200	0.00000
18:	4 3 1 3 3 0									26987.26750		26987.27227		-0.00477	0.00200	0.00000
19:	4 2 2 3 2 1									28268.53210		28268.53311		-0.00101	0.00200	0.00000
20:	4 1 3 3 1 2									28342.73080		28342.72934		0.00146	0.00200	0.00000
21:	5 0 5 4 0 4									29514.62680		29514.62672		0.00008	0.00200	0.00000
22:	5 2 4 4 2 3									32419.85840		32419.85959		-0.00119	0.00200	0.00000

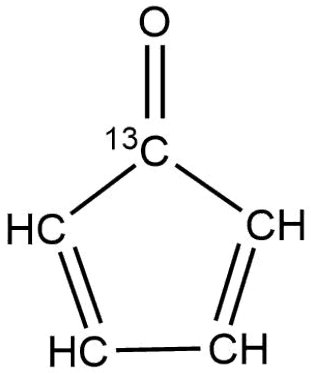
```
  23:   5  3  3  4  3  2                    33562.73290   33562.72631    0.00659    0.00200   0.00000
  24:   6  1  6  5  1  5                    34392.74500   34392.74567   -0.00067    0.00200   0.00000
  25:   6  0  6  5  0  5                    34702.75420   34702.75339    0.00081    0.00200   0.00000
  26:   5  1  4  4  1  3                    34753.04080   34753.04014    0.00066    0.00200   0.00000
  27:   5  2  3  4  2  2                    35856.19480   35856.19611   -0.00131    0.00200   0.00000
  28:   6  2  5  5  2  4                    38469.93960   38469.94134   -0.00174    0.00200   0.00000
NORMALIZED DIAGONAL:
   1   1.00000E+00    2   7.62005E-01    3   4.08475E-01    4   9.97394E-01    5   4.46286E-02    6   4.64232E-01
   7   3.12451E-01    8   8.49504E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000                  8152.1616( 69)           0.0000
  2         20000                 3939.549807(286)        -0.000000
  3         30000                 2655.799018(174)        -0.000000
  4           200                     -0.2442( 87)E-03       0.0000E-03
  5          2000                       -0.71(165)E-03        -0.00E-03
  6          1100                      -1.758( 35)E-03       -0.000E-03
  7         40100                      -0.0972( 39)E-03       0.0000E-03
  8         50000                      -0.0369( 33)E-03      -0.0000E-03
 MICROWAVE AVG =        0.000044 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001711 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.85530         0.85530
```

Molecule 116

IUPAC Name: 2,4-cyclopentadien-1-one (13C1)

Common name: cyclopentadienone (13C1)

SMILES: C1=CC(=O)C=C1



116: Fit file

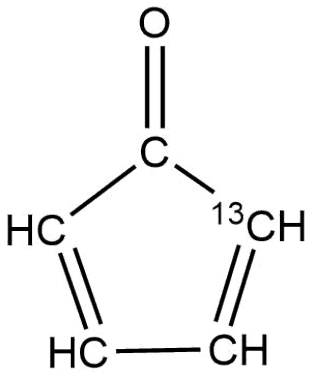
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                    12891.87070   12891.87233   -0.00163    0.00200   0.00072
    2:   2  1  1  1  1  0                    14412.76470   14412.76389    0.00081    0.00200   0.00117
    3:   3  1  3  2  1  2                    17655.37590   17655.37549    0.00041    0.00200   0.00195
    4:   3  0  3  2  0  2                    18776.19390   18776.19501   -0.00111    0.00200   0.00106
    5:   3  1  2  2  1  1                    21446.67450   21446.67441    0.00009    0.00200   0.00160
    6:   4  0  4  3  0  3                    24220.19720   24220.19633    0.00087    0.00200   0.00176
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.76934E-01    3   3.67512E-01    4   6.23865E-01    5   6.45597E-01    6   9.88712E-01
    7   8.97960E-01    8   9.97589E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  8152.5991(149)          -0.0000
   2         20000                 3921.68832( 48)         -0.00000
   3         30000                 2647.71626( 56)          0.00000
   4           200                    -0.2490( 83)E-03       0.0000E-03
   5          2000                   -0.01549(164)         -0.00000
   6          1100                     -1.669( 35)E-03       -0.000E-03
   7         40100                    -0.0836( 38)E-03      -0.0000E-03
   8         50000                    -0.0371( 33)E-03       0.0000E-03
 MICROWAVE AVG =       -0.000094 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000956 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        0.49704         0.49704
```

Molecule 117

IUPAC Name: 2,4-cyclopentadien-1-one (13C2)

Common name: cyclopentadienone (13C2)

SMILES: C1=CC(=O)C=C1



117: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                    11846.32160   11846.32050    0.00110    0.00200   0.00000
    2:   2  0  2  1  0  1                    12881.33220   12881.33260   -0.00040    0.00200   0.00000
    3:   2  1  1  1  1  0                    14453.06380   14453.06521   -0.00141    0.00200   0.00000
    4:   3  1  3  2  1  2                    17615.99290   17615.99400   -0.00110    0.00200   0.00000
    5:   3  0  3  2  0  2                    18718.57260   18718.57255    0.00005    0.00200   0.00000
    6:   3  1  2  2  1  1                    21490.67160   21490.67005    0.00155    0.00200   0.00000
    7:   4  1  3  3  1  2                    28252.77770   28252.77806   -0.00036    0.00200   0.00000
    8:   5  1  5  4  1  4                    28746.10200   28746.10172    0.00028    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.18417E-01    3   5.96388E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  7967.8951(129)           0.0000
   2         20000                 3939.11466( 37)          0.00000
   3         30000                2635.739193(281)        -0.000000
   4           200               -0.244217429(  0)E-03 -0.000000000E-03
   5          2000               -0.705171475(  0)E-03 -0.000000000E-03
   6          1100               -1.758031179(  0)E-03  0.000000000E-03
   7         40100               -0.097201081(  0)E-03 -0.000000000E-03
   8         50000               -0.036930690(  0)E-03 -0.000000000E-03
 MICROWAVE AVG =       -0.000037 MHz, IR AVG =        0.00000
```

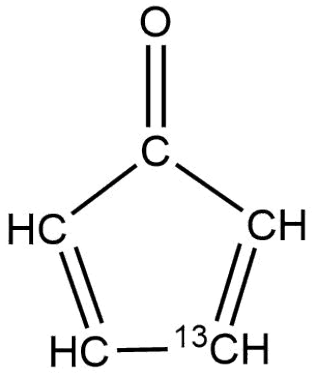
```
MICROWAVE RMS =        0.000947 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.47336         0.47336
```

Molecule 118

IUPAC Name: 2,4-cyclopentadien-1-one (13C3)

Common name: cyclopentadienone (13C3)

SMILES: C1=CC(=O)C=C1



118: Fit file

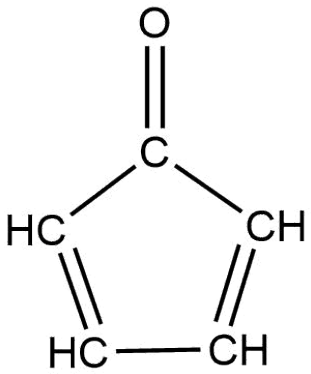
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                    11744.84210   11744.84298   -0.00088    0.00200   0.00000
    2:   2  0  2  1  0  1                    12760.82740   12760.82841   -0.00101    0.00200   0.00000
    3:   2  1  1  1  1  0                    14262.88100   14262.87856    0.00244    0.00200   0.00000
    4:   3  1  3  2  1  2                    17477.59960   17477.59898    0.00062    0.00200   0.00000
    5:   3  0  3  2  0  2                    18588.07430   18588.07374    0.00056    0.00200   0.00000
    6:   3  1  2  2  1  1                    21224.65090   21224.65245   -0.00155    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.61695E-01    3   5.85144E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  8081.7992(166)           0.0000
   2         20000                 3880.47935( 46)          0.00000
   3         30000                 2621.45845( 44)         -0.00000
   4           200               -0.244217429(  0)E-03 -0.000000000E-03
   5          2000               -0.705171475(  0)E-03 -0.000000000E-03
   6          1100               -1.758031179(  0)E-03  0.000000000E-03
   7         40100               -0.097201081(  0)E-03 -0.000000000E-03
   8         50000               -0.036930690(  0)E-03 -0.000000000E-03
 MICROWAVE AVG =        0.000031 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001343 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.67159         0.67159
```

Molecule 119

IUPAC Name: 2,4-cyclopentadien-1-one (ve1)

Common name: cyclopentadienone (ve1)

SMILES: C1=CC(=O)C=C1



119: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                    12943.66830   12943.66790    0.00040    0.00200   0.00000
    2:   3  0  3  2  0  2                    18844.87860   18844.87792    0.00068    0.00200   0.00000
    3:   4  0  4  3  0  3                    24302.83210   24302.83105    0.00105    0.00200   0.00000
    4:   5  0  5  4  0  4                    29527.96660   29527.96645    0.00015    0.00200   0.00000
    5:   2  1  2  1  1  1                    11913.42140   11913.42440   -0.00300    0.00200   0.00000
    6:   2  1  1  1  1  0                    14476.77870   14476.77836    0.00034    0.00200   0.00000
    7:   3  1  3  2  1  2                    17725.81280   17725.81294   -0.00014    0.00200   0.00000
    8:   3  1  2  2  1  1                    21539.28040   21539.27915    0.00125    0.00200   0.00000
    9:   4  1  4  3  1  3                    23404.63660   23404.63592    0.00068    0.00200   0.00000
   10:   4  1  3  3  1  2                    28347.01020   28347.00838    0.00182    0.00200   0.00000
   11:   5  1  5  4  1  4                    28957.75130   28957.75152   -0.00022    0.00200   0.00000
   12:   6  1  6  5  1  5                    34412.75380   34412.75491   -0.00111    0.00200   0.00000
   13:   6  0  6  5  0  5                    34720.70650   34720.70472    0.00178    0.00200   0.00000
   14:   5  1  4  4  1  3                    34757.85730   34757.86043   -0.00313    0.00200   0.00000
   15:   7  0  7  6  0  6                    39952.64940   39952.64985   -0.00045    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.93992E-01    3   4.69926E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  8135.7930( 58)          -0.0000
   2         20000                 3939.619104(265)         0.000000
```

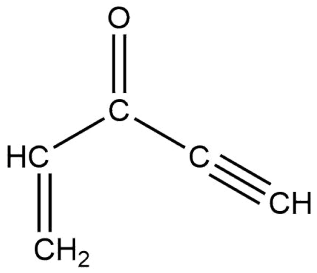
```
  3         30000                 2657.939010(158)         0.000000
  4           200                -0.244217429(  0)E-03  0.000000000E-03
  5          2000                -0.705171475(  0)E-03 -0.000000000E-03
  6          1100                -1.758031179(  0)E-03 -0.000000000E-03
  7         40100                -0.097201081(  0)E-03 -0.000000000E-03
  8         50000                -0.036930690(  0)E-03 -0.000000000E-03
MICROWAVE AVG =        0.000008 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001430 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.71524         0.71524
```

Molecule 120

IUPAC Name: 1-penten-4-yn-3-one (anti)

Common name: ethynyl vinyl ketone (anti)

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



120: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  2  3  0  3                      8919.83480    8919.83471    0.00009    0.00200   0.00000
 ***** NEXT LINE NOT USED IN FIT
    2:   3  0  3  2  0  2                     10563.76640   14728.75906 -999.99999    0.00200   0.00000
    3:   3  0  3  2  1  2                     14115.60020   14115.60189   -0.00169    0.00200   0.00000
 ***** NEXT LINE NOT USED IN FIT
    4:   4  0  4  3  0  3                     14728.75730   18749.02053 -999.99999    0.00200   0.00000
    5:   4  0  4  3  0  3                     18749.01880   18749.02053   -0.00173    0.00200   0.00000
    6:   4  0  4  3  1  3                     18558.11150   18558.11006    0.00144    0.00200   0.00000
    7:   4  1  4  3  0  3                     18797.76870   18797.76927   -0.00057    0.00200   0.00000
    8:   5  0  5  4  1  4                     22792.07850   22792.07758    0.00092    0.00200   0.00000
    9:   5  1  5  4  0  4                     22852.01150   22852.01183   -0.00033    0.00200   0.00000
   10:   2  1  2  1  0  1                     11176.92480   11176.92413    0.00067    0.00200   0.00000
   11:   1  1  1  0  0  0                      7028.87360    7028.87404   -0.00044    0.00200   0.00000
   12:   2  0  2  1  1  1                      9180.02100    9180.02075    0.00025    0.00200   0.00000
   13:   3  1  3  2  0  2                     14919.66980   14919.66952    0.00028    0.00200   0.00000
   14:   2  2  1  2  1  2                      8642.41360    8642.41520   -0.00160    0.00200   0.00000
   15:   2  2  1  1  1  0                     16938.51390   16938.51254    0.00136    0.00200   0.00000
   16:   2  2  0  1  1  1                     19162.03290   19162.03257    0.00033    0.00200   0.00000
    2 Lines rejected from fit
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.70575E-01    3   9.96268E-01    4   4.60214E-02    5   1.23340E-01    6   3.01757E-01
    7   3.78759E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       4954.85077(209)          0.00000
```

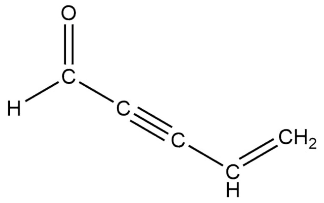
```
  2         20000          B       3571.11215(134)         -0.00000
  3         30000          C      2074.023896(270)         0.000000
  4           200    Delta_J           -2.052( 51)E-03        0.000E-03
  5          1100   Delta_JK            7.267(311)E-03       -0.000E-03
  6          2000    Delta_K        -0.010779(288)         0.000000
  7         40100     -del_J          -0.9591(309)E-03       0.0000E-03
  8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
MICROWAVE AVG =       -0.000074 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001018 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.50889         0.50889
```

Molecule 121

IUPAC Name: 4-penten-2-ynal (syn)

Common name: 4-penten-2-ynal (syn)

SMILES: C=CC#CC=O



121: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                      8127.74120    8127.74255   -0.00135    0.00200   0.00000
    2:   3  0  3  2  0  2                      8273.15590    8273.15644   -0.00054    0.00200   0.00000
    3:   3  1  2  2  1  1                      8421.59070    8421.59076   -0.00006    0.00200   0.00000
    4:   4  1  4  3  1  3                     10836.49890   10836.49889    0.00001    0.00200   0.00000
    5:   4  0  4  3  0  3                     11028.96950   11028.97027   -0.00077    0.00200   0.00000
    6:   4  1  3  3  1  2                     11228.27910   11228.27879    0.00031    0.00200   0.00000
    7:   5  1  5  4  1  4                     13544.83750   13544.83741    0.00009    0.00200   0.00000
    8:   5  0  5  4  0  4                     13783.15320   13783.15268    0.00052    0.00200   0.00000
    9:   5  1  4  4  1  3                     14034.52640   14034.52763   -0.00123    0.00200   0.00000
   10:   6  1  6  5  1  5                     16252.65770   16252.65761    0.00009    0.00200   0.00000
   11:   6  0  6  5  0  5                     16535.30140   16535.29856    0.00284    0.00200   0.00000
   12:   6  1  5  5  1  4                     16840.22350   16840.22375   -0.00025    0.00200   0.00000
   13:   7  1  7  6  1  6                     18959.86240   18959.86164    0.00076    0.00200   0.00000
   14:   7  0  7  6  0  6                     19285.00500   19285.00613   -0.00113    0.00200   0.00000
   15:   7  1  6  6  1  5                     19645.25220   19645.25112    0.00108    0.00200   0.00000
   16:   8  0  8  7  0  7                     22031.87820   22031.87910   -0.00090    0.00200   0.00000
   17:   9  0  9  8  0  8                     24775.52930   24775.52956   -0.00026    0.00200   0.00000
   18:   4  1  3  4  0  4                     18413.65470   18413.65465    0.00005    0.00200   0.00000
   19:   4  1  4  3  0  3                     28463.13910   28463.13928   -0.00018    0.00200   0.00000
   20:   2  1  1  2  0  2                     18065.91270   18065.91182    0.00088    0.00200   0.00000
   21:   3  1  2  3  0  3                     18214.34540   18214.34614   -0.00074    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.43953E-01    3   3.93987E-01    4   9.99574E-01    5   1.00000E+00    6   6.74295E-01
    7   9.78668E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                19297.55870(159)          0.00000
```

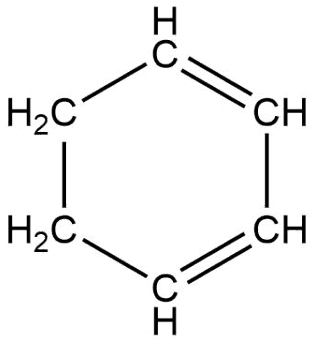
```
  2         20000                 1428.109140(237)         0.000000
  3         30000                 1330.155242(185)         0.000000
  4           200                    -0.28194(115)E-03     -0.00000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                    0.025825( 88)        -0.000000
  7         40100                    -0.05767(143)E-03      0.00000E-03
  8         50000                -0.328707538(  0)E-24  0.000000000E-24
MICROWAVE AVG =       -0.000038 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000926 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.46304         0.46304
```

Molecule 122

IUPAC Name: 1,3-cyclohexadiene

Common name: 1,3-cyclohexadiene

SMILES: C1CC=CC=C1

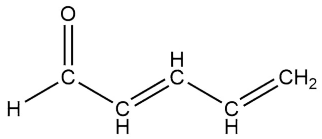


Molecule 123

IUPAC Name: (2E)-2,4-pentadienal (syn)

Common name: 2,4-pentadienal (syn-(2E))

SMILES: C=CC=CC=O



123: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  1  0  1  0  1                    12575.65420   12575.65066    0.00354    0.00200   0.00000
    2:   2  1  1  2  0  2                    12743.99690   12743.99647    0.00043    0.00200   0.00000
    3:   3  1  2  3  0  3                    12999.62760   12999.63502   -0.00742    0.00200   0.00000
    4:   4  1  3  4  0  4                    13346.29410   13346.28888    0.00522    0.00200   0.00000
    5:   5  1  4  5  0  5                    13788.88090   13788.87589    0.00501    0.00200   0.00000
    6:   2  1  2  1  0  1                    18374.61110   18374.60787    0.00323    0.00200   0.00000
    7:   3  1  3  2  0  2                    21191.40500   21191.40655   -0.00155    0.00200   0.00000
    8:   4  1  4  3  0  3                    23927.60460   23927.61305   -0.00845    0.00200   0.00000
    9:   6  1  6  5  0  5                    29173.02260   29173.02260    0.00000    0.00200   0.00000
   10:   3  1  3  2  1  2                     8947.36170    8947.36376   -0.00206    0.00200   0.00000
   11:   3  0  3  2  0  2                     9191.67420    9191.66848    0.00572    0.00200   0.00000
   12:   3  1  2  2  1  1                     9447.30490    9447.30703   -0.00213    0.00200   0.00000
   13:   4  1  4  3  1  3                    11927.87540   11927.87498    0.00042    0.00200   0.00000
   14:   4  0  4  3  0  3                    12247.76870   12247.76349    0.00521    0.00200   0.00000
   15:   4  1  3  3  1  2                    12594.40620   12594.41735   -0.01115    0.00200   0.00000
   16:   5  1  5  4  1  4                    14906.75670   14906.75154    0.00516    0.00200   0.00000
   17:   5  0  5  4  0  4                    15297.20580   15297.20177    0.00403    0.00200   0.00000
   18:   5  1  4  4  1  3                    15739.78070   15739.78878   -0.00808    0.00200   0.00000
   19:   6  1  6  5  1  5                    17883.63460   17883.62327    0.01133    0.00200   0.00000
   20:   6  0  6  5  0  5                    18338.37480   18338.37312    0.00168    0.00200   0.00000
   21:   7  0  7  6  0  6                    21369.73810   21369.73908   -0.00098    0.00200   0.00000
   22:   8  0  8  7  0  7                    24389.87710   24389.88050   -0.00340    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.74830E-01    3   9.91708E-01    4   4.42954E-01    5   1.00000E+00    6   5.67742E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                14025.37112(107)          0.00000
   2         20000                1616.385315(152)         0.000000
```

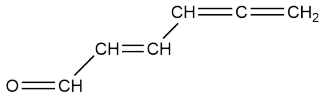
```
  3         30000                 1449.734085(130)         0.000000
  4           200                    -0.19970(147)E-03      0.00000E-03
  5          2000                 1.765680624(  0)E-21 -0.000000000E-21
  6          1100                      6.814( 54)E-03       -0.000E-03
  7         40100                -0.291686973(  0)E-24 -0.000000000E-24
  8         50000                -0.212827842(  0)E-21  0.000000000E-21
MICROWAVE AVG =        0.000262 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.005432 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        2.71608         2.71608
```

Molecule 124

IUPAC Name: (2E)-2,4,5-hexatrienal (anti)

Common name: 2,4,5-hexatrienal (anti-(2E))

SMILES: C=C=CC=CC=O



124: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   4  0  4  3  0  3                      6856.34530    6856.34543   -0.00013    0.00200   0.00000
    2:   5  0  5  4  0  4                      8570.16530    8570.16508    0.00022    0.00200   0.00000
    3:   6  0  6  5  0  5                     10283.80660   10283.80696   -0.00036    0.00200   0.00000
    4:   7  0  7  6  0  6                     11997.23530   11997.23555   -0.00025    0.00200   0.00000
    5:   8  0  8  7  0  7                     13710.41590   13710.41536    0.00054    0.00200   0.00000
    6:   9  0  9  8  0  8                     15423.31110   15423.31096    0.00014    0.00200   0.00000
    7:  10  0 10  9  0  9                     17135.88680   17135.88702   -0.00022    0.00200   0.00000
    8:   4  1  4  3  1  3                      6796.12380    6796.12643   -0.00263    0.00200   0.00000
    9:   5  1  5  4  1  4                      8495.08500    8495.08673   -0.00173    0.00200   0.00000
   10:   6  1  6  5  1  5                     10193.99760   10193.99962   -0.00202    0.00200   0.00000
   11:   7  1  7  6  1  6                     11892.85350   11892.85577   -0.00227    0.00200   0.00000
   12:   8  1  8  7  1  7                     13591.65180   13591.64590    0.00590    0.00200   0.00000
   13:   4  1  3  3  1  2                      6917.24880    6917.24505    0.00375    0.00200   0.00000
   14:   5  1  4  4  1  3                      8646.48770    8646.48467    0.00303    0.00200   0.00000
   15:   6  1  5  5  1  4                     10375.67760   10375.67639    0.00121    0.00200   0.00000
   16:   7  1  6  6  1  5                     12104.80970   12104.81049   -0.00079    0.00200   0.00000
   17:   8  1  7  7  1  6                     13833.87320   13833.87718   -0.00398    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.20782E-01    3   3.92260E-01    4   1.38546E-01    5   9.89305E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            20669( 34)               0
   2         20000          B       872.227548(174)        -0.000000
   3         30000          C       841.947855(174)        -0.000000
   4           200    Delta_J         -0.03556(213)E-03     -0.00000E-03
   5          1100   Delta_JK            7.831(209)E-03        0.000E-03
   6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   7         40100     -del_J     -0.697612116(  0)E-24  0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
```

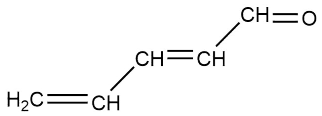
```
MICROWAVE AVG =        0.000023 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002373 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.18629         1.18629
```

Molecule 125

IUPAC Name: (2E)-2,4-pentadienal (anti)

Common name: 2,4-pentadienal (anti-(2E))

SMILES: C=CC=CC=O



125: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  0  3  2  0  2                    7882.77630    7882.77514    0.00116    0.00200   0.00000
    2:   3  1  2  2  1  1                    7973.26930    7973.26687    0.00243    0.00200   0.00000
    3:   4  1  4  3  1  3                   10390.50850   10390.50865   -0.00015    0.00200   0.00000
    4:   4  0  4  3  0  3                   10509.89510   10509.89498    0.00012    0.00200   0.00000
    5:   5  1  5  4  1  4                   12987.93960   12987.94014   -0.00054    0.00200   0.00000
    6:   5  0  5  4  0  4                   13136.61030   13136.61039   -0.00009    0.00200   0.00000
    7:   5  1  4  4  1  3                   13288.43020   13288.42802    0.00218    0.00200   0.00000
    8:   6  1  6  5  1  5                   15585.24160   15585.24177   -0.00017    0.00200   0.00000
    9:   6  0  6  5  0  5                   15762.82070   15762.82036    0.00034    0.00200   0.00000
   10:   6  1  5  5  1  4                   15945.82440   15945.82403    0.00037    0.00200   0.00000
   11:   7  1  7  6  1  6                   18182.38660   18182.38811   -0.00151    0.00200   0.00000
   12:   7  0  7  6  0  6                   18388.42150   18388.42399   -0.00249    0.00200   0.00000
   13:   7  1  6  6  1  5                   18603.05820   18603.06112   -0.00292    0.00200   0.00000
   14:   8  0  8  7  0  7                   21013.32210   21013.32061    0.00149    0.00200   0.00000
   15:   9  1  9  8  1  8                   23376.11660   23376.11494    0.00166    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.85455E-01    3   3.36440E-01    4   2.23707E-01    5   1.00000E+00    6   9.58707E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    28424.6(210)             -0.0
   2         20000                1343.912376(223)         0.000000
   3         30000                1283.814364(224)        -0.000000
   4           200                   -0.05012(193)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                      1.258(234)E-03        0.000E-03
   7         40100                -0.047468413(  0)E-24 -0.000000000E-24
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000125 MHz, IR AVG =        0.00000
```

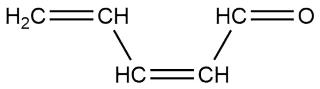
```
MICROWAVE RMS =        0.001518 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.75898         0.75898
```

Molecule 126

IUPAC Name: (2Z)-2,4-pentadienal (anti)

Common name: 2,4-pentadienal (anti-(2Z))

SMILES: C=CC=CC=O



126: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                     8899.80750    8899.80572    0.00178    0.00200   0.00000
    2:   3  0  3  2  0  2                     9123.11870    9123.11964   -0.00094    0.00200   0.00000
    3:   3  1  2  2  1  1                     9355.05950    9355.05902    0.00048    0.00200   0.00000
    4:   4  1  4  3  1  3                    11864.92700   11864.92721   -0.00021    0.00200   0.00000
    5:   4  0  4  3  0  3                    12158.22590   12158.22615   -0.00025    0.00200   0.00000
    6:   4  2  3  3  2  2                    12170.09070   12170.09230   -0.00160    0.00200   0.00000
    7:   4  2  2  3  2  1                    12182.77390   12182.76953    0.00437    0.00200   0.00000
    8:   4  1  3  3  1  2                    12471.89350   12471.89399   -0.00049    0.00200   0.00000
    9:   5  1  5  4  1  4                    14828.79810   14828.79964   -0.00154    0.00200   0.00000
   10:   5  0  5  4  0  4                    15188.26040   15188.26017    0.00023    0.00200   0.00000
   11:   5  2  4  4  2  3                    15210.99790   15210.99877   -0.00087    0.00200   0.00000
   12:   5  2  3  4  2  2                    15236.33500   15236.33625   -0.00125    0.00200   0.00000
   13:   5  1  4  4  1  3                    15587.40810   15587.40793    0.00017    0.00200   0.00000
   14:   6  1  6  5  1  5                    17791.13460   17791.13537   -0.00077    0.00200   0.00000
   15:   6  0  6  5  0  5                    18211.98290   18211.98276    0.00014    0.00200   0.00000
   16:   6  1  5  5  1  4                    18701.24540   18701.24559   -0.00019    0.00200   0.00000
   17:   7  1  7  6  1  6                    20751.66440   20751.66294    0.00146    0.00200   0.00000
   18:   7  0  7  6  0  6                    21228.19450   21228.19371    0.00079    0.00200   0.00000
   19:   7  1  6  6  1  5                    21813.03590   21813.03494    0.00096    0.00200   0.00000
   20:   8  1  8  7  1  7                    23710.12950   23710.12992   -0.00042    0.00200   0.00000
   21:   8  0  8  7  0  7                    24235.75730   24235.75752   -0.00022    0.00200   0.00000
   22:   8  1  7  7  1  6                    24922.38230   24922.38360   -0.00130    0.00200   0.00000
   23:   9  0  9  8  0  8                    27233.63750   27233.63755   -0.00005    0.00200   0.00000
   24:   9  1  8  8  1  7                    28028.87530   28028.87538   -0.00008    0.00200   0.00000
   25:  10  1  9  9  1  8                    31132.06720   31132.06678    0.00042    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.51111E-01    3   4.13330E-01    4   2.74863E-01    5   9.65906E-01    6   1.00000E+00
    7   9.97950E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
```

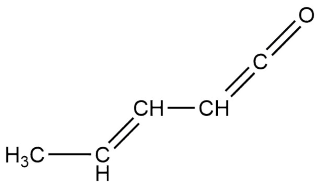
```
  1         10000          A        15139.288(299)            0.000
  2         20000          B      1597.246235(236)         0.000000
  3         30000          C      1445.490775(262)        -0.000000
  4           200    Delta_J         -0.17436( 99)E-03      0.00000E-03
  5          1100   Delta_JK            5.480( 43)E-03       -0.000E-03
  6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
  7         40100     -del_J         -0.02992(105)E-03     -0.00000E-03
  8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000025 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001225 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.61231         0.61231
```

Molecule 127

IUPAC Name: (3E)-1,3-pentadien-1-one (anti)

Common name: 1,3-pentadien-1-one (anti-(3E)), trans-propenylketene

SMILES: CC=CC=C=O



127: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	3 0 3 2 0 2							7797.27010		7797.27327		-0.00317		0.00200	0.00067
2:	3 0 3 2 0 2							7797.27640		7797.27327		0.00313		0.00200	0.00067
3:	4 1 4 3 1 3							10268.81950		10268.83392		-0.01442		0.00200	0.00096
4:	4 1 4 3 1 3							10268.86890		10268.83392		0.03498		0.00200	0.00096
5:	4 0 4 3 0 3							10395.67380		10395.67850		-0.00470		0.00200	0.00075
6:	4 0 4 3 0 3							10395.68540		10395.67850		0.00690		0.00200	0.00075
7:	4 1 3 3 1 2							10525.04030		10525.08620		-0.04590		0.00200	0.00095
8:	4 1 3 3 1 2							10525.10900		10525.08620		0.02280		0.00200	0.00095
9:	5 1 5 4 1 4							12835.73820		12835.75015		-0.01195		0.00200	0.00084
10:	5 1 5 4 1 4							12835.75970		12835.75015		0.00955		0.00200	0.00084
11:	5 0 5 4 0 4							12993.49060		12993.49596		-0.00536		0.00200	0.00074
12:	5 0 5 4 0 4							12993.50220		12993.49596		0.00624		0.00200	0.00074
13:	5 1 4 4 1 3							13156.04370		13156.06277		-0.01907		0.00200	0.00084
14:	5 1 4 4 1 3							13156.08770		13156.06277		0.02493		0.00200	0.00084
15:	6 1 6 5 1 5							15402.46100		15402.47265		-0.01165		0.00200	0.00118
16:	6 1 6 5 1 5							15402.47260		15402.47265		-0.00005		0.00200	0.00118
17:	6 0 6 5 0 5							15590.56960		15590.57899		-0.00939		0.00200	0.00066
18:	6 0 6 5 0 5							15590.58640		15590.57899		0.00741		0.00200	0.00066
19:	6 1 5 5 1 4							15786.82940		15786.84159		-0.01219		0.00200	0.00117
20:	6 1 5 5 1 4							15786.86430		15786.84159		0.02271		0.00200	0.00117
21:	7 0 7 6 0 6							18186.77260		18186.78124		-0.00864		0.00200	0.00073
22:	7 0 7 6 0 6							18186.78760		18186.78124		0.00636		0.00200	0.00073
23:	8 0 8 7 0 7							20781.94620		20781.95692		-0.01072		0.00200	0.00122
24:	8 0 8 7 0 7							20781.96950		20781.95692		0.01258		0.00200	0.00122

NORMALIZED DIAGONAL:

1 1.00000E+00 2 4.21833E-01 3 4.03534E-01 4 9.62731E-02 5 9.93174E-01 6 1.00000E+00
7 1.00000E+00 8 1.00000E+00

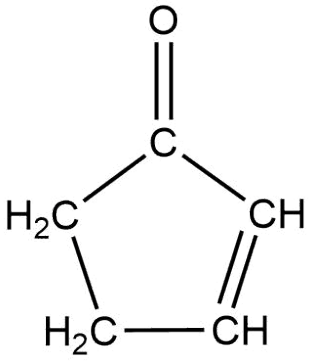
```
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A          22708.3(185)              0.0
   2         20000          B      1331.675485(174)        -0.000000
   3         30000          C      1267.612113(174)        -0.000000
   4           200    Delta_J          -0.1336( 48)E-03      -0.0000E-03
   5          1100   Delta_JK         0.016426(251)         0.000000
   6          2000    Delta_K      0.060148253(  0)E-21 -0.000000000E-21
   7         40100     -del_J      0.390714074(  0)E-24  0.000000000E-24
   8         41000     -del_K     -0.129449902(  0)E-21 -0.000000000E-21
 MICROWAVE AVG =        0.000015 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.016790 MHz, IR RMS =        0.00000
 END OF ITERATION  2 OLD, NEW RMS ERROR=        8.39511         8.39511
```

Molecule 128

IUPAC Name: 2-cyclopenten-1-one

Common name: 2-cyclopentenone

SMILES: C1CC(=O)C=C1



128: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                    11064.00880   11063.99956    0.00924    0.00200   0.00000
    2:   2  0  2  1  0  1                    11954.86090   11954.84430    0.01660    0.00200   0.00000
    3:   2  1  1  1  1  0                    13251.57600   13251.57334    0.00266    0.00200   0.00000
    4:   3  1  3  2  1  2                    16479.06100   16479.05970    0.00130    0.00200   0.00000
    5:   3  0  3  2  0  2                    17467.24460   17467.23303    0.01157    0.00200   0.00000
    6:   3  2  1  2  2  0                    19006.08470   19006.09392   -0.00922    0.00200   0.00000
    7:   3  1  2  2  1  1                    19736.38050   19736.39369   -0.01319    0.00200   0.00000
    8:   4  1  4  3  1  3                    21784.17740   21784.18513   -0.00773    0.00200   0.00000
    9:   4  0  4  3  0  3                    22603.15040   22603.15064   -0.00024    0.00200   0.00000
   10:   4  2  3  3  2  2                    24156.55290   24156.54694    0.00596    0.00200   0.00000
   11:   4  2  2  3  2  1                    25866.36730   25866.36186    0.00544    0.00200   0.00000
   12:   5  1  5  4  1  4                    26983.59880   26983.61178   -0.01298    0.00200   0.00000
   13:   5  0  5  4  0  4                    27523.51480   27523.52590   -0.01110    0.00200   0.00000
   14:   6  1  6  5  1  5                    32098.17240   32098.16647    0.00593    0.00200   0.00000
   15:   6  0  6  5  0  5                    32400.97530   32400.96816    0.00714    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99406E-01    3   2.66969E-01    4   8.25971E-02    5   1.00000E+00    6   4.73473E-01
    7   1.72667E-01    8   8.33318E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  7410.1735( 81)          -0.0000
   2         20000                 3586.34025( 67)          0.00000
```

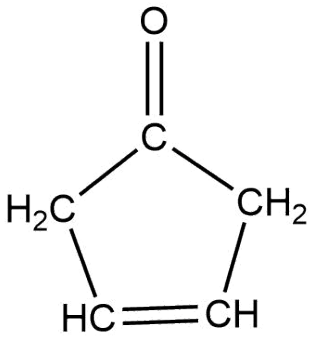
```
  3         30000                  2492.55005( 39)         -0.00000
  4           200                      0.0169(159)E-03       0.0000E-03
  5          2000                -1.530050170(  0)E-21 -0.000000000E-21
  6          1100                       1.326(151)E-03       -0.000E-03
  7         40100                      -0.1035( 87)E-03      -0.0000E-03
  8         50000                      -0.5244( 91)E-03      -0.0000E-03
MICROWAVE AVG =        0.000758 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.009185 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        4.59259         4.59259
```

Molecule 131

IUPAC Name: 3-cyclopenten-1-one

Common name: 3-cyclopentenone

SMILES: C1C=CCC1=O



131: Fit file

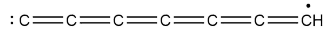
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                    11125.95850   11125.95932   -0.00082    0.00200   0.00000
    2:   2  0  2  1  0  1                    12025.60210   12025.59364    0.00846    0.00200   0.00000
    3:   2  1  1  1  1  0                    13349.18910   13349.19167   -0.00257    0.00200   0.00000
    4:   3  1  3  2  1  2                    16567.02100   16567.02204   -0.00104    0.00200   0.00000
    5:   3  0  3  2  0  2                    17554.88150   17554.88384   -0.00234    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.53508E-01    3   5.46145E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  7378.3192(170)           0.0000
   2         20000                 3615.20196( 73)          0.00000
   3         30000                 2503.58579( 49)          0.00000
   4           200               -1.736283902(  0)E-24 -0.000000000E-24
   5          2000               -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                0.054854237(  0)E-21  0.000000000E-21
   7         40100               -0.328666732(  0)E-24  0.000000000E-24
   8         50000               -0.212827842(  0)E-21  0.000000000E-21
 MICROWAVE AVG =        0.000338 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.004134 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        2.06686         2.06686
```

Molecule 132

IUPAC Name: 1,2,3,4,5,6-heptahexaene-1,1,7-trienyl radical

Common name: 1,2,3,4,5,6-heptahexaene-1,1,7-trienyl radical

SMILES: [C]=C=C=C=C=C=[CH]

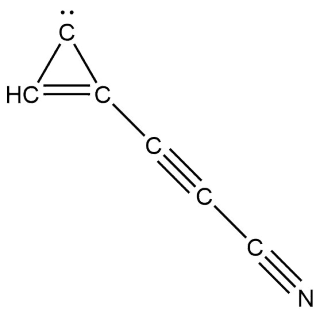


Molecule 133

IUPAC Name: cyanoacetylcycloprop-1-ene-2,2-diyl

Common name: cyanoacetylcyclopropenylidene

SMILES: [C]1C=C1C#CC#N

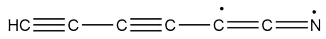


Molecule 134

IUPAC Name: 2,4-cyanopentadiyne-2,2-diyl

Common name: 2,4-cyanopentadiyne-2,2-diyl

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



Molecule 135

IUPAC Name: 6-oxo-1,2,3,4,5-hexapentaenylidene

Common name: hexacarbonmonoxide

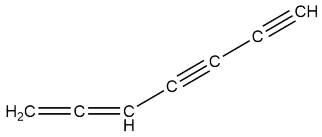
SMILES: [C]=C=C=C=C=C=O

Molecule 136

IUPAC Name: 1,2-heptadiene-4,6-diyne

Common name: allenyldiacetylene

SMILES: C=C=CC#CC#C



136: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	4 1	4 3	1 3								7285.53000		7285.52944		0.00056	0.00200	0.00000
2:	4 0	4 3	0 3								7383.53400		7383.53456		-0.00056	0.00200	0.00000
3:	4 1	3 3	1 2								7483.94300		7483.94214		0.00086	0.00200	0.00000
4:	5 1	5 4	1 4								9106.65800		9106.65743		0.00057	0.00200	0.00000
5:	5 0	5 4	0 4								9228.45300		9228.45262		0.00038	0.00200	0.00000
6:	5 1	4 4	1 3								9354.66100		9354.65948		0.00152	0.00200	0.00000
7:	6 1	6 5	1 5								10927.61800		10927.61699		0.00101	0.00200	0.00000
8:	6 0	6 5	0 5								11072.72800		11072.72756		0.00044	0.00200	0.00000
9:	6 1	5 5	1 4								11225.19800		11225.19699		0.00101	0.00200	0.00000
10:	7 1	7 6	1 6								12748.37600		12748.37558		0.00042	0.00200	0.00000
11:	7 0	7 6	0 6								12916.23100		12916.23161		-0.00061	0.00200	0.00000
12:	7 1	6 6	1 5								13095.51800		13095.51769		0.00031	0.00200	0.00000
13:	8 1	8 7	1 7								14568.90200		14568.90129		0.00071	0.00200	0.00000
14:	8 0	8 7	0 7								14758.83700		14758.83771		-0.00071	0.00200	0.00000
15:	8 1	7 7	1 6								14965.58500		14965.58404		0.00096	0.00200	0.00000
16:	9 1	9 8	1 8								16389.16300		16389.16292		0.00008	0.00200	0.00000
17:	9 0	9 8	0 8								16600.41900		16600.41995		-0.00095	0.00200	0.00000
18:	9 1	8 8	1 7								16835.35700		16835.35783		-0.00083	0.00200	0.00000
19:	10 1	10 9	1 9								18209.13100		18209.13010		0.00090	0.00200	0.00000
20:	10 0	10 9	0 9								18440.85400		18440.85400		-0.00000	0.00200	0.00000
21:	11 0	11 10	0 10								20280.01700		20280.01774		-0.00074	0.00200	0.00000
22:	11 1	10 10	1 9								20573.87200		20573.87110		0.00090	0.00200	0.00000
23:	12 1	12 11	1 11								21848.06600		21848.06424		0.00176	0.00200	0.00000
24:	12 0	12 11	0 11								22117.79100		22117.79192		-0.00092	0.00200	0.00000
25:	12 1	11 11	1 10								22442.53000		22442.53003		-0.00003	0.00200	0.00000
26:	13 1	13 12	1 12								23666.97500		23666.97537		-0.00037	0.00200	0.00000
27:	13 0	13 12	0 12								23954.05900		23954.06109		-0.00209	0.00200	0.00000
28:	13 1	12 12	1 11								24310.73600		24310.73514		0.00086	0.00200	0.00000
29:	5 2	4 4	2 3								9231.67500		9231.67476		0.00024	0.00200	0.00000

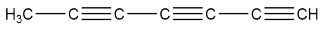
```
  30:   5  2  3  4  2  2                    9234.17800    9234.17973   -0.00173    0.00200   0.00000
  31:   7  2  6  6  2  5                   12923.66100   12923.66161   -0.00061    0.00200   0.00000
  32:   6  2  5  5  2  4                   11077.74100   11077.74134   -0.00034    0.00200   0.00000
  33:   6  2  4  5  2  3                   11082.12200   11082.12409   -0.00209    0.00200   0.00000
  34:   7  2  5  6  2  4                   12930.67100   12930.67187   -0.00087    0.00200   0.00000
  35:   8  2  7  7  2  6                   14769.41000   14769.41126   -0.00126    0.00200   0.00000
  36:   8  2  6  7  2  5                   14779.92100   14779.92226   -0.00126    0.00200   0.00000
  37:   9  2  8  8  2  7                   16614.96600   16614.96602   -0.00002    0.00200   0.00000
  38:   9  2  7  8  2  6                   16629.97200   16629.97333   -0.00133    0.00200   0.00000
  39:  10  2  9  9  2  8                   18460.30800   18460.30164    0.00636    0.00200   0.00000
  40:  10  2  8  9  2  7                   18480.92000   18480.92161   -0.00161    0.00200   0.00000
  41:   1  1  0  1  0  1                   14755.76800   14755.76598    0.00202    0.00200   0.00000
  42:   1  1  1  0  0  0                   16552.36300   16552.36441   -0.00141    0.00200   0.00000
  43:   2  1  2  1  0  1                   18349.05900   18349.05961   -0.00061    0.00200   0.00000
  44:  11  2 10 10  2  9                   20305.39500   20305.39394    0.00106    0.00200   0.00000
  45:  11  2  9 10  2  8                   20332.86000   20332.86142   -0.00142    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99999E-01    3   2.42897E-01    4   4.09032E-01    5   6.88135E-01    6   9.68309E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 15654.01571(116)         -0.00000
   2         20000                  947.906826(145)        -0.000000
   3         30000                  898.299385(136)         0.000000
   4           200                   -0.146925(205)E-03    -0.000000E-03
   5          1100                    0.0248883(117)        0.0000000
   6         40100                   -0.031001(269)E-03     0.000000E-03
 MICROWAVE AVG =        0.000013 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001400 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.69994         0.69994
```

Molecule 137

IUPAC Name: 1,3,5-heptatriyne

Common name: methyltriacetylene

SMILES: CC#CC#CC#C

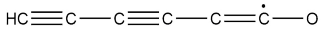


Molecule 138

IUPAC Name: 1-hexene-3,5-diyn-1-on-2-yl radical

Common name: 1-hexene-3,5-diyn-1-on-2-yl radical

SMILES: C#CC#C[C]=C=O

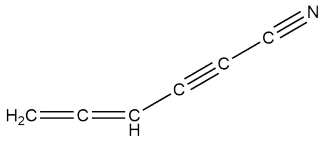


Molecule 139

IUPAC Name: 4,5-hexadien-2-ynenitrile

Common name: cyanoacetylene allene, allyl cyanoacetylene

SMILES: C=C=CC#CC#N

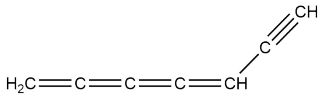


Molecule 140

IUPAC Name: 1,2,3,4-heptatetraen-6-yne

Common name: 1,2,3,4-heptatetraen-6-yne

SMILES: C=C=C=C=CC#C



140: Fit file

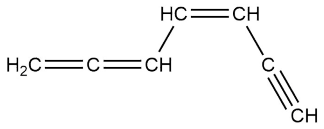
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   4  1  4  3  1  3                    7220.73920    7220.73990   -0.00070    0.00200   0.00000
    2:   4  0  4  3  0  3                    7307.43360    7307.43362   -0.00002    0.00200   0.00000
    3:   4  1  3  3  1  2                    7395.78990    7395.78873    0.00117    0.00200   0.00000
    4:   5  1  5  4  1  4                    9025.74870    9025.74693    0.00177    0.00200   0.00000
    5:   5  0  5  4  0  4                    9133.60830    9133.60856   -0.00026    0.00200   0.00000
    6:   5  1  4  4  1  3                    9244.55080    9244.55139   -0.00059    0.00200   0.00000
    7:   6  1  6  5  1  5                   10830.63530   10830.63599   -0.00069    0.00200   0.00000
    8:   6  0  6  5  0  5                   10959.32830   10959.32810    0.00020    0.00200   0.00000
    9:   6  1  5  5  1  4                   11093.19020   11093.19044   -0.00024    0.00200   0.00000
   10:   7  1  7  6  1  6                   12635.38320   12635.38412   -0.00092    0.00200   0.00000
   11:   7  0  7  6  0  6                   12784.50120   12784.50153   -0.00033    0.00200   0.00000
   12:   7  1  6  6  1  5                   12941.67990   12941.68055   -0.00065    0.00200   0.00000
   13:   8  1  8  7  1  7                   14439.96930   14439.96874    0.00056    0.00200   0.00000
   14:   8  0  8  7  0  7                   14609.03920   14609.03848    0.00072    0.00200   0.00000
   15:   8  1  7  7  1  6                   14789.99660   14789.99606    0.00054    0.00200   0.00000
   16:   9  0  9  8  0  8                   16432.84870   16432.84906   -0.00036    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   2.51071E-01    3   2.10067E-01    4   1.69267E-01    5   9.78504E-01    6   9.97495E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    16995.6(123)             0.0
   2         20000                   935.42538( 36)          0.00000
   3         30000                   891.66121( 34)          0.00000
   4           200                    -0.07656(216)E-03      0.00000E-03
   5          1100                    0.014525(231)         -0.000000
   6         40100                    -0.01400(158)E-03      0.00000E-03
 MICROWAVE AVG =        0.000013 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000734 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.36695         0.36695
```

Molecule 141

IUPAC Name: (4Z)-1,2,4-heptatrien-6-yne (anti)

Common name: 1,2,4-heptatrien-6-yne (anti-(4Z))

SMILES: C=C=CC=CC#C



141: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	- DIFF.	- WT.	
1:	4	1	4	3	1	3					8676.92460	8676.92413	0.00047	0.00200	0.00000
2:	4	0	4	3	0	3					8925.76830	8925.76887	-0.00057	0.00200	0.00000
3:	4	2	3	3	2	2					8941.02760	8941.02834	-0.00074	0.00200	0.00000
4:	4	2	2	3	2	1					8957.42860	8957.43021	-0.00161	0.00200	0.00000
5:	4	1	3	3	1	2					9200.91790	9200.91709	0.00081	0.00200	0.00000
6:	5	1	5	4	1	4					10843.13720	10843.13760	-0.00040	0.00200	0.00000
7:	5	0	5	4	0	4					11144.92490	11144.92473	0.00017	0.00200	0.00000
8:	5	2	4	4	2	3					11174.20140	11174.20045	0.00095	0.00200	0.00000
9:	5	2	3	4	2	2					11206.95450	11206.95555	-0.00105	0.00200	0.00000
10:	5	1	4	4	1	3					11497.94090	11497.94046	0.00044	0.00200	0.00000
11:	6	1	6	5	1	5					13007.40890	13007.40925	-0.00035	0.00200	0.00000
12:	6	0	6	5	0	5					13355.99580	13355.99554	0.00026	0.00200	0.00000
13:	6	2	5	5	2	4					13405.98480	13405.98344	0.00136	0.00200	0.00000
14:	6	2	4	5	2	3					13463.15200	13463.15304	-0.00104	0.00200	0.00000
15:	6	1	5	5	1	4					13792.75570	13792.75536	0.00034	0.00200	0.00000
16:	7	1	7	6	1	6					15169.41950	15169.41946	0.00004	0.00200	0.00000
17:	7	0	7	6	0	6					15557.54050	15557.54077	-0.00027	0.00200	0.00000
18:	7	2	6	6	2	5					15636.10320	15636.10086	0.00234	0.00200	0.00000
19:	7	2	5	6	2	4					15727.17730	15727.17945	-0.00215	0.00200	0.00000
20:	7	1	6	6	1	5					16084.84860	16084.84829	0.00031	0.00200	0.00000
21:	8	1	8	7	1	7					17328.88450	17328.88448	0.00002	0.00200	0.00000
22:	8	0	8	7	0	7					17748.29780	17748.29899	-0.00119	0.00200	0.00000
23:	8	1	7	7	1	6					18373.66630	18373.66609	0.00021	0.00200	0.00000
24:	9	1	9	8	1	8					19485.56180	19485.56093	0.00087	0.00200	0.00000
25:	9	0	9	8	0	8					19927.27180	19927.27251	-0.00071	0.00200	0.00000
26:	9	1	8	8	1	7					20658.60920	20658.60930	-0.00010	0.00200	0.00000
27:	10	1	10	9	1	9					21639.25030	21639.24934	0.00096	0.00200	0.00000
28:	10	0	10	9	0	9					22093.81730	22093.81754	-0.00024	0.00200	0.00000
29:	10	1	9	9	1	8					22939.02650	22939.02600	0.00050	0.00200	0.00000

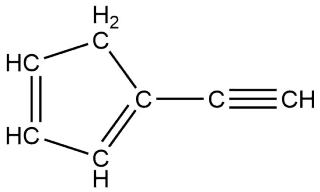
```
  30:  11  1 11 10  1 10                    23789.79760   23789.79680    0.00080    0.00200   0.00000
  31:  11  0 11 10  0 10                    24247.72460   24247.72429    0.00031    0.00200   0.00000
  32:  11  1 10 10  1  9                    25214.20640   25214.20654   -0.00014    0.00200   0.00000
  33:  12  1 12 11  1 11                    25937.09750   25937.09834   -0.00084    0.00200   0.00000
  34:  12  0 12 11  0 11                    26389.26730   26389.26773   -0.00043    0.00200   0.00000
NORMALIZED DIAGONAL:
   1   1.00000E+00    2   4.44235E-01    3   2.33381E-01    4   2.95758E-01    5   1.00000E+00    6   9.87330E-01
   7   8.60170E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000                   8959.174( 52)            0.000
  2         20000                1183.288622(194)         0.000000
  3         30000                1052.265826(152)        -0.000000
  4           200                   -0.18350( 40)E-03     -0.00000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                     4.2034(263)E-03      -0.0000E-03
  7         40100                   -0.04118( 42)E-03     -0.00000E-03
  8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =       -0.000019 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000872 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.43591         0.43591
```

Molecule 142

IUPAC Name: 1-ethynyl-1,3-cyclopentadiene

Common name: 1-ethynyl-1,3-cyclopentadiene

SMILES: C#CC1=CC=CC1



142: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2	1	2	1	1	1				6526.55170		6526.55300		-0.00130	0.00200	0.00000
2:	1	1	0	1	0	1				6824.99280		6824.99240		0.00040	0.00200	0.00000
3:	2	0	2	1	0	1				6844.38370		6844.38232		0.00138	0.00200	0.00000
4:	2	1	1	1	1	0				7186.71970		7186.71995		-0.00025	0.00200	0.00000
5:	5	1	4	5	0	5				9468.72860		9468.72617		0.00243	0.00200	0.00000
6:	3	1	3	2	1	2				9782.30110		9782.29989		0.00121	0.00200	0.00000
7:	1	1	1	0	0	0				9923.22900		9923.23237		-0.00337	0.00200	0.00000
8:	3	0	3	2	0	2				10236.02470		10236.02251		0.00219	0.00200	0.00000
9:	3	2	1	2	2	0				10333.84780		10333.85100		-0.00320	0.00200	0.00000
10:	3	1	2	2	1	1				10772.26300		10772.26335		-0.00035	0.00200	0.00000
11:	2	1	2	1	0	1				13021.46160		13021.46154		0.00006	0.00200	0.00000
12:	4	1	4	3	1	3				13029.40620		13029.40465		0.00155	0.00200	0.00000
13:	4	0	4	3	0	3				13591.65160		13591.65067		0.00093	0.00200	0.00000
14:	4	2	3	3	2	2				13703.66390		13703.66138		0.00252	0.00200	0.00000
15:	4	3	2	3	3	1				13736.79710		13736.79823		-0.00113	0.00200	0.00000
16:	4	3	1	3	3	0				13738.50670		13738.50690		-0.00020	0.00200	0.00000
17:	4	2	2	3	2	1				13825.28720		13825.28898		-0.00178	0.00200	0.00000
18:	4	1	3	3	1	2				14348.02300		14348.02371		-0.00071	0.00200	0.00000
19:	5	1	5	4	1	4				16265.62630		16265.62602		0.00028	0.00200	0.00000
20:	5	0	5	4	0	4				16901.27870		16901.27840		0.00030	0.00200	0.00000
21:	5	2	4	4	2	3				17114.24950		17114.24513		0.00437	0.00200	0.00000
22:	5	2	3	4	2	2				17354.51420		17354.51881		-0.00461	0.00200	0.00000
23:	5	1	4	4	1	3				17910.06010		17910.06067		-0.00057	0.00200	0.00000
24:	6	1	6	5	1	5				19489.23270		19489.23394		-0.00124	0.00200	0.00000
25:	6	0	6	5	0	5				20158.19160		20158.19171		-0.00011	0.00200	0.00000
26:	6	2	5	5	2	4				20514.65540		20514.64688		0.00852	0.00200	0.00000
27:	6	2	4	5	2	3				20926.15300		20926.16015		-0.00715	0.00200	0.00000

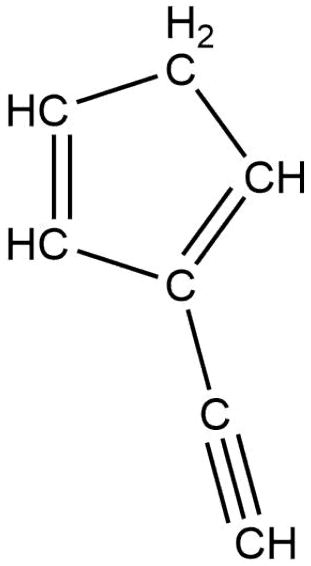
```
   28:   6  1  5  5  1  4                    21453.84660   21453.84582    0.00078    0.00200   0.00000
   29:   7  0  7  6  0  6                    23360.77670   23360.77780   -0.00110    0.00200   0.00000
   30:   7  1  6  6  1  5                    24974.13240   24974.13191    0.00049    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.20131E-01    3   3.75426E-01    4   9.99187E-01    5   1.00000E+00    6   8.10302E-01
    7   9.80373E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  8374.11750(106)         -0.00000
   2         20000                 1879.204009(241)         0.000000
   3         30000                 1549.120018(200)        -0.000000
   4           200                    -0.04824(170)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                     -2.5097(206)E-03      -0.0000E-03
   7         40100                    -0.01609(177)E-03     -0.00000E-03
   8         50000                -0.072268847(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000011 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002710 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.35523         1.35523
```

Molecule 143

IUPAC Name: 5-ethynyl-1,3-cyclopentadiene

Common name: 5-ethynyl-1,3-cyclopentadiene

SMILES: C#CC1=CCC=C1



143: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 1 2 1 1 1									6505.82270		6505.82579		-0.00309	0.00200	0.00000
2:	1 1 0 1 0 1									6719.17160		6719.16935		0.00225	0.00200	0.00000
3:	2 0 2 1 0 1									6826.20080		6826.19994		0.00086	0.00200	0.00000
4:	2 1 1 2 0 2									7064.90460		7064.90326		0.00134	0.00200	0.00000
5:	2 1 1 1 1 0									7171.93700		7171.93385		0.00315	0.00200	0.00000
6:	3 1 2 3 0 3									7607.02220		7607.01913		0.00307	0.00200	0.00000
7:	4 0 4 3 1 3									7942.97450		7942.97066		0.00384	0.00200	0.00000
8:	4 1 3 4 0 4									8372.60590		8372.60169		0.00421	0.00200	0.00000
9:	5 1 4 5 0 5									9394.85450		9394.85662		-0.00212	0.00200	0.00000
10:	1 1 1 0 0 0									9805.56380		9805.56078		0.00302	0.00200	0.00000
11:	3 1 3 2 1 2									9750.94970		9750.95082		-0.00112	0.00200	0.00000
12:	3 0 3 2 0 2									10207.69620		10207.69458		0.00162	0.00200	0.00000
13:	3 2 2 2 2 1									10258.27450		10258.27154		0.00296	0.00200	0.00000
14:	3 2 1 2 2 0									10308.90780		10308.90975		-0.00195	0.00200	0.00000
15:	3 1 2 2 1 1									10749.81260		10749.81045		0.00215	0.00200	0.00000
16:	5 0 5 4 1 4									11804.62730		11804.62245		0.00485	0.00200	0.00000

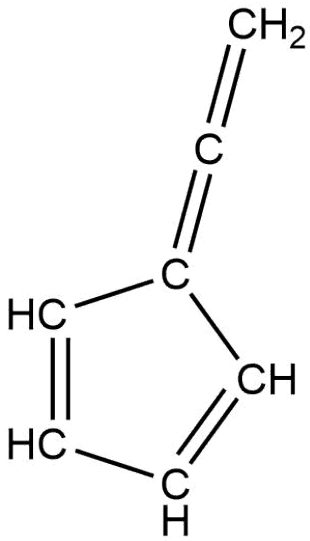
```
  17:   2  1  2  1  0  1                  12891.94020   12891.94111   -0.00091    0.00200   0.00000
  18:   4  1  4  3  1  3                  12987.14820   12987.14761    0.00059    0.00200   0.00000
  19:   4  0  4  3  0  3                  13551.96810   13551.96807    0.00003    0.00200   0.00000
  20:   4  2  3  3  2  2                  13667.82170   13667.81753    0.00417    0.00200   0.00000
  21:   4  3  2  3  3  1                  13702.09070   13702.08587    0.00483    0.00200   0.00000
  22:   4  3  1  3  3  0                  13703.88820   13703.89898   -0.01078    0.00200   0.00000
  23:   4  2  2  3  2  1                  13793.61660   13793.61635    0.00025    0.00200   0.00000
  24:   4  1  3  3  1  2                  14317.55130   14317.55064    0.00066    0.00200   0.00000
  25:   6  0  6  5  1  5                  15684.00220   15684.00339   -0.00119    0.00200   0.00000
  26:   5  1  5  4  1  4                  16212.11870   16212.11765    0.00105    0.00200   0.00000
  27:   5  0  5  4  0  4                  16848.79790   16848.79940   -0.00150    0.00200   0.00000
  28:   5  2  4  4  2  3                  17068.91490   17068.91029    0.00461    0.00200   0.00000
  29:   5  3  3  4  3  2                  17137.50810   17137.50593    0.00217    0.00200   0.00000
  30:   5  3  2  4  3  1                  17143.84170   17143.83931    0.00239    0.00200   0.00000
  31:   5  2  3  4  2  2                  17317.26790   17317.27242   -0.00452    0.00200   0.00000
  32:   5  1  4  4  1  3                  17871.05080   17871.05433   -0.00353    0.00200   0.00000
  33:   4  1  4  3  0  3                  18596.14150   18596.14502   -0.00352    0.00200   0.00000
  34:   6  1  6  5  1  5                  19424.10490   19424.10286    0.00204    0.00200   0.00000
  35:   6  0  6  5  0  5                  20091.49590   20091.49859   -0.00269    0.00200   0.00000
  36:   6  1  5  5  1  4                  21405.58770   21405.59754   -0.00984    0.00200   0.00000
  37:   7  1  7  6  1  6                  22621.96360   22621.96198    0.00162    0.00200   0.00000
  38:   7  1  6  6  1  5                  24915.67870   24915.69563   -0.01693    0.01000   0.00000
  39:   8  1  8  7  1  7                  25805.20410   25805.20134    0.00276    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.98359E-01    3   9.02346E-01    4   4.41945E-01    5   1.00000E+00    6   7.80571E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   8262.37025( 68)          0.00000
   2         20000                  1876.249824(109)         0.000001
   3         30000                  1543.195792(119)         0.000001
   4           200                     -0.03746(132)E-03     -0.00001E-03
   5          2000                  -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                       -2.5524(136)E-03      -0.0001E-03
   7         40100                  -2.130453416(  0)E-24 -0.000000000E-24
   8         50000                  -0.328707538(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000083 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.004450 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.78516         1.78516
```

Molecule 144

IUPAC Name: 5-ethenylidene-1,3-cyclopentadiene

Common name: fulvenallene

SMILES: C=C=C1C=CC=C1



144: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 1 2 1 1 1									6533.99750		6534.00155		-0.00405	0.00200	0.00000
2:	2 0 2 1 0 1									6858.35320		6858.35368		-0.00048	0.00200	0.00000
3:	2 1 1 1 1 0									7209.11780		7209.11417		0.00363	0.00200	0.00000
4:	3 1 3 2 1 2									9792.89210		9792.89520		-0.00310	0.00200	0.00000
5:	3 0 3 2 0 2									10254.62110		10254.62160		-0.00050	0.00200	0.00000
6:	3 2 2 2 2 1									10307.28150		10307.28004		0.00146	0.00200	0.00000
7:	3 2 1 2 2 0									10360.00990		10360.01046		-0.00056	0.00200	0.00000
8:	3 1 2 2 1 1									10805.24270		10805.24044		0.00226	0.00200	0.00000
9:	4 1 4 3 1 3									13042.50470		13042.50658		-0.00188	0.00200	0.00000
10:	4 0 4 3 0 3									13612.17200		13612.17339		-0.00139	0.00200	0.00000
11:	4 2 3 3 2 2									13732.75380		13732.75169		0.00211	0.00200	0.00000
12:	4 3 2 3 3 1									13768.40190		13768.40260		-0.00070	0.00200	0.00000
13:	4 3 1 3 3 0									13770.33900		13770.34291		-0.00391	0.00200	0.00000
14:	4 2 2 3 2 1									13863.70140		13863.70258		-0.00118	0.00200	0.00000
15:	4 1 3 3 1 2									14390.79300		14390.79152		0.00148	0.00200	0.00000
16:	5 1 5 4 1 4									16280.46640		16280.46575		0.00065	0.00200	0.00000
17:	5 0 5 4 0 4									16920.49880		16920.49927		-0.00047	0.00200	0.00000

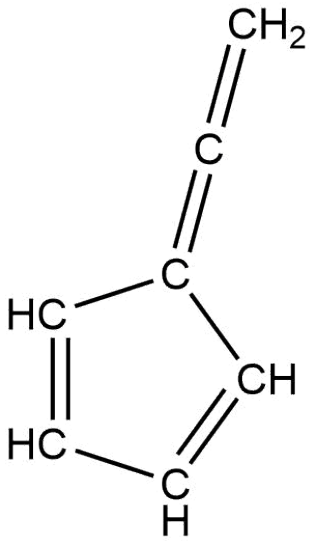
```
   18:   5  2  4  4  2  3                    17149.42480   17149.41957    0.00523    0.00200   0.00000
   19:   5  3  3  4  3  2                    17220.75690   17220.75535    0.00155    0.00200   0.00000
   20:   5  3  2  4  3  1                    17227.53240   17227.53234    0.00006    0.00200   0.00000
   21:   5  2  3  4  2  2                    17407.77120   17407.77299   -0.00179    0.00200   0.00000
   22:   5  1  4  4  1  3                    17961.47050   17961.47020    0.00030    0.00200   0.00000
   23:   6  1  6  5  1  5                    19504.98240   19504.97878    0.00362    0.00200   0.00000
   24:   6  0  6  5  0  5                    20172.93260   20172.93316   -0.00056    0.00200   0.00000
   25:   6  1  5  5  1  4                    21512.31130   21512.31189   -0.00059    0.00200   0.00000
   26:   7  1  6  6  1  5                    25037.53860   25037.54109   -0.00249    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   6.21845E-01    3   5.18899E-01    4   3.46493E-01    5   1.00000E+00    6   9.92459E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   8180.792( 33)            0.000
   2         20000                1886.670989(207)         0.000000
   3         30000                1549.114676(173)        -0.000000
   4           200                   -0.04610(228)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                    -2.9989(185)E-03      -0.0000E-03
   7         40100                -2.130453416(  0)E-24 -0.000000000E-24
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =       -0.000050 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002238 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.11887         1.11887
```

Molecule 145

IUPAC Name: 5-ethenylidene-1,3-cyclopentadiene (1v22)

Common name: fulvenallene (1v22)

SMILES: C=C=C1C=CC=C1



145: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	3 1 3 2 1 2									9802.59380		9802.59708		-0.00328	0.00200	0.00000
2:	3 0 3 2 0 2									10264.48080		10264.47918		0.00162	0.00200	0.00000
3:	3 1 2 2 1 1									10815.98650		10815.98165		0.00485	0.00200	0.00000
4:	4 1 4 3 1 3									13055.32770		13055.32790		-0.00020	0.00200	0.00000
5:	4 0 4 3 0 3									13624.83360		13624.83283		0.00077	0.00200	0.00000
6:	4 1 3 3 1 2									14404.97940		14404.97524		0.00416	0.00200	0.00000
7:	5 1 5 4 1 4									16296.32160		16296.32260		-0.00100	0.00200	0.00000
8:	5 0 5 4 0 4									16935.60620		16935.60635		-0.00015	0.00200	0.00000
9:	5 1 4 4 1 3									17978.96510		17978.96277		0.00233	0.00200	0.00000
10:	6 1 6 5 1 5									19523.78290		19523.78281		0.00009	0.00200	0.00000
11:	6 0 6 5 0 5									20190.16050		20190.16126		-0.00076	0.00200	0.00000
12:	7 1 7 6 1 6									22736.57380		22736.57401		-0.00021	0.00200	0.00000
13:	7 0 7 6 0 6									23387.81530		23387.81623		-0.00093	0.00200	0.00000
14:	7 1 6 6 1 5									25061.02140		25061.02796		-0.00656	0.00200	0.00000
15:	8 1 8 7 1 7									25934.25440		25934.25374		0.00066	0.00200	0.00000
16:	8 0 8 7 0 7									26534.70410		26534.70437		-0.00027	0.00200	0.00000
17:	10 0 10 9 0 9									32724.85010		32724.84805		0.00205	0.00200	0.00000

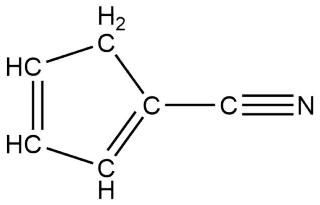
```
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.60224E-01    3   3.15535E-01    4   1.35573E-01    5   1.00000E+00    6   5.38402E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   8142.845( 39)            0.000
   2         20000                1888.559897(230)         0.000000
   3         30000                1550.655462(179)         0.000000
   4           200                   -0.03446(259)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                     -3.092(242)E-03       -0.000E-03
   7         40100                -0.411750199(  0)E-24 -0.000000000E-24
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000185 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002550 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.27490         1.27490
```

Molecule 146

IUPAC Name: 1,3-cyclopentadiene-1-carbonitrile

Common name: 1-cyano-1,3-cyclopentadiene

SMILES: C1C=CC=C1C#N



146: Fit file

	EXP.FREQ.			CALC.FREQ.			DIFF.		EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.		
1:	2	1	1	2	1	1	0	1			7277.05350	7277.05870	-0.00520	0.00200	0.00065		
2:	2	1	1	2	1	1	0	2			7277.61800	7277.62076	-0.00276	0.00200	0.00082		
3:	2	1	1	3	1	1	0	2			7278.36080	7278.36161	-0.00081	0.00200	0.00042		
4:	2	0	2	2	1	0	1	2			6924.97370	6924.97513	-0.00143	0.00200	0.00067		
5:	2	0	2	1	1	0	1	0			6925.17420	6925.17661	-0.00241	0.00200	0.00057		
6:	2	0	2	2	1	0	1	1			6926.22730	6926.22883	-0.00153	0.00200	0.00023		
7:	2	0	2	3	1	0	1	2			6926.31450	6926.31356	0.00094	0.00200	0.00023		
8:	2	0	2	1	1	0	1	1			6928.31080	6928.31121	-0.00041	0.00200	0.00109		
9:	3	1	3	3	2	1	2	3			9891.66890	9891.66979	-0.00089	0.00200	0.00103		
10:	3	1	3	3	2	1	2	2			9892.26950	9892.27214	-0.00264	0.00200	0.00046		
11:	3	1	3	4	2	1	2	3			9892.64210	9892.64124	0.00086	0.00200	0.00044		
12:	3	1	3	2	2	1	2	2			9893.58110	9893.58392	-0.00282	0.00200	0.00130		
13:	3	0	3	2	2	0	2	1			10356.72890	10356.72920	-0.00030	0.00200	0.00032		
14:	3	0	3	3	2	0	2	2			10356.94980	10356.94762	0.00218	0.00200	0.00031		
15:	3	0	3	4	2	0	2	3			10356.99010	10356.98971	0.00039	0.00200	0.00030		
16:	3	2	2	3	2	2	1	2			10407.74240	10407.74312	-0.00072	0.00200	0.00066	10407.74312	-0.00072
17:	3	2	2	3	2	2	1	2			10407.74240	10407.74312	-0.00072	0.00200	0.00066	10407.74312	-0.00072
18:	3	2	2	4	2	2	1	3			10409.08760	10409.08635	0.00125	0.00200	0.00041		
19:	3	2	1	4	2	2	0	3			10460.98910	10460.99091	-0.00181	0.00200	0.00043		
20:	3	2	1	2	2	2	0	1			10461.73330	10461.73912	-0.00582	0.00200	0.00066		
21:	3	1	2	3	2	1	1	3			10907.85780	10907.85821	-0.00041	0.00200	0.00099		
22:	3	1	2	3	2	1	1	2			10908.59940	10908.59907	0.00033	0.00200	0.00052		
23:	3	1	2	2	2	1	1	1			10908.95520	10908.95163	0.00357	0.00200	0.00052		
24:	3	1	2	4	2	1	1	3			10908.97470	10908.97317	0.00153	0.00200	0.00051		
25:	3	1	2	2	2	1	1	2			10910.10160	10910.10452	-0.00292	0.00200	0.00131		
26:	4	1	4	4	3	1	3	3			13175.47380	13175.47108	0.00272	0.00200	0.00052		
27:	4	1	4	3	3	1	3	2			13175.58400	13175.58479	-0.00079	0.00200	0.00052		

```
  28:   4  1  4  5  3  1  3  4              13175.63340   13175.63337    0.00003    0.00200   0.00051
  29:   4  0  4  3  3  0  3  2              13749.42290   13749.42393   -0.00103    0.00200   0.00039
  30:   4  0  4  4  3  0  3  3              13749.52430   13749.52532   -0.00102    0.00200   0.00039
  31:   4  0  4  5  3  0  3  4              13749.54830   13749.54669    0.00161    0.00200   0.00038
  32:   4  2  3  4  3  2  2  3              13867.84200   13867.84054    0.00146    0.00200   0.00048
  33:   4  2  3  5  3  2  2  4              13868.41030   13868.40926    0.00104    0.00200   0.00043
  34:   4  2  3  3  3  2  2  2              13868.55780   13868.55542    0.00238    0.00200   0.00045
  35:   4  2  2  5  3  2  1  4              13997.33970   13997.33951    0.00019    0.00200   0.00050
  36:   4  1  3  4  3  1  2  3              14529.11700   14529.11553    0.00147    0.00200   0.00054
  37:   4  1  3  3  3  1  2  2              14529.21910   14529.21962   -0.00052    0.00200   0.00054
  38:   4  1  3  5  3  1  2  4              14529.28280   14529.28075    0.00205    0.00200   0.00054
  39:   5  1  5  5  4  1  4  4              16447.06810   16447.06796    0.00014    0.00200   0.00055
  40:   5  1  5  4  4  1  4  3              16447.11120   16447.11197   -0.00077    0.00200   0.00055
  41:   5  1  5  6  4  1  4  5              16447.15430   16447.15490   -0.00060    0.00200   0.00055
  42:   5  0  5  4  4  0  4  3              17093.45790   17093.45695    0.00095    0.00200   0.00051
  43:   5  0  5  5  4  0  4  4              17093.52020   17093.52060   -0.00040    0.00200   0.00051
  44:   5  0  5  6  4  0  4  5              17093.53260   17093.52999    0.00261    0.00200   0.00051
  45:   5  1  4  5  4  1  3  4              18134.92110   18134.92047    0.00063    0.00200   0.00054
  46:   5  1  4  4  4  1  3  3              18134.95930   18134.95851    0.00079    0.00200   0.00054
  47:   5  1  4  6  4  1  3  5              18135.01030   18135.00894    0.00136    0.00200   0.00054
  48:   7  1  7  7  6  1  6  6              22949.16330   22949.16491   -0.00161    0.00200   0.00084
  49:   7  1  7  6  6  1  6  5              22949.17470   22949.17181    0.00289    0.00200   0.00084
  50:   7  1  7  8  6  1  6  7              22949.19890   22949.19833    0.00057    0.00200   0.00084
  51:   7  0  7  6  6  0  6  5              23614.25080   23614.24693    0.00387    0.00200   0.00078
  52:   7  0  7  8  6  0  6  7              23614.28230   23614.28208    0.00022    0.00200   0.00078   23614.28332   -0.00102
  53:   7  0  7  7  6  0  6  6              23614.28230   23614.28456   -0.00226    0.00200   0.00078   23614.28332   -0.00102
  54:   7  2  6  7  6  2  5  6              24186.13130   24186.13191   -0.00061    0.00200   0.00105
  55:   7  2  6  6  6  2  5  5              24186.22940   24186.23342   -0.00402    0.00200   0.00105
  56:   7  2  6  8  6  2  5  7              24186.24690   24186.24301    0.00389    0.00200   0.00105
  57:   7  3  5  8  6  3  4  7              24376.32710   24376.33090   -0.00380    0.00200   0.00127
  58:   7  3  5  6  6  3  4  5              24376.35710   24376.35289    0.00421    0.00200   0.00127
  59:   7  2  5  7  6  2  4  6              24858.33370   24858.32903    0.00467    0.00200   0.00109
  60:   7  2  5  6  6  2  4  5              24858.44140   24858.44620   -0.00480    0.00200   0.00108
  61:   7  2  5  8  6  2  4  7              24858.45550   24858.45486    0.00064    0.00200   0.00108
  62:   7  1  6  7  6  1  5  6              25282.43920   25282.43756    0.00164    0.00200   0.00108   25282.43867    0.00053
  63:   7  1  6  6  6  1  5  5              25282.43920   25282.43979   -0.00059    0.00200   0.00108   25282.43867    0.00053
  64:   7  1  6  8  6  1  5  7              25282.46690   25282.47008   -0.00318    0.00200   0.00108
  65:   8  0  8  9  7  0  7  8              26795.33360   26795.33449   -0.00089    0.00200   0.00097   26795.33685   -0.00325
  66:   8  0  8  8  7  0  7  7              26795.33360   26795.33920   -0.00560    0.00200   0.00097   26795.33685   -0.00325
  67:   9  0  9 10  8  0  8  9              29936.24350   29936.24075    0.00275    0.00200   0.00149   29936.24346    0.00004
  68:   9  0  9  9  8  0  8  8              29936.24350   29936.24617   -0.00267    0.00200   0.00149   29936.24346    0.00004
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   6.73152E-01    3   2.86458E-01    4   3.59801E-01    5   1.00000E+00    6   9.98191E-01
    7   6.02488E-01    8   1.35673E-01    9   9.22519E-01   10   9.99991E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  8352.9822(160)          -0.0000
   2         20000                  1904.25132( 34)          0.00000
   3         30000                 1565.366032(307)        -0.000000
```

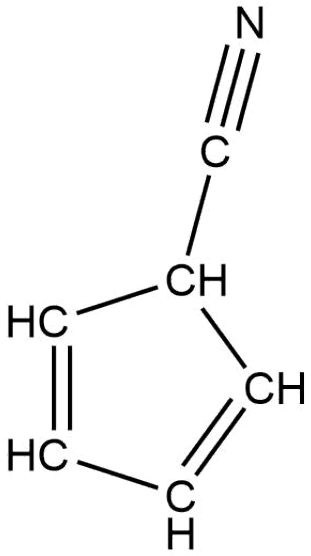
```
  4           200                   -0.07004(152)E-03     -0.00000E-03
  5          2000                -1.573881133(  0)E-27 -0.000000000E-27
  6          1100                    -2.3624(146)E-03       0.0000E-03
  7         40100     -del_J         -0.01161(107)E-03     -0.00000E-03
  8         41000     -del_K           -1.186(124)E-03       -0.000E-03
  9     110010000     chi_aa         -4.17946(211)         -0.00000
 10     110020000     chi_bb          2.30509(257)          0.00000
MICROWAVE AVG =       -0.000135 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002283 MHz, IR RMS =        0.00000
END OF ITERATION  2 OLD, NEW RMS ERROR=        1.14157         1.14157
```

Molecule 147

IUPAC Name: 2,4-cyclopentadiene-1-carbonitrile

Common name: 1-cyano-2,4-cyclopentadiene

SMILES: C1=CC(C=C1)C#N



147: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2	1	1	3	1	1	0	2		7266.11580		7266.11428		0.00152	0.00200	0.00000
2:	3	1	3	3	2	1	2	3		9862.32280		9862.32365		-0.00085	0.00200	0.00000
3:	3	1	3	3	2	1	2	2		9862.96330		9862.96551		-0.00221	0.00200	0.00000
4:	3	1	3	4	2	1	2	3		9863.34160		9863.34104		0.00056	0.00200	0.00000
5:	3	1	3	2	2	1	2	2		9864.33660		9864.33932		-0.00272	0.00200	0.00000
6:	3	0	3	2	2	0	2	1		10331.03540		10331.03636		-0.00096	0.00200	0.00000
7:	3	0	3	3	2	0	2	2		10331.25340		10331.25473		-0.00133	0.00200	0.00000
8:	3	0	3	4	2	0	2	3		10331.29980		10331.29973		0.00007	0.00200	0.00000
9:	3	2	2	3	2	2	1	2		10384.04990		10384.04688		0.00302	0.00200	0.00000
10:	3	2	2	4	2	2	1	3		10385.41170		10385.40754		0.00416	0.00200	0.00000
11:	3	1	2	3	2	1	1	2		10889.89760		10889.89663		0.00097	0.00200	0.00000
12:	3	1	2	2	2	1	1	1		10890.25820		10890.25936		-0.00116	0.00200	0.00000
13:	3	1	2	4	2	1	1	3		10890.27720		10890.27492		0.00228	0.00200	0.00000
14:	4	1	4	3	3	1	3	2		13135.96740		13135.97054		-0.00314	0.00200	0.00000
15:	4	1	4	5	3	1	3	4		13136.02370		13136.02246		0.00124	0.00200	0.00000
16:	4	1	4	3	3	1	3	3		13137.34410		13137.34435		-0.00025	0.00200	0.00000
17:	4	0	4	3	3	0	3	2		13712.90930		13712.90872		0.00058	0.00200	0.00000

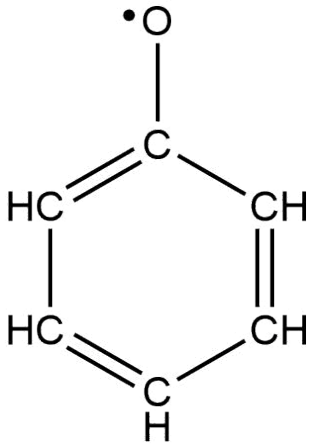
```
  18:   4  0  4  4  3  0  3  3              13713.00910   13713.00779    0.00131    0.00200   0.00000
  19:   4  0  4  5  3  0  3  4              13713.03190   13713.03261   -0.00071    0.00200   0.00000
  20:   4  2  3  4  3  2  2  3              13835.86350   13835.86425   -0.00075    0.00200   0.00000
  21:   4  2  3  5  3  2  2  4              13836.44210   13836.44072    0.00138    0.00200   0.00000
  22:   4  2  3  3  3  2  2  2              13836.58820   13836.58887   -0.00067    0.00200   0.00000
  23:   4  2  2  4  3  2  1  3              13969.72150   13969.72331   -0.00181    0.00200   0.00000
  24:   4  2  2  5  3  2  1  4              13970.30430   13970.30704   -0.00274    0.00200   0.00000
  25:   4  2  2  3  3  2  1  2              13970.45310   13970.45623   -0.00313    0.00200   0.00000
  26:   4  1  3  4  3  1  2  3              14503.54370   14503.54356    0.00014    0.00200   0.00000
  27:   4  1  3  3  3  1  2  2              14503.65540   14503.65208    0.00332    0.00200   0.00000
  28:   4  1  3  5  3  1  2  4              14503.71200   14503.71098    0.00102    0.00200   0.00000
  29:   5  1  5  5  4  1  4  4              16396.74220   16396.73997    0.00223    0.00200   0.00000
  30:   5  1  5  4  4  1  4  3              16396.78640   16396.78441    0.00199    0.00200   0.00000
  31:   5  1  5  6  4  1  4  5              16396.83160   16396.82946    0.00214    0.00200   0.00000
  32:   5  1  5  4  4  1  4  4              16398.27450   16398.27216    0.00234    0.00200   0.00000
  33:   5  0  5  4  4  0  4  3              17044.42340   17044.42757   -0.00417    0.00200   0.00000
  34:   5  0  5  5  4  0  4  4              17044.48530   17044.48771   -0.00241    0.00200   0.00000
  35:   5  0  5  6  4  0  4  5              17044.50230   17044.50113    0.00117    0.00200   0.00000
  36:   5  1  4  5  4  1  3  4              18101.86500   18101.86489    0.00011    0.00200   0.00000
  37:   5  1  4  4  4  1  3  3              18101.90480   18101.90584   -0.00104    0.00200   0.00000
  38:   5  1  4  6  4  1  3  5              18101.95440   18101.95509   -0.00069    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   5.34335E-01    3   4.66259E-01    4   2.81213E-01    5   1.00000E+00    6   9.98153E-01
    7   1.00000E+00    8   1.00000E+00    9   9.94975E-01   10   3.33553E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    8235.657( 44)            0.000
   2         20000                 1902.071773(190)         0.000000
   3         30000                 1559.650238(193)         0.000000
   4           200                    -0.0561( 37)E-03       0.0000E-03
   5          2000                -1.573881133(  0)E-27 -0.000000000E-27
   6          1100                     -2.286( 46)E-03       -0.000E-03
   7         40100     -del_J      3.007784780(  0)E-27 -0.000000000E-27
   8         41000     -del_K      2.687998204(  1)E-27  0.000000000E-27
   9     110010000     chi_aa          -4.2337( 56)           0.0000
  10     110020000     chi_bb           2.2364( 72)          -0.0000
 MICROWAVE AVG =        0.000021 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001966 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.98318         0.98318
```

Molecule 148

IUPAC Name: 1-oxidanylbenzene

Common name: phenoxy radical

SMILES: C1=CC=C(C=C1)[O]

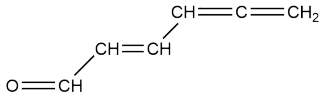


Molecule 149

IUPAC Name: (2E)-2,4,5-hexatrienal (anti) (ve1)

Common name: 2,4,5-hexatrienal (anti-(2E)) (ve1)

SMILES: C=C=CC=CC=O



149: Fit file

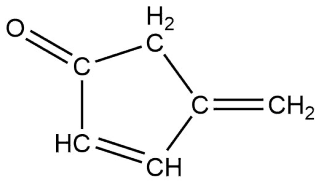
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   4  0  4  3  0  3                     6869.21890    6869.21993   -0.00103    0.00200   0.00000
    2:   5  0  5  4  0  4                     8586.24570    8586.24546    0.00024    0.00200   0.00000
    3:   6  0  6  5  0  5                    10303.08450   10303.08473   -0.00023    0.00200   0.00000
    4:   7  0  7  6  0  6                    12019.70090   12019.70050    0.00040    0.00200   0.00000
    5:   8  0  8  7  0  7                    13736.05690   13736.05562    0.00128    0.00200   0.00000
    6:   9  0  9  8  0  8                    15452.11200   15452.11297   -0.00097    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.65437E-02    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A  20668.915538460(  0)      0.000000000
   2         20000          B         874.2046( 75)          -0.0000
   3         30000          C         843.1937( 72)           0.0000
   4           200    Delta_J      -0.03555906( 48)E-03  -0.00000000E-03
   5          1100   Delta_JK      7.831126880(267)E-03 -0.000000000E-03
   6          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
   7         40100     -del_J     -0.697612116(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
 MICROWAVE AVG =       -0.000052 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000805 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.40252         0.40252
```

Molecule 150

IUPAC Name: 4-methylidene-2-cyclopenten-1-one

Common name: 4-methylidene-2-cyclopenten-1-one

SMILES: C=C1CC(=O)C=C1



150: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      7582.11810    7582.11626    0.00184    0.00200   0.00000
    2:   2  1  1  1  1  0                      8140.86630    8140.86142    0.00488    0.00200   0.00000
    3:   3  1  3  2  1  2                     10636.79710   10636.79794   -0.00084    0.00200   0.00000
    4:   3  0  3  2  0  2                     11268.99800   11268.99871   -0.00071    0.00200   0.00000
    5:   3  1  2  2  1  1                     12183.59990   12183.59798    0.00192    0.00200   0.00000
    6:   3  2  2  2  2  1                     11436.79080   11436.79176   -0.00096    0.00200   0.00000
    7:   3  2  1  2  2  0                     11604.59000   11604.58838    0.00162    0.00200   0.00000
    8:   4  2  3  3  2  2                     15216.00210   15216.00174    0.00036    0.00200   0.00000
    9:   4  2  2  3  2  1                     15623.87540   15623.87717   -0.00177    0.00200   0.00000
   10:   4  1  4  3  1  3                     14137.73620   14137.73631   -0.00011    0.00200   0.00000
   11:   4  0  4  3  0  3                     14841.08140   14841.08351   -0.00211    0.00200   0.00000
   12:   4  1  3  3  1  2                     16189.98700   16189.98955   -0.00255    0.00200   0.00000
   13:   5  1  5  4  1  4                     17606.39090   17606.38944    0.00146    0.00200   0.00000
   14:   5  0  5  4  0  4                     18287.57940   18287.58113   -0.00173    0.00200   0.00000
   15:   6  0  6  5  0  5                     21627.15340   21627.15190    0.00150    0.00200   0.00000
   16:   2  1  2  1  0  1                     11553.28920   11553.28869    0.00051    0.00200   0.00000
   17:   3  1  3  2  0  2                     14607.96910   14607.97037   -0.00127    0.00200   0.00000
   18:   4  1  4  3  0  3                     17476.70880   17476.70797    0.00083    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99316E-01    3   2.81910E-01    4   7.39032E-01    5   5.79163E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       6609.38374(184)         -0.00000
   2         20000          B      2164.298312(276)        -0.000000
   3         30000          C       1647.96938( 32)          0.00000
   4           200    Delta_J          -0.0717( 46)E-03       0.0000E-03
```

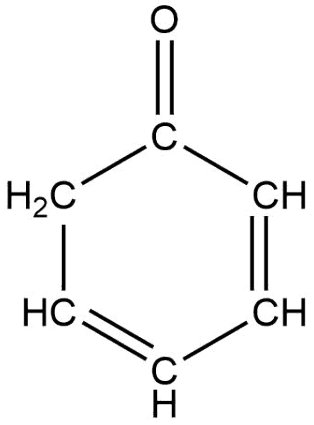
```
  5          1100   Delta_JK           -0.148( 54)E-03       -0.000E-03
  6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
  7         40100     -del_J     -1.158454703(  0)E-24 -0.000000000E-24
  8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
MICROWAVE AVG =        0.000159 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001822 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.91103         0.91103
```

Molecule 151

IUPAC Name: 2,4-cyclohexadien-1-one

Common name: 2,4-cyclohexadienone

SMILES: C1C=CC=CC1=O



151: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 1 2 1 1 1									8075.56550		8075.56685		-0.00135	0.00200	0.00000
2:	2 0 2 1 0 1									8772.84020		8772.84201		-0.00181	0.00200	0.00000
3:	2 1 1 1 1 0									9882.22140		9882.21952		0.00188	0.00200	0.00000
4:	3 1 3 2 1 2									11996.44100		11996.44262		-0.00162	0.00200	0.00000
5:	3 0 3 2 0 2									12706.23050		12706.23134		-0.00084	0.00200	0.00000
6:	3 2 2 2 2 1									13468.33000		13468.32844		0.00156	0.00200	0.00000
7:	3 2 1 2 2 0									14230.43010		14230.42881		0.00129	0.00200	0.00000
8:	3 1 2 2 1 1									14676.10670		14676.10451		0.00219	0.00200	0.00000
9:	4 1 4 3 1 3									15814.19490		15814.19462		0.00028	0.00200	0.00000
10:	4 0 4 3 0 3									16331.43200		16331.43316		-0.00116	0.00200	0.00000
11:	4 1 3 3 1 2									19252.26110		19252.25875		0.00235	0.00200	0.00000
12:	6 1 6 5 1 5									23202.58320		23202.58259		0.00061	0.00200	0.00000
13:	6 0 6 5 0 5									23345.29820		23345.29841		-0.00021	0.00200	0.00000
14:	5 3 2 4 3 1									23461.99760		23462.00038		-0.00278	0.00200	0.00000
15:	2 1 2 1 0 1									10542.51220		10542.51564		-0.00344	0.00200	0.00000
16:	4 2 3 3 2 2									17795.41780		17795.41691		0.00089	0.00200	0.00000
17:	4 2 2 3 2 1									19418.06130		19418.06314		-0.00184	0.00200	0.00000
18:	5 2 4 4 2 3									21991.35680		21991.35467		0.00213	0.00200	0.00000
19:	5 3 3 4 3 2									22897.41920		22897.41959		-0.00039	0.00200	0.00000
20:	5 2 3 4 2 2									24574.54580		24574.54680		-0.00100	0.00200	0.00000

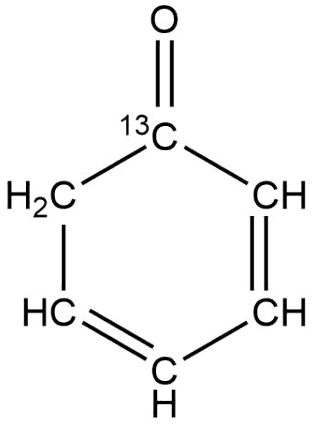
```
   21:   7  1  7  6  1  6                    26824.92050   26824.91988    0.00062    0.00200   0.00000
   22:   7  0  7  6  0  6                    26887.78880   26887.78729    0.00151    0.00200   0.00000
   23:   8  1  8  7  1  7                    30426.74480   30426.74501   -0.00021    0.00200   0.00000
   24:   8  0  8  7  0  7                    30452.80700   30452.80898   -0.00198    0.00200   0.00000
   25:   7  1  6  6  1  5                    30855.27200   30855.27053    0.00147    0.00200   0.00000
   26:   3  1  3  2  0  2                    13766.11630   13766.11625    0.00005    0.00200   0.00000
   27:   4  0  4  3  1  3                    15271.54820   15271.54824   -0.00004    0.00200   0.00000
   28:   4  1  4  3  0  3                    16874.07950   16874.07953   -0.00003    0.00200   0.00000
   29:   2  2  1  1  1  0                    17283.06540   17283.06539    0.00001    0.00200   0.00000
   30:   3  3  1  2  2  0                    27972.23410   27972.23412   -0.00002    0.00200   0.00000
   31:   3  3  0  2  2  1                    28208.59730   28208.59730    0.00000    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99796E-01    3   3.66808E-01    4   1.36359E-01    5   1.00000E+00    6   4.29189E-01
    7   9.92609E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  5163.33741( 46)          0.00000
   2         20000                 2696.388539(240)         0.000000
   3         30000                 1793.060696(144)         0.000000
   4           200                     -0.1481( 35)E-03      -0.0000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                     -0.1364(288)E-03      -0.0000E-03
   7         40100                    -0.04711(197)E-03     -0.00000E-03
   8         50000                -0.328707538(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000061 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001464 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.73185         0.73185
```

Molecule 153

IUPAC Name: 2,4-cyclohexadien-1-one (13C1)

Common name: 2,4-cyclohexadienone (13C1)

SMILES: C1C=CC=CC1=O



153: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8739.83240    8739.83016    0.00224    0.00200   0.00000
    2:   2  1  1  1  1  0                     9868.38760    9868.38635    0.00125    0.00200   0.00000
    3:   3  1  3  2  1  2                    11942.19610   11942.19480    0.00130    0.00200   0.00000
    4:   3  0  3  2  0  2                    12639.48130   12639.48159   -0.00029    0.00200   0.00000
    5:   3  1  2  2  1  1                    14647.52330   14647.52381   -0.00051    0.00200   0.00000
    6:   4  1  4  3  1  3                    15735.22710   15735.22712   -0.00002    0.00200   0.00000
    7:   4  0  4  3  0  3                    16230.71530   16230.71602   -0.00072    0.00200   0.00000
    8:   4  1  3  3  1  2                    19196.24250   19196.24171    0.00079    0.00200   0.00000
    9:   5  0  5  4  0  4                    19710.23040   19710.23108   -0.00068    0.00200   0.00000
   10:   3  2  2  2  2  1                    13433.40980   13433.41288   -0.00308    0.00200   0.00000
   11:   5  1  5  4  1  4                    19436.07940   19436.07935    0.00005    0.00200   0.00000
   12:   6  0  6  5  0  5                    23201.78450   23201.78388    0.00062    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.71817E-01    3   4.25190E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 5080.7013( 64)          -0.0000
   2         20000                2695.291195(288)         0.000000
   3         30000                1782.519606(226)         0.000000
```

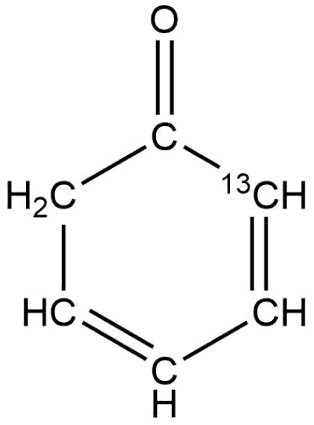
```
  4           200                -0.149471251(  0)E-03 -0.000000000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                -0.141008520(  0)E-03  0.000000000E-03
  7         40100                -0.046669381(  0)E-03 -0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000079 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001294 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.64687         0.64687
```

Molecule 154

IUPAC Name: 2,4-cyclohexadien-1-one (13C2)

Common name: 2,4-cyclohexadienone (13C2)

SMILES: C1C=CC=CC1=O



154: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8700.28710    8700.28714   -0.00004    0.00200   0.00000
    2:   2  1  1  1  1  0                     9815.17960    9815.17861    0.00099    0.00200   0.00000
    3:   3  1  3  2  1  2                    11891.33130   11891.32909    0.00221    0.00200   0.00000
    4:   3  2  2  3  0  3                    12402.71800   12402.71766    0.00034    0.00200   0.00000
    5:   3  0  3  2  0  2                    12589.29450   12589.29605   -0.00155    0.00200   0.00000
    6:   3  1  2  2  1  1                    14571.55390   14571.55388    0.00002    0.00200   0.00000
    7:   4  1  4  3  1  3                    15670.96670   15670.96362    0.00308    0.00200   0.00000
    8:   4  0  4  3  0  3                    16171.65310   16171.65592   -0.00282    0.00200   0.00000
    9:   4  2  3  3  2  2                    17656.07550   17656.07537    0.00013    0.00200   0.00000
   10:   4  1  3  3  1  2                    19103.61740   19103.61858   -0.00118    0.00200   0.00000
   11:   5  0  5  4  0  4                    19639.31280   19639.31296   -0.00016    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.08743E-01    3   9.95597E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 5081.38838( 55)          0.00000
   2         20000                2679.797030(298)        -0.000000
   3         30000                1775.794121(152)         0.000000
   4           200               -0.143084823(  0)E-03 -0.000000000E-03
```

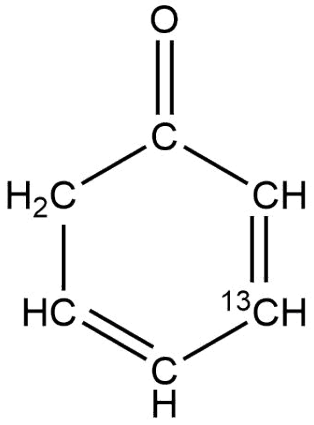
```
  5          2000                -0.015738811(  0)E-18  0.000000000E-18
  6          1100                -0.127041358(  0)E-03  0.000000000E-03
  7         40100                -0.047163922(  0)E-03 -0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000093 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001574 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.78711         0.78711
```

Molecule 155

IUPAC Name: 2,4-cyclohexadien-1-one (13C3)

Common name: 2,4-cyclohexadienone (13C3)

SMILES: C1C=CC=CC1=O



155: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8647.33780    8647.33836   -0.00056    0.00200   0.00000
    2:   3  1  3  2  1  2                    11834.95100   11834.94929    0.00171    0.00200   0.00000
    3:   3  0  3  2  0  2                    12544.96990   12544.96966    0.00024    0.00200   0.00000
    4:   3  1  2  2  1  1                    14437.36250   14437.36332   -0.00082    0.00200   0.00000
    5:   4  1  4  3  1  3                    15609.36080   15609.36104   -0.00024    0.00200   0.00000
    6:   4  0  4  3  0  3                    16141.22540   16141.22554   -0.00014    0.00200   0.00000
    7:   3  1  2  2  1  1                    14437.36460   14437.36332    0.00128    0.00200   0.00000
    8:   4  1  3  3  1  2                    18958.45160   18958.45204   -0.00044    0.00200   0.00000
    9:   5  1  5  4  1  4                    19295.94970   19295.95089   -0.00119    0.00200   0.00000
   10:   5  0  5  4  0  4                    19607.95060   19607.94998    0.00062    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.42999E-01    3   4.62440E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  5163.3418( 73)           0.0000
   2         20000                 2648.071523(293)         0.000000
   3         30000                 1771.581063(248)        -0.000000
   4           200                -0.148077412(  0)E-03 -0.000000000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
```

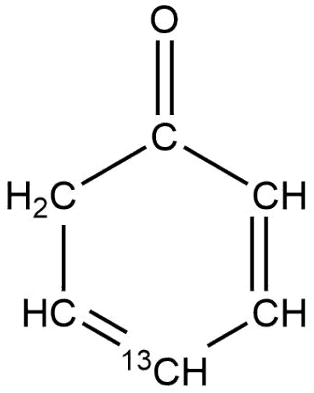
```
  6          1100                -0.136409284(  0)E-03  0.000000000E-03
  7         40100                -0.047109659(  0)E-03 -0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000046 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000875 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.43770         0.43770
```

Molecule 156

IUPAC Name: 2,4-cyclohexadien-1-one (13C4)

Common name: 2,4-cyclohexadienone (13C4)

SMILES: C1C=CC=CC1=O



156: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8690.10220    8690.10373   -0.00153    0.00200   0.00000
    2:   2  1  1  1  1  0                     9796.61260    9796.61166    0.00094    0.00200   0.00000
    3:   3  1  3  2  1  2                    11880.14780   11880.14533    0.00247    0.00200   0.00000
    4:   3  0  3  2  0  2                    12580.31870   12580.31899   -0.00029    0.00200   0.00000
    5:   3  2  2  2  2  1                    13346.31540   13346.31529    0.00011    0.00200   0.00000
    6:   3  2  1  2  2  0                    14112.31500   14112.31487    0.00013    0.00200   0.00000
    7:   3  1  2  2  1  1                    14546.43020   14546.42956    0.00064    0.00200   0.00000
    8:   4  1  4  3  1  3                    15658.49100   15658.49183   -0.00083    0.00200   0.00000
    9:   4  0  4  3  0  3                    16164.66190   16164.66236   -0.00046    0.00200   0.00000
   10:   4  2  3  3  2  2                    17631.58140   17631.58376   -0.00236    0.00200   0.00000
   11:   4  1  3  3  1  2                    19076.30720   19076.30663    0.00057    0.00200   0.00000
   12:   5  0  5  4  0  4                    19631.61530   19631.61443    0.00087    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.70928E-01    3   4.68276E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   5094.8662( 56)          -0.0000
   2         20000                  2673.920134(272)        -0.000000
   3         30000                  1774.858053(264)         0.000000
   4           200                 -0.148077412(  0)E-03  0.000000000E-03
```

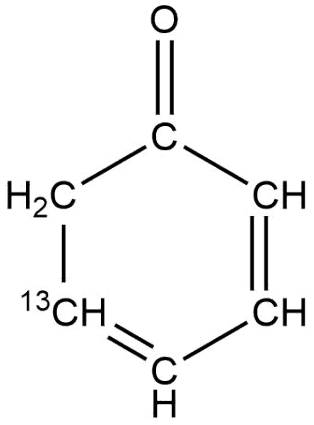
```
  5          2000                -0.015738811(  0)E-18  0.000000000E-18
  6          1100                -0.136409284(  0)E-03  0.000000000E-03
  7         40100                -0.047109659(  0)E-03  0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000021 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001205 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.60246         0.60246
```

Molecule 157

IUPAC Name: 2,4-cyclohexadien-1-one (13C5)

Common name: 2,4-cyclohexadienone (13C5)

SMILES: C1C=CC=CC1=O



157: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8739.46270    8739.46431   -0.00161    0.00200   0.00000
    2:   2  1  1  1  1  0                     9869.07450    9869.08074   -0.00624    0.00200   0.00000
    3:   3  1  3  2  1  2                    11941.29510   11941.29623   -0.00113    0.00200   0.00000
    4:   3  0  3  2  0  2                    12638.04360   12638.04362   -0.00002    0.00200   0.00000
    5:   3  2  2  2  2  1                    13433.61760   13433.61781   -0.00021    0.00200   0.00000
    6:   3  2  1  2  2  0                    14229.19530   14229.19545   -0.00015    0.00200   0.00000
    7:   3  1  2  2  1  1                    14648.16370   14648.16094    0.00276    0.00200   0.00000
    8:   4  1  4  3  1  3                    15733.68390   15733.68493   -0.00103    0.00200   0.00000
    9:   4  0  4  3  0  3                    16228.18150   16228.18131    0.00019    0.00200   0.00000
   10:   4  2  3  3  2  2                    17740.90080   17740.89891    0.00189    0.00200   0.00000
   11:   4  2  2  3  2  1                    19420.01460   19420.01373    0.00087    0.00200   0.00000
   12:   5  1  5  4  1  4                    19433.82800   19433.82716    0.00084    0.00200   0.00000
   13:   5  0  5  4  0  4                    19707.06140   19707.06140    0.00000    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.88416E-01    3   4.31216E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  5077.4123( 58)           0.0000
   2         20000                 2695.604211(311)         0.000000
```

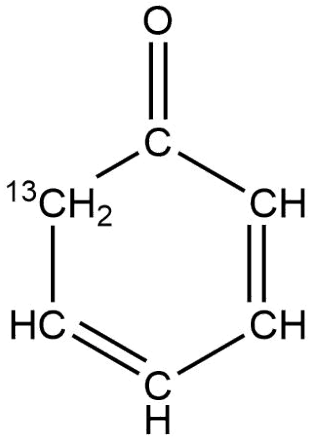
```
  3         30000                 1782.274985(256)        -0.000000
  4           200                -0.151198693(  0)E-03 -0.000000000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                -0.143764136(  0)E-03  0.000000000E-03
  7         40100                -0.045900276(  0)E-03  0.000000000E-03
  8         50000                -0.328707538(  0)E-24  0.000000000E-24
MICROWAVE AVG =       -0.000294 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002086 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.04324         1.04324
```

Molecule 158

IUPAC Name: 2,4-cyclohexadien-1-one (13C6)

Common name: 2,4-cyclohexadienone (13C6)

SMILES: C1C=CC=CC1=O



158: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      8733.90990    8733.90888    0.00102    0.00200   0.00000
    2:   3  1  3  2  1  2                     11946.37030   11946.37148   -0.00118    0.00200   0.00000
    3:   3  0  3  2  0  2                     12656.40540   12656.40524    0.00016    0.00200   0.00000
    4:   3  2  2  2  2  1                     13403.16810   13403.16625    0.00185    0.00200   0.00000
    5:   3  1  2  2  1  1                     14601.79420   14601.79432   -0.00012    0.00200   0.00000
    6:   4  1  4  3  1  3                     15750.76640   15750.76696   -0.00056    0.00200   0.00000
    7:   4  0  4  3  0  3                     16272.73560   16272.73524    0.00036    0.00200   0.00000
    8:   4  1  3  3  1  2                     19161.06030   19161.06138   -0.00108    0.00200   0.00000
    9:   5  1  5  4  1  4                     19465.17510   19465.17519   -0.00009    0.00200   0.00000
   10:   5  0  5  4  0  4                     19765.00080   19765.00052    0.00028    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.44961E-01    3   4.72322E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  5163.6082( 67)           0.0000
   2         20000                 2681.31139( 32)          -0.00000
   3         30000                1786.417112(240)         -0.000000
   4           200               -0.148077412(  0)E-03 -0.000000000E-03
   5          2000               -0.015738811(  0)E-18  0.000000000E-18
```

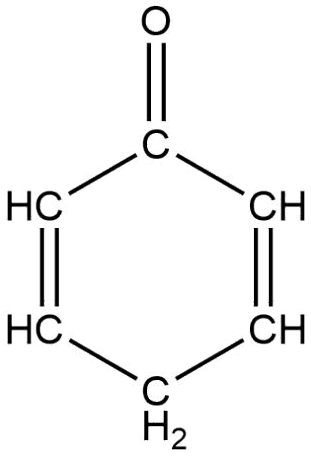
```
  6          1100                -0.136409284(  0)E-03  0.000000000E-03
  7         40100                -0.047109659(  0)E-03  0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000064 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000872 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.43582         0.43582
```

Molecule 159

IUPAC Name: 2,5-cyclohexadien-1-one

Common name: 2,5-cyclohexadienone

SMILES: O=C1C=CCC=C1



159: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 1 2 1 1 1									8041.03510		8041.03442		0.00068	0.00200	0.00000
2:	2 0 2 1 0 1									8733.61440		8733.61530		-0.00090	0.00200	0.00000
3:	2 1 1 1 1 0									9814.53080		9814.52555		0.00525	0.00200	0.00000
4:	3 1 3 2 1 2									11951.02990		11951.02936		0.00054	0.00200	0.00000
5:	3 0 3 2 0 2									12669.47240		12669.47447		-0.00207	0.00200	0.00000
6:	3 1 2 2 1 1									14583.90840		14583.90925		-0.00085	0.00200	0.00000
7:	4 1 4 3 1 3									15762.16890		15762.16809		0.00081	0.00200	0.00000
8:	4 0 4 3 0 3									16300.41940		16300.42220		-0.00280	0.00200	0.00000
9:	5 1 5 4 1 4									19484.46220		19484.46143		0.00077	0.00200	0.00000
10:	5 0 5 4 0 4									19800.25820		19800.26057		-0.00237	0.00200	0.00000
11:	5 2 4 4 2 3									21889.71820		21889.71507		0.00313	0.00200	0.00000
12:	6 0 6 5 0 5									23299.33050		23299.33172		-0.00122	0.00200	0.00000
13:	5 1 4 4 1 3									23403.08010		23403.08346		-0.00336	0.00200	0.00000
14:	7 1 7 6 1 6									26758.10220		26758.10120		0.00100	0.00200	0.00000
15:	7 0 7 6 0 6									26829.63000		26829.63007		-0.00007	0.00200	0.00000
16:	6 1 5 5 1 4									27268.91900		27268.92329		-0.00429	0.00200	0.00000
17:	8 1 8 7 1 7									30352.92260		30352.92133		0.00127	0.00200	0.00000
18:	8 0 8 7 0 7									30383.39870		30383.39800		0.00070	0.00200	0.00000
19:	7 1 6 6 1 5									30814.94640		30814.94620		0.00020	0.00200	0.00000

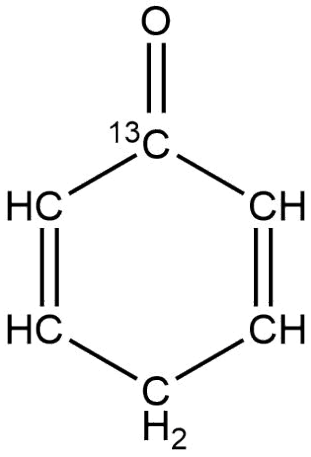
```
  20:   9  1  9  8  1  8                    33937.24180   33937.24190   -0.00010    0.00200   0.00000
  21:   9  0  9  8  0  8                    33949.69630   33949.69585    0.00045    0.00200   0.00000
  22:   8  1  7  7  1  6                    34227.40100   34227.39528    0.00572    0.00200   0.00000
  23:  10  1 10  9  1  9                    37516.93640   37516.93670   -0.00030    0.00200   0.00000
  24:  10  0 10  9  0  9                    37521.87210   37521.87440   -0.00230    0.00200   0.00000
  25:   3  2  2  2  2  1                    13391.65890   13391.65824    0.00066    0.00200   0.00000
  26:   3  2  1  2  2  0                    14113.84810   14113.84716    0.00094    0.00200   0.00000
  27:   4  2  3  3  2  2                    17702.71170   17702.71116    0.00054    0.00200   0.00000
  28:   4  3  2  3  3  1                    18175.40770   18175.40548    0.00222    0.00200   0.00000
  29:   4  3  1  3  3  0                    18334.01840   18334.01831    0.00009    0.00200   0.00000
  30:   4  2  2  3  2  1                    19254.64570   19254.64485    0.00085    0.00200   0.00000
  31:   5  3  3  4  3  2                    22751.57030   22751.57016    0.00014    0.00200   0.00000
  32:   5  3  2  4  3  1                    23266.30390   23266.30323    0.00067    0.00200   0.00000
  33:   5  2  3  4  2  2                    24383.94330   24383.94401   -0.00071    0.00200   0.00000
  34:   6  3  4  5  3  3                    27269.74750   27269.74543    0.00207    0.00200   0.00000
  35:   6  4  3  5  4  2                    27410.74970   27410.75077   -0.00107    0.00200   0.00000
  36:   6  4  2  5  4  1                    27518.42960   27518.43425   -0.00465    0.00200   0.00000
  37:   6  3  3  5  3  2                    28459.43650   28459.43608    0.00042    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.96377E-01    3   2.45458E-01    4   9.80406E-02    5   1.00000E+00    6   4.81510E-01
    7   8.81092E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 5220.70505(188)         -0.00000
   2         20000                2675.319781(273)        -0.000000
   3         30000                1788.572737(153)         0.000000
   4           200                   -0.13113(237)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                    -0.2147(136)E-03      -0.0000E-03
   7         40100                   -0.04616(144)E-03      0.00000E-03
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000056 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002123 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.06146         1.06146
```

Molecule 160

IUPAC Name: 2,5-cyclohexadien-1-one (13C1)

Common name: 2,5-cyclohexadienone (13C1)

SMILES: O=C1C=CCC=C1



160: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                      8005.74180    8005.74355   -0.00175    0.00200   0.00000
    2:   2  0  2  1  0  1                      8694.23260    8694.23398   -0.00138    0.00200   0.00000
    3:   2  1  1  1  1  0                      9762.49720    9762.49642    0.00078    0.00200   0.00000
    4:   3  1  3  2  1  2                     11900.41920   11900.42016   -0.00096    0.00200   0.00000
    5:   3  0  3  2  0  2                     12618.70720   12618.70893   -0.00173    0.00200   0.00000
    6:   3  1  2  2  1  1                     14509.15380   14509.15481   -0.00101    0.00200   0.00000
    7:   4  1  4  3  1  3                     15697.91410   15697.91373    0.00037    0.00200   0.00000
    8:   4  0  4  3  0  3                     16240.60860   16240.61024   -0.00164    0.00200   0.00000
    9:   4  1  3  3  1  2                     19058.22690   19058.22587    0.00103    0.00200   0.00000
   10:   5  1  5  4  1  4                     19407.56830   19407.56772    0.00058    0.00200   0.00000
   11:   5  0  5  4  0  4                     19729.01030   19729.01228   -0.00198    0.00200   0.00000
   12:   6  0  6  5  0  5                     23214.37340   23214.37016    0.00324    0.00200   0.00000
   13:   5  1  4  4  1  3                     23300.96030   23300.95945    0.00085    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.71775E-01    3   5.03551E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   5220.9510( 53)          -0.0000
```

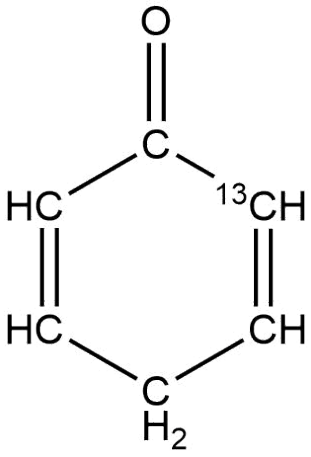
```
  2         20000                 2660.220217(286)         0.000000
  3         30000                 1781.842302(186)         0.000000
  4           200                -0.131129919(  0)E-03  0.000000000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                -0.214676345(  0)E-03 -0.000000000E-03
  7         40100                -0.046164929(  0)E-03 -0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =       -0.000276 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001515 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.75773         0.75773
```

Molecule 161

IUPAC Name: 2,5-cyclohexadien-1-one (13C2)

Common name: 2,5-cyclohexadienone (13C2)

SMILES: O=C1C=CCC=C1



161: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8701.98040    8701.97886    0.00154    0.00200   0.00000
    2:   2  1  1  1  1  0                     9801.35860    9801.35667    0.00193    0.00200   0.00000
    3:   3  1  3  2  1  2                    11898.42540   11898.42508    0.00032    0.00200   0.00000
    4:   3  0  3  2  0  2                    12605.40100   12605.40041    0.00059    0.00200   0.00000
    5:   3  2  2  2  2  1                    13357.91370   13357.91806   -0.00436    0.00200   0.00000
    6:   3  2  1  2  2  0                    14110.44140   14110.44206   -0.00066    0.00200   0.00000
    7:   3  1  2  2  1  1                    14556.89370   14556.89174    0.00196    0.00200   0.00000
    8:   4  1  4  3  1  3                    15685.65120   15685.65183   -0.00063    0.00200   0.00000
    9:   4  0  4  3  0  3                    16202.74080   16202.74027    0.00053    0.00200   0.00000
   10:   4  2  3  3  2  2                    17650.39180   17650.38965    0.00215    0.00200   0.00000
   11:   4  1  3  3  1  2                    19097.92570   19097.92891   -0.00321    0.00200   0.00000
   12:   5  0  5  4  0  4                    19678.05190   19678.05285   -0.00095    0.00200   0.00000
   13:   5  2  4  4  2  3                    21813.39480   21813.39301    0.00179    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.53742E-01    3   2.14353E-01    4   1.69428E-01    5   1.00000E+00    6   4.83931E-01
    7   6.65083E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   5137.5293( 84)          -0.0000
```

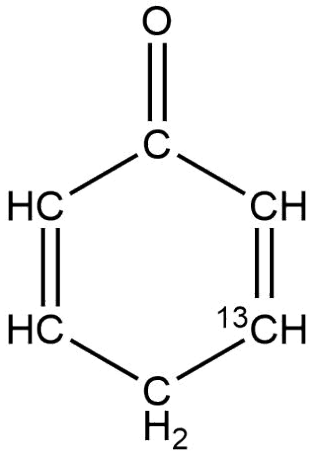
```
  2         20000                  2674.35857( 63)         -0.00000
  3         30000                  1778.28704( 56)          0.00000
  4           200                     -0.1148(130)E-03       0.0000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                      -0.265(103)E-03       -0.000E-03
  7         40100                     -0.0418( 90)E-03       0.0000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000076 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001952 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.97620         0.97620
```

Molecule 162

IUPAC Name: 2,5-cyclohexadien-1-one (13C3)

Common name: 2,5-cyclohexadienone (13C3)

SMILES: O=C1C=CCC=C1



162: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      8662.41330    8662.41574   -0.00244    0.00200   0.00050
    2:   3  1  3  2  1  2                     11847.67510   11847.67569   -0.00059    0.00200   0.00105
    3:   3  0  3  2  0  2                     12554.97040   12554.97145   -0.00105    0.00200   0.00087
    4:   3  2  2  2  2  1                     13291.55970   13291.55425    0.00545    0.00200   0.00082
    5:   3  2  1  2  2  0                     14028.14040   14028.14170   -0.00130    0.00200   0.00154
    6:   3  1  2  2  1  1                     14481.07690   14481.07786   -0.00096    0.00200   0.00153
    7:   4  1  4  3  1  3                     15621.44970   15621.45048   -0.00078    0.00200   0.00130
    8:   4  0  4  3  0  3                     16143.57050   16143.57040    0.00010    0.00200   0.00117
    9:   5  0  5  4  0  4                     19607.36570   19607.36511    0.00059    0.00200   0.00135
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.74383E-01    3   3.71049E-01    4   8.29942E-01    5   1.00000E+00    6   9.97118E-01
    7   9.03234E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                   5138.7034( 73)           0.0000
   2         20000                  2658.93766( 42)          0.00000
   3         30000                  1771.58662( 36)         -0.00000
   4           200                    -0.12905(231)E-03      0.00000E-03
   5          2000                -0.015738811(  0)E-18 -0.000000000E-18
```

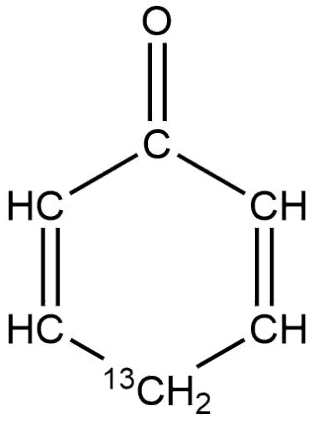
```
  6          1100                    -0.1936(135)E-03      -0.0000E-03
  7         40100                    -0.04683(142)E-03      0.00000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =       -0.000109 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002126 MHz, IR RMS =        0.00000
END OF ITERATION  2 OLD, NEW RMS ERROR=        1.06911         1.06911
```

Molecule 163

IUPAC Name: 2,5-cyclohexadien-1-one (13C4)

Common name: 2,5-cyclohexadienone (13C4)

SMILES: O=C1C=CCC=C1



163: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                     7925.95500    7925.91532    0.03968    0.05000   0.00000
    2:   2  0  2  1  0  1                     8605.06700    8605.13141   -0.06441    0.05000   0.00000
    3:   3  1  3  2  1  2                    11785.77700   11785.70257    0.07443    0.05000   0.00000
    4:   3  0  3  2  0  2                    12503.20000   12503.12912    0.07088    0.05000   0.00000
    5:   3  1  2  2  1  1                    14340.62200   14340.98798   -0.36598    0.05000   0.00000
    6:   4  1  4  3  1  3                    15552.08900   15551.96998    0.11902    0.05000   0.00000
    7:   4  0  4  3  0  3                    16104.26000   16104.06852    0.19148    0.05000   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.00000E+00    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000              5220.705000000(  0)      0.000000000
   2         20000              2626.394900000(  0)     -0.000000000
   3         30000              1766.508000000(  0)      0.000000000
   4           200                -0.131129919(  0)E-03  0.000000000E-03
   5          2000                -0.015738811(  0)E-18  0.000000000E-18
   6          1100                -0.214676345(  0)E-03  0.000000000E-03
   7         40100                -0.046164929(  0)E-03 -0.000000000E-03
   8         50000                -0.328707538(  0)E-24  0.000000000E-24
```

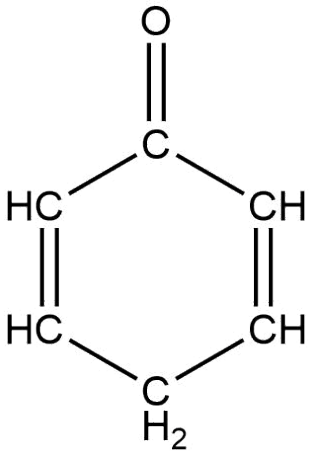
```
MICROWAVE AVG =        0.009299 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.169477 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        3.38955         3.38955
```

Molecule 164

IUPAC Name: 2,5-cyclohexadien-1-one (1v20)

Common name: 2,5-cyclohexadienone (1v20)

SMILES: O=C1C=CCC=C1



164: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8732.07510    8732.07548   -0.00038    0.00200   0.00000
    2:   3  0  3  2  0  2                    12667.55320   12667.55354   -0.00034    0.00200   0.00000
    3:   4  0  4  3  0  3                    16298.58370   16298.58336    0.00034    0.00200   0.00000
    4:   3  1  3  2  1  2                    11950.47610   11950.47528    0.00082    0.00200   0.00000
    5:   3  1  2  2  1  1                    14579.58430   14579.58418    0.00012    0.00200   0.00000
    6:   4  1  4  3  1  3                    15761.58960   15761.59020   -0.00060    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.54487E-01    3   4.73774E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  5213.9981( 94)          -0.0000
   2         20000                 2674.26948( 52)          0.00000
   3         30000                 1788.77990( 36)          0.00000
   4           200               -0.131129919(271)E-03 -0.000000000E-03
   5          2000               -0.015738811(  0)E-18 -0.000000000E-18
   6          1100                -0.21467635( 37)E-03   0.00000000E-03
   7         40100               -0.046164929(205)E-03  0.000000000E-03
   8         50000               -0.328707538(  0)E-24  0.000000000E-24
```

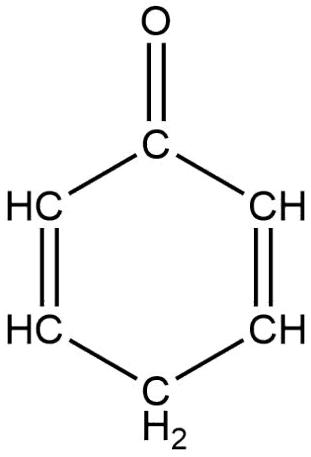
```
MICROWAVE AVG =       -0.000006 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000487 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.24350         0.24350
```

Molecule 165

IUPAC Name: 2,5-cyclohexadien-1-one (1v22)

Common name: 2,5-cyclohexadienone (1v22)

SMILES: O=C1C=CCC=C1



165: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     8740.50730    8740.50701    0.00029    0.00200   0.00000
    2:   2  1  1  1  1  0                     9823.48000    9823.47924    0.00076    0.00200   0.00000
    3:   3  1  3  2  1  2                    11961.41090   11961.41395   -0.00305    0.00200   0.00000
    4:   3  0  3  2  0  2                    12677.53340   12677.53619   -0.00279    0.00200   0.00000
    5:   3  1  2  2  1  1                    14596.32020   14596.32060   -0.00040    0.00200   0.00000
    6:   4  1  4  3  1  3                    15775.14500   15775.14608   -0.00108    0.00200   0.00000
    7:   4  0  4  3  0  3                    16309.64890   16309.65157   -0.00267    0.00200   0.00000
    8:   4  1  3  3  1  2                    19164.73370   19164.73221    0.00149    0.00200   0.00000
    9:   5  1  5  4  1  4                    19499.88280   19499.88235    0.00045    0.00200   0.00000
   10:   5  0  5  4  0  4                    19812.16500   19812.16502   -0.00002    0.00200   0.00000
   11:   6  0  6  5  0  5                    23314.90940   23314.90547    0.00393    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.60773E-01    3   4.08284E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                 5208.0483( 72)           0.0000
   2         20000                2677.755828(304)        -0.000000
   3         30000                1790.218543(239)        -0.000000
```

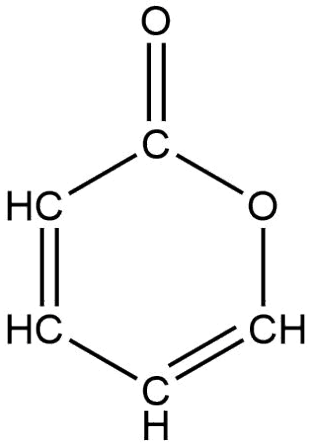
```
  4           200                -0.148077412(271)E-03  0.000000000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                 -0.13640928( 37)E-03   0.00000000E-03
  7         40100                -0.047109659(205)E-03 -0.000000000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =       -0.000282 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002001 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.00069         1.00069
```

Molecule 166

IUPAC Name: 2-pyranone

Common name: 2H-pyran-2-one, alpha-pyrone

SMILES: C1=CC(=O)OC=C1



166: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  1  2  1  1  1                      8618.63610    8618.63702   -0.00092    0.00200   0.00000
    2:   2  0  2  1  0  1                      9377.00150    9376.99941    0.00209    0.00200   0.00000
    3:   2  1  1  1  1  0                     10558.86110   10558.85753    0.00357    0.00200   0.00000
    4:   3  1  3  2  1  2                     12807.39570   12807.39638   -0.00068    0.00200   0.00000
    5:   3  0  3  2  0  2                     13595.19950   13595.19870    0.00080    0.00200   0.00000
    6:   3  1  2  2  1  1                     15687.99560   15687.99874   -0.00314    0.00200   0.00000
    7:   4  1  4  3  1  3                     16888.20680   16888.20831   -0.00151    0.00200   0.00000
    8:   4  0  4  3  0  3                     17479.66400   17479.66400   -0.00000    0.00200   0.00000
    9:   5  1  5  4  1  4                     20871.86790   20871.86614    0.00176    0.00200   0.00000
   10:   5  0  5  4  0  4                     21219.69740   21219.69804   -0.00064    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.97447E-01    3   2.58804E-01    4   5.08044E-01    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        5677.6273( 74)          -0.0000
   2         20000          B       2882.24249( 41)          0.00000
   3         30000          C       1912.13224( 44)          0.00000
   4           200    Delta_J          -0.0684( 82)E-03      -0.0000E-03
   5          1100   Delta_JK      0.578664556(  0)E-21 -0.000000000E-21
```

```
  6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
  7         40100     -del_J     -0.803383257(  0)E-24  0.000000000E-24
  8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000134 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.001864 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.93219         0.93219
```

Molecule 167

IUPAC Name: 2,4,6-heptatriynenitrile

Common name: cyanohexatriyne

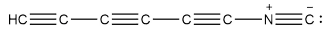
SMILES: C#CC#CC#CC#N

Molecule 168

IUPAC Name: isocyano-1,3,5-hexatriyne

Common name: isocyanotriacetylene

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



Molecule 169

IUPAC Name: 7-oxo-1,2,3,4,5,6-heptahexaenylidene

Common name: heptacarbonmonoxide

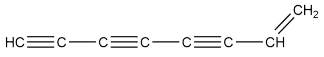
SMILES: [C]=C=C=C=C=C=O

Molecule 170

IUPAC Name: 1-octene-3,5,7-triyne

Common name: vinyltriacetylene

SMILES: C=CC#CC#CC#C

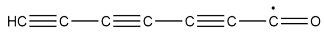


Molecule 171

IUPAC Name: 2,4,6-heptatriyn-1-on-1-yl

Common name: hepta-2,4,6-triyn-1-on-1-yl

SMILES: C#CC#CC#C[C]=O

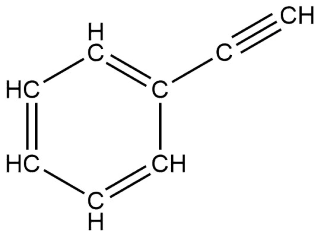


Molecule 172

IUPAC Name: ethynylbenzene

Common name: phenylacetylene

SMILES: C#CC1=CC=CC=C1

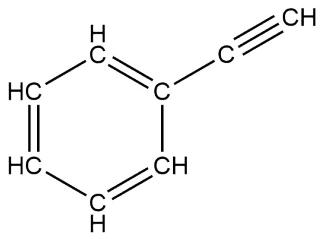


Molecule 173

IUPAC Name: ethynylbenzene (1v16)

Common name: phenylacetylene (1v16)

SMILES: C#CC1=CC=CC=C1



173: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                     7709.24560    7709.24712   -0.00152    0.00200   0.00000
    2:   3  0  3  2  0  2                     8134.09660    8134.09556    0.00104    0.00200   0.00000
    3:   3  1  2  2  1  1                     8681.65560    8681.65352    0.00208    0.00200   0.00000
    4:   4  0  4  3  0  3                    10762.95200   10762.95326   -0.00126    0.00200   0.00000
    5:   4  1  3  3  1  2                    11552.63120   11552.63057    0.00063    0.00200   0.00000
    6:   5  1  5  4  1  4                    12793.72650   12793.72720   -0.00070    0.00200   0.00000
    7:   5  0  5  4  0  4                    13328.55970   13328.56026   -0.00056    0.00200   0.00000
    8:   5  1  4  4  1  3                    14401.99070   14401.99088   -0.00018    0.00200   0.00000
    9:   6  1  6  5  1  5                    15311.46010   15311.45889    0.00121    0.00200   0.00000
   10:   6  0  6  5  0  5                    15828.96670   15828.96576    0.00094    0.00200   0.00000
   11:   6  1  5  5  1  4                    17221.87000   17221.87133   -0.00133    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.82756E-01    3   3.34887E-01    4   1.54147E-01    5   1.00000E+00    6   8.26471E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    5674.829( 55)            0.000
   2         20000                  1529.99464( 38)         -0.00000
   3         30000                 1205.643651(307)        -0.000000
   4           200                     -0.0291( 73)E-03      -0.0000E-03
   5          2000                 0.100000000(  0)E-21 -0.000000000E-21
   6          1100                      -1.05( 43)E-03         0.00E-03
   7         40100                 -5.36425720( 28)E-30   0.00000000E-30
   8         41000                 -4.95790905( 40)E-30  -0.00000000E-30
 MICROWAVE AVG =        0.000032 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001154 MHz, IR RMS =        0.00000
```

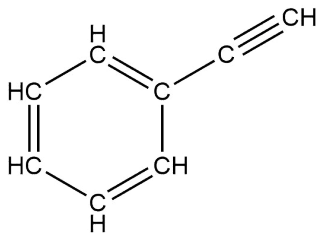
```
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.57709         0.57709
```

Molecule 174

IUPAC Name: ethynylbenzene (1v23)

Common name: phenylacetylene (1v23)

SMILES: C#CC1=CC=CC=C1



174: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 1 1 1 1 0									5796.97700		5796.97135		0.00565	0.00200	0.00000
2:	3 1 3 2 1 2									7710.99640		7710.99890		-0.00250	0.00200	0.00000
3:	3 0 3 2 0 2									8135.80150		8135.80110		0.00040	0.00200	0.00000
4:	3 2 2 2 2 1									8208.78850		8208.78964		-0.00114	0.00200	0.00000
5:	3 2 1 2 2 0									8281.80590		8281.80244		0.00346	0.00200	0.00000
6:	3 1 2 2 1 1									8683.65020		8683.64425		0.00595	0.00200	0.00000
7:	4 1 4 3 1 3									10261.38100		10261.38354		-0.00254	0.00200	0.00000
8:	4 0 4 3 0 3									10765.01710		10765.01663		0.00047	0.00200	0.00000
9:	4 2 3 3 2 2									10930.76820		10930.76686		0.00134	0.00200	0.00000
10:	4 3 2 3 3 1									10979.83920		10979.83665		0.00255	0.00200	0.00000
11:	4 3 1 3 3 0									10983.73000		10983.72807		0.00193	0.00200	0.00000
12:	4 2 2 3 2 1									11110.81520		11110.81343		0.00177	0.00200	0.00000
13:	4 1 3 3 1 2									11555.22520		11555.21915		0.00605	0.00200	0.00000
14:	5 1 5 4 1 4									12796.50940		12796.51277		-0.00337	0.00200	0.00000
15:	5 0 5 4 0 4									13330.85390		13330.85406		-0.00016	0.00200	0.00000
16:	5 2 4 4 2 3									13640.54430		13640.54232		0.00198	0.00200	0.00000
17:	5 4 2 4 4 1									13721.95030		13721.95187		-0.00157	0.00200	0.00000
18:	5 4 1 4 4 0									13722.10360		13722.10438		-0.00078	0.00200	0.00000
19:	5 3 3 4 3 2									13737.77680		13737.77647		0.00033	0.00200	0.00000
20:	5 3 2 4 3 1									13751.33680		13751.33683		-0.00003	0.00200	0.00000
21:	5 2 3 4 2 2									13990.88350		13990.88392		-0.00042	0.00200	0.00000
22:	5 1 4 4 1 3									14405.11520		14405.11069		0.00451	0.00200	0.00000
23:	6 1 6 5 1 5									15314.70910		15314.71242		-0.00332	0.00200	0.00000
24:	6 0 6 5 0 5									15831.41630		15831.41722		-0.00092	0.00200	0.00000
25:	6 2 5 5 2 4									16335.17730		16335.17502		0.00228	0.00200	0.00000
26:	6 2 4 5 2 3									16920.67820		16920.68409		-0.00589	0.00200	0.00000

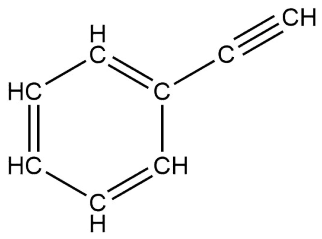
```
  27:   6  1  5  5  1  4                    17225.42880   17225.42678    0.00202    0.00200   0.00000
  28:   7  1  7  6  1  6                    17815.44750   17815.45032   -0.00282    0.00200   0.00000
  29:   7  0  7  6  0  6                    18275.76940   18275.77004   -0.00064    0.00200   0.00000
  30:   7  1  6  6  1  5                    20006.81400   20006.81766   -0.00366    0.00200   0.00000
  31:   8  1  8  7  1  7                    20299.26580   20299.26658   -0.00078    0.00200   0.00000
  32:   8  0  8  7  0  7                    20680.99690   20680.99696   -0.00006    0.00200   0.00000
  33:   8  1  7  7  1  6                    22738.70560   22738.71406   -0.00846    0.00200   0.00000
  34:   9  0  9  8  0  8                    23065.66900   23065.66544    0.00356    0.00200   0.00000
  35:  10  1 10  9  1  9                    25222.38400   25222.37915    0.00485    0.00200   0.00000
NORMALIZED DIAGONAL:
   1   1.00000E+00    2   7.02237E-01    3   3.35059E-01    4   5.33038E-01    5   1.00000E+00    6   9.97581E-01
   7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000                  5665.5108( 86)          -0.0000
  2         20000                 1530.351997(112)         0.000000
  3         30000                 1205.920239(134)         0.000000
  4           200                    -0.02601( 77)E-03      0.00000E-03
  5          2000                10.000000000(  0)E-03 -0.000000000E-03
  6          1100                     -1.0108( 97)E-03      -0.0000E-03
  7         40100                 -5.36425720( 28)E-30  -0.00000000E-30
  8         41000                 -4.95790905( 40)E-30   0.00000000E-30
 MICROWAVE AVG =        0.000288 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.003253 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.62635         1.62635
```

Molecule 175

IUPAC Name: ethynylbenzene (2v23)

Common name: phenylacetylene (2v23)

SMILES: C#CC1=CC=CC=C1



175: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                     7716.15660    7716.16512   -0.00852    0.00200   0.00087
    2:   3  0  3  2  0  2                     8140.40870    8140.39938    0.00932    0.00200   0.00044
    3:   3  1  2  2  1  1                     8687.88340    8687.87685    0.00655    0.00200   0.00075
    4:   4  1  4  3  1  3                    10268.24540   10268.24473    0.00067    0.00200   0.00111
    5:   4  0  4  3  0  3                    10771.04720   10771.03879    0.00841    0.00200   0.00057
    6:   4  1  3  3  1  2                    11560.82440   11560.82370    0.00070    0.00200   0.00093
    7:   5  1  5  4  1  4                    12805.05180   12805.05294   -0.00114    0.00200   0.00133
    8:   5  0  5  4  0  4                    13338.25470   13338.25153    0.00317    0.00200   0.00100
    9:   5  1  4  4  1  3                    14412.04470   14412.04648   -0.00178    0.00200   0.00107
   10:   6  0  6  5  0  5                    15840.19540   15840.19875   -0.00335    0.00200   0.00163
   11:   6  1  5  5  1  4                    17233.62730   17233.63435   -0.00705    0.00200   0.00122
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.05505E-01    3   5.05514E-01    4   9.99025E-01    5   1.00000E+00    6   9.99903E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  5651.6941(237)           0.0000
   2         20000                1530.981076(192)         0.000000
   3         30000                1206.859674(218)        -0.000000
   4           200                  -0.036790( 64)E-03     0.000000E-03
   5          2000                10.000000000(  0)E-03 -0.000000000E-03
   6          1100                   1.00781(195)E-03     -0.00000E-03
   7         40100                -5.36425720( 28)E-30  -0.00000000E-30
   8         41000                -4.95790905( 40)E-30  -0.00000000E-30
 MICROWAVE AVG =        0.000634 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005636 MHz, IR RMS =        0.00000
```

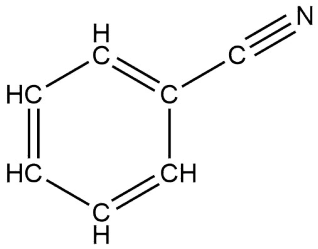
```
END OF ITERATION  2 OLD, NEW RMS ERROR=        2.81839         2.81839
```

Molecule 176

IUPAC Name: benzonitrile

Common name: cyanobenzene

SMILES: C1=CC=C(C=C1)C#N

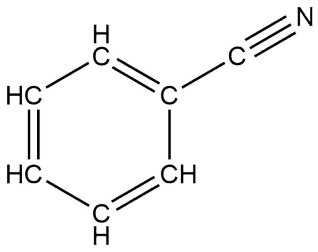


Molecule 177

IUPAC Name: benzonitrile (1v12)

Common name: cyanobenzene (1v12)

SMILES: C1=CC=C(C=C1)C#N



177: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.				
1:	3	0	3	2	2	0	2	1		8204.91260		8204.91489		-0.00229		0.00200	0.00000	
2:	3	0	3	3	2	0	2	2		8205.14320		8205.14344		-0.00024		0.00200	0.00000	
3:	3	0	3	4	2	0	2	3		8205.18140		8205.18364		-0.00224		0.00200	0.00000	
4:	4	1	4	4	3	1	3	3		10340.28340		10340.28192		0.00148		0.00200	0.00000	
5:	4	1	4	3	3	1	3	2		10340.39860		10340.39650		0.00210		0.00200	0.00000	
6:	4	1	4	5	3	1	3	4		10340.44780		10340.44856		-0.00076		0.00200	0.00000	
7:	4	0	4	3	3	0	3	2		10852.67660		10852.67667		-0.00007		0.00200	0.00000	
8:	4	0	4	4	3	0	3	3		10852.78310		10852.78526		-0.00216		0.00200	0.00000	
9:	4	0	4	5	3	0	3	4		10852.80430		10852.80348		0.00082		0.00200	0.00000	
10:	4	1	3	4	3	1	2	3		11668.06590		11668.06608		-0.00018		0.00200	0.00000	
11:	4	1	3	3	3	1	2	2		11668.17090		11668.17303		-0.00213		0.00200	0.00000	
12:	4	1	3	5	3	1	2	4		11668.22950		11668.23432		-0.00482		0.00200	0.00000	
13:	5	1	5	5	4	1	4	4		12893.56710		12893.56838		-0.00128		0.00200	0.00000	
14:	5	1	5	4	4	1	4	3		12893.61240		12893.61181		0.00059		0.00200	0.00000	
15:	5	1	5	6	4	1	4	5		12893.65880		12893.65723		0.00157		0.00200	0.00000	
16:	5	1	4	5	4	1	3	4		14543.80390		14543.79827		0.00563		0.00200	0.00000	
17:	5	1	4	6	4	1	3	5		14543.89110		14543.88709		0.00401		0.00200	0.00000	
18:	5	0	5	4	4	0	4	3		13433.85060		13433.85440		-0.00380		0.00200	0.00000	
19:	5	0	5	5	4	0	4	4		13433.91950		13433.92376		-0.00426		0.00200	0.00000	
20:	5	0	5	6	4	0	4	5		13433.92850		13433.92983		-0.00133		0.00200	0.00000	
21:	6	0	6	5	5	0	5	4		15947.31110		15947.31113		-0.00003		0.00200	0.00000	
22:	6	0	6	6	5	0	5	5		15947.36240		15947.36174		0.00066		0.00200	0.00000	15947.36159	0.00081
23:	6	0	6	7	5	0	5	6		15947.36240		15947.36144		0.00096		0.00200	0.00000	15947.36159	0.00081
24:	7	0	7	6	6	0	6	5		18403.58090		18403.57767		0.00323		0.00200	0.00000	
25:	7	0	7	7	6	0	6	6		18403.61520		18403.61610		-0.00090		0.00200	0.00000	18403.61459	0.00061
26:	7	0	7	8	6	0	6	7		18403.61520		18403.61308		0.00212		0.00200	0.00000	18403.61459	0.00061

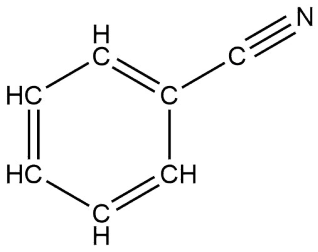
```
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.23950E-01    3   4.15158E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   9.96995E-01   10   8.82733E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        5655.5985(130)           0.0000
   2         20000          B      1546.911676(160)         0.000000
   3         30000          C      1213.899053(149)        -0.000000
   4           200     -Del_J     -0.045550279(150)E-03  0.000000000E-03
   5          1100    -Del_JK      -0.93304105( 56)E-03   0.00000000E-03
   6          2000     -Del_K     -0.271827665(100)E-03  0.000000000E-03
   7         40100     -del_J      -0.01109396( 41)E-03  -0.00000000E-03
   8         41000     -del_K      -0.61408849( 53)E-03  -0.00000000E-03
   9     110010000     chi_aa          -4.3004(276)          -0.0000
  10     110020000     chi_bb           2.3068(237)           0.0000
 MICROWAVE AVG =       -0.000198 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002489 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.24461         1.24461
```

Molecule 178

IUPAC Name: benzonitrile (1v15)

Common name: cyanobenzene (1v15)

SMILES: C1=CC=C(C=C1)C#N



178: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.				
1:	3	0	3	2	2	0	2	1		8209.58480		8209.58408		0.00072		0.00200	0.00000	
2:	3	0	3	4	2	0	2	3		8209.84820		8209.84878		-0.00058		0.00200	0.00000	
3:	4	1	4	4	3	1	3	3		10348.16780		10348.16759		0.00021		0.00200	0.00000	
4:	4	1	4	3	3	1	3	2		10348.28460		10348.28051		0.00409		0.00200	0.00000	
5:	4	1	4	5	3	1	3	4		10348.33080		10348.33140		-0.00060		0.00200	0.00000	
6:	4	0	4	3	3	0	3	2		10859.27130		10859.27131		-0.00001		0.00200	0.00000	
7:	4	0	4	4	3	0	3	3		10859.37710		10859.37896		-0.00186		0.00200	0.00000	
8:	4	0	4	5	3	0	3	4		10859.39850		10859.39625		0.00225		0.00200	0.00000	10859.39625	0.00225
9:	4	0	4	5	3	0	3	4		10859.39850		10859.39625		0.00225		0.00200	0.00000	10859.39625	0.00225
10:	4	1	3	4	3	1	2	3		11672.07280		11672.07134		0.00146		0.00200	0.00000	
11:	4	1	3	3	3	1	2	2		11672.17640		11672.17614		0.00026		0.00200	0.00000	
12:	4	1	3	5	3	1	2	4		11672.23820		11672.23690		0.00130		0.00200	0.00000	
13:	5	1	5	5	4	1	4	4		12903.55390		12903.55692		-0.00302		0.00200	0.00000	
14:	5	1	5	4	4	1	4	3		12903.59920		12903.59963		-0.00043		0.00200	0.00000	
15:	5	1	5	6	4	1	4	5		12903.64450		12903.64414		0.00036		0.00200	0.00000	
16:	5	0	5	4	4	0	4	3		13442.63510		13442.63697		-0.00187		0.00200	0.00000	
17:	5	0	5	5	4	0	4	4		13442.70430		13442.70611		-0.00181		0.00200	0.00000	
18:	5	0	5	6	4	0	4	5		13442.71280		13442.71131		0.00149		0.00200	0.00000	
19:	5	1	4	5	4	1	3	4		14548.99310		14548.99106		0.00204		0.00200	0.00000	
20:	5	1	4	4	4	1	3	3		14549.02370		14549.02779		-0.00409		0.00200	0.00000	
21:	5	1	4	6	4	1	3	5		14549.07810		14549.07832		-0.00022		0.00200	0.00000	
22:	6	0	6	5	5	0	5	4		15958.51050		15958.51091		-0.00041		0.00200	0.00000	
23:	6	0	6	6	5	0	5	5		15958.56160		15958.56162		-0.00002		0.00200	0.00000	15958.56106	0.00054
24:	6	0	6	7	5	0	5	6		15958.56160		15958.56050		0.00110		0.00200	0.00000	15958.56106	0.00054
25:	7	0	7	6	6	0	6	5		18417.33690		18417.33619		0.00071		0.00200	0.00000	
26:	7	0	7	7	6	0	6	6		18417.37350		18417.37491		-0.00141		0.00200	0.00000	18417.37304	0.00046

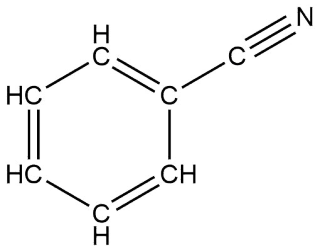
```
   27:   7  0  7  8  6  0  6  7              18417.37350   18417.37117    0.00233    0.00200   0.00000   18417.37304    0.00046
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.34301E-01    3   4.19668E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   9.98098E-01   10   8.85988E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        5649.9153(130)          -0.0000
   2         20000          B      1547.145261(147)         0.000000
   3         30000          C      1215.108892(147)         0.000000
   4           200     -Del_J     -0.045550279(150)E-03 -0.000000000E-03
   5          1100    -Del_JK      -0.93304105( 56)E-03   0.00000000E-03
   6          2000     -Del_K     -0.271827665(100)E-03 -0.000000000E-03
   7         40100     -del_J      -0.01109396( 41)E-03  -0.00000000E-03
   8         41000     -del_K      -0.61408849( 53)E-03   0.00000000E-03
   9     110010000     chi_aa          -4.2338(275)          -0.0000
  10     110020000     chi_bb           2.2844(244)           0.0000
 MICROWAVE AVG =        0.000041 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001720 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.86002         0.86002
```

Molecule 179

IUPAC Name: benzonitrile (1v21)

Common name: cyanobenzene (1v21)

SMILES: C1=CC=C(C=C1)C#N



179: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.			
1:	3	1	3	3	2	1	2	3		7777.47570		7777.47519		0.00051	0.00200	0.00000		
2:	3	1	3	3	2	1	2	2		7778.10920		7778.10838		0.00082	0.00200	0.00000		
3:	3	1	3	4	2	1	2	3		7778.48380		7778.48376		0.00004	0.00200	0.00000	7778.48419	-0.0003
4:	3	1	3	2	2	1	2	1		7778.48380		7778.48463		-0.00083	0.00200	0.00000	7778.48419	-0.0003
5:	3	1	3	2	2	1	2	2		7779.46850		7779.47037		-0.00187	0.00200	0.00000		
6:	3	0	3	3	2	0	2	3		8209.77740		8209.78068		-0.00328	0.00200	0.00000		
7:	3	0	3	2	2	0	2	1		8210.91170		8210.91342		-0.00172	0.00200	0.00000		
8:	3	0	3	3	2	0	2	2		8211.13770		8211.13916		-0.00146	0.00200	0.00000		
9:	3	0	3	4	2	0	2	3		8211.17840		8211.17891		-0.00051	0.00200	0.00000		
10:	3	0	3	2	2	0	2	2		8213.02520		8213.02708		-0.00188	0.00200	0.00000		
11:	3	2	2	3	2	2	1	2		8287.11100		8287.11698		-0.00598	0.05000	0.00000		
12:	3	2	2	4	2	2	1	3		8288.44400		8288.48231		-0.03831	0.05000	0.00000		
13:	3	2	2	2	2	2	1	1		8289.24400		8289.24119		0.00281	0.05000	0.00000		
14:	3	1	2	3	2	1	1	2		8773.49670		8773.49626		0.00044	0.00200	0.00000		
15:	3	1	2	4	2	1	1	3		8773.87590		8773.87504		0.00086	0.00200	0.00000		
16:	3	1	2	2	2	1	1	2		8774.99500		8774.99629		-0.00129	0.00200	0.00000		
17:	4	1	4	4	3	1	3	3		10350.04250		10350.04244		0.00006	0.00200	0.00000		
18:	4	1	4	3	3	1	3	2		10350.15660		10350.15563		0.00097	0.00200	0.00000		
19:	4	1	4	5	3	1	3	4		10350.20810		10350.20708		0.00102	0.00200	0.00000		
20:	4	0	4	4	3	0	3	4		10859.63180		10859.63258		-0.00078	0.00200	0.00000		
21:	4	0	4	3	3	0	3	2		10860.92340		10860.92360		-0.00020	0.00200	0.00000		
22:	4	0	4	4	3	0	3	3		10861.02850		10861.03081		-0.00231	0.00200	0.00000		
23:	4	0	4	5	3	0	3	4		10861.04980		10861.04887		0.00093	0.00200	0.00000		
24:	4	0	4	3	3	0	3	3		10862.81270		10862.81152		0.00118	0.00200	0.00000		
25:	4	2	3	4	3	2	2	3		11035.37800		11035.39504		-0.01704	0.05000	0.00000		
26:	4	2	3	5	3	2	2	4		11036.00000		11035.97264		0.02736	0.05000	0.00000	11036.02738	-0.0273

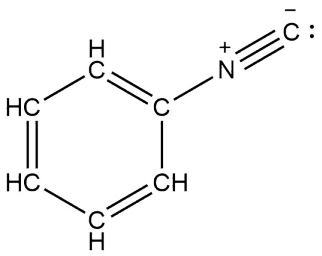
```
  27:   4  2  3  3  3  2  2  2              11036.00000   11036.12105   -0.12105    0.05000   0.00000   11036.02738   -0.02738
  28:   4  2  2  4  3  2  1  3              11225.24400   11225.27262   -0.02862    0.05000   0.00000
  29:   4  2  2  5  3  2  1  4              11225.86700   11225.86436    0.00264    0.05000   0.00000
  30:   4  2  2  3  3  2  1  2              11226.04400   11226.01476    0.02924    0.05000   0.00000
  31:   4  1  3  4  3  1  2  3              11673.93010   11673.92882    0.00128    0.00200   0.00000
  32:   4  1  3  3  3  1  2  2              11674.03290   11674.03451   -0.00161    0.00200   0.00000
  33:   4  1  3  5  3  1  2  4              11674.09580   11674.09503    0.00077    0.00200   0.00000
  34:   5  1  5  5  4  1  4  4              12905.85910   12905.85978   -0.00068    0.00200   0.00000
  35:   5  1  5  4  4  1  4  3              12905.90370   12905.90269    0.00101    0.00200   0.00000
  36:   5  1  5  6  4  1  4  5              12905.94590   12905.94757   -0.00167    0.00200   0.00000
  37:   5  0  5  4  4  0  4  3              13444.54410   13444.54288    0.00122    0.00200   0.00000
  38:   5  0  5  5  4  0  4  4              13444.60970   13444.61133   -0.00163    0.00200   0.00000
  39:   5  0  5  6  4  0  4  5              13444.62000   13444.61739    0.00261    0.00200   0.00000
  40:   6  1  6  6  5  1  5  5              15443.95200   15443.95266   -0.00066    0.00200   0.00000
  41:   6  1  6  5  5  1  5  4              15443.97210   15443.96975    0.00235    0.00200   0.00000
  42:   6  1  6  7  5  1  5  6              15444.00570   15444.00494    0.00076    0.00200   0.00000
  43:   6  0  6  5  5  0  5  4              15960.63760   15960.63873   -0.00113    0.00200   0.00000
  44:   6  0  6  7  5  0  5  6              15960.68870   15960.68842    0.00028    0.00200   0.00000   15960.68854    0.00016
  45:   6  0  6  6  5  0  5  5              15960.68870   15960.68866    0.00004    0.00200   0.00000   15960.68854    0.00016
  46:   6  1  5  6  5  1  4  5              17397.07920   17397.07918    0.00002    0.00200   0.00000
  47:   6  1  5  5  5  1  4  4              17397.09260   17397.09056    0.00204    0.00200   0.00000
  48:   6  1  5  7  5  1  4  6              17397.12950   17397.12967   -0.00017    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.48601E-01    3   5.55449E-01    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   8.02990E-01   10   9.99992E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        5643.7338(130)           0.0000
   2         20000          B      1547.385289(131)         0.000000
   3         30000          C      1215.350090(101)         0.000000
   4           200      -Del_J     -0.045550285(150)E-03  0.000000000E-03
   5          1100     -Del_JK      -0.93304105( 56)E-03   0.00000000E-03
   6          2000      -Del_K     -0.271827665(100)E-03  0.000000000E-03
   7         40100      -del_J      -0.01109396( 41)E-03  -0.00000000E-03
   8         41000      -del_K      -0.61408849( 53)E-03  -0.00000000E-03
   9     110010000      chi_aa         -4.24836(235)         -0.00000
  10     110020000      chi_bb           2.2779( 34)           0.0000
 MICROWAVE AVG =       -0.001930 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.009777 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.64947         0.64947
```

Molecule 180

IUPAC Name: isocyanobenzene

Common name: phenylisocyanide

SMILES: [C-]#[N+]C1=CC=CC=C1

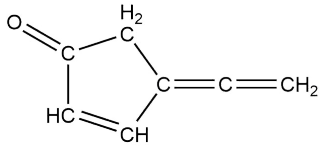


Molecule 181

IUPAC Name: 4-ethenylidene-2-cyclopenten-1-one

Common name: 4-vinylidenecyclopentenone

SMILES: C=C=C1C=CC(=O)C1



181: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  1  3  2  1  2                     6642.96000    6642.96208   -0.00208    0.05200   0.00000
    2:   4  1  4  3  1  3                     8851.10330    8851.10488   -0.00158    0.00200   0.00000
    3:   4  0  4  3  0  3                     9194.46230    9194.45848    0.00382    0.00200   0.00000
    4:   4  1  3  3  1  2                     9625.01700    9625.01661    0.00039    0.00200   0.00000
    5:   5  1  5  4  1  4                    11054.23470   11054.23663   -0.00193    0.00200   0.00000
    6:   5  0  5  4  0  4                    11452.92080   11452.91814    0.00266    0.00200   0.00000
    7:   5  1  4  4  1  3                    12020.32050   12020.31805    0.00245    0.00200   0.00000
    8:   6  1  6  5  1  5                    13251.44850   13251.44958   -0.00108    0.00200   0.00000
    9:   6  1  5  5  1  4                    14407.77060   14407.77132   -0.00072    0.00200   0.00000
   10:   6  0  6  5  0  5                    13686.28850   13686.28619    0.00231    0.00200   0.00000
   11:   7  1  7  6  1  6                    15442.04670   15442.04766   -0.00096    0.00200   0.00000
   12:   7  0  7  6  0  6                    15892.15150   15892.15015    0.00135    0.00200   0.00000
   13:   7  1  6  6  1  5                    16785.25180   16785.25778   -0.00598    0.00200   0.00000
   14:   8  1  8  7  1  7                    17625.56770   17625.56794   -0.00024    0.00200   0.00000
   15:   8  0  8  7  0  7                    18070.24710   18070.24728   -0.00018    0.00200   0.00000
   16:   9  1  9  8  1  8                    19801.79110   19801.78877    0.00233    0.00200   0.00000
   17:   9  0  9  8  0  8                    20222.73370   20222.73332    0.00038    0.00200   0.00000
   18:   3  1  3  2  0  2                    11483.91560   11483.91012    0.00548    0.00200   0.00000
   19:   4  1  4  3  0  3                    13420.14310   13420.14383   -0.00073    0.00200   0.00000
   20:   5  1  5  4  0  4                    15279.91700   15279.92198   -0.00498    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.96673E-01    3   3.00548E-01    4   7.17451E-01    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       6282.02946(169)         -0.00000
   2         20000          B      1252.941807(140)        -0.000000
   3         30000          C      1059.318267(169)         0.000000
```

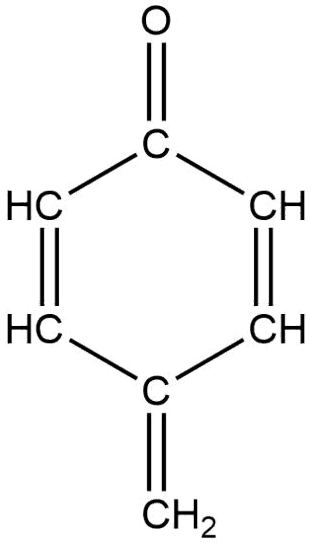
```
  4           200    Delta_J         -0.02427(106)E-03     -0.00000E-03
  5          1100   Delta_JK     -7.949395092(  0)E-24 -0.000000000E-24
  6          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
  7         40100     -del_J     -0.803383257(  0)E-24  0.000000000E-24
  8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000035 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002693 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.32619         1.32619
```

Molecule 182

IUPAC Name: 4-methylidene-2,5-cyclohexadien-1-one

Common name: p-quinomethane

SMILES: C=C1C=CC(=O)C=C1



182: Fit file

	EXP.FREQ.			CALC.FREQ.			DIFF.	EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	3	1	3	2	1	2				8079.59600	8079.59629	-0.00029	0.00200	0.00000
2:	4	1	4	3	1	3				10740.82110	10740.82195	-0.00085	0.00200	0.00000
3:	5	1	5	4	1	4				13378.67090	13378.67210	-0.00120	0.00200	0.00000
4:	6	1	6	5	1	5				15991.79950	15991.80097	-0.00147	0.00200	0.00000
5:	7	1	7	6	1	6				18580.96310	18580.96443	-0.00133	0.00200	0.00000
6:	3	0	3	2	0	2				8565.30520	8565.30579	-0.00059	0.00200	0.00000
7:	3	1	2	2	1	1				9252.25800	9252.25188	0.00612	0.00200	0.00000
8:	4	0	4	3	0	3				11288.23330	11288.23508	-0.00178	0.00200	0.00000
9:	4	1	3	3	1	2				12297.58990	12297.58519	0.00471	0.00200	0.00000
10:	5	0	5	4	0	4				13918.71080	13918.71280	-0.00200	0.00200	0.00000
11:	5	1	4	4	1	3				15305.24830	15305.24645	0.00185	0.00200	0.00000
12:	6	0	6	5	0	5				16467.14850	16467.14853	-0.00003	0.00200	0.00000
13:	6	1	5	5	1	4				18260.48100	18260.48217	-0.00117	0.00200	0.00000
14:	7	0	7	6	0	6				18960.42440	18960.42239	0.00201	0.00200	0.00000
15:	7	1	6	6	1	5				21146.09470	21146.10064	-0.00594	0.00200	0.00000
16:	8	0	8	7	0	7				21428.39490	21428.39046	0.00444	0.00200	0.00000

NORMALIZED DIAGONAL:

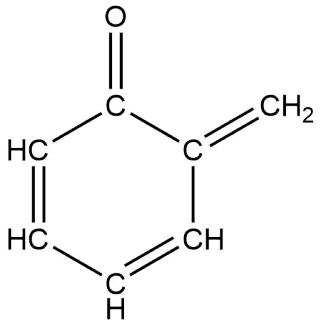
```
   1   1.00000E+00    2   8.06664E-01    3   4.62117E-01    4   1.16949E-01    5   3.08857E-01    6   1.00000E+00
   7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
  1         10000          A        5246.5968(161)           0.0000
  2         20000          B      1643.160354(309)        -0.000000
  3         30000          C      1251.788613(182)        -0.000000
  4           200    Delta_J          -0.0259( 47)E-03      -0.0000E-03
  5          1100   Delta_JK           -0.775(294)E-03        0.000E-03
  6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
  7         40100     -del_J     -0.803383257(  0)E-24  0.000000000E-24
  8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =        0.000155 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002928 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.46410         1.46410
```

Molecule 183

IUPAC Name: 6-methylidene-2,4-cyclohexadien-1-one

Common name: o-quinomethane

SMILES: C=C1C=CC=CC1=O



183: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-AVG.	CALC.FREQ.	-	DIFF.	-	WT.	
1:	2 0 2 1 0 1						7060.74250	7060.74210		0.00040		0.00200	0.00000
2:	2 1 2 1 0 1						7450.29080	7450.29162		-0.00082		0.00200	0.00000
3:	2 1 1 1 1 0						8565.30420	8565.30724		-0.00304		0.00200	0.00000
4:	3 0 3 2 1 2						9447.94210	9447.94255		-0.00045		0.00200	0.00000
5:	3 1 3 2 1 2						9566.08130	9566.08044		0.00086		0.00200	0.00000
6:	3 0 3 2 0 2						9837.49220	9837.49207		0.00013		0.00200	0.00000
7:	3 1 3 2 0 2						9955.62960	9955.62996		-0.00036		0.00200	0.00000
8:	2 2 1 1 1 0						11259.70340	11259.70455		-0.00115		0.00200	0.00000
9:	3 2 2 2 2 1						11338.09710	11338.09196		0.00514		0.00200	0.00000
10:	3 1 2 2 1 1						12407.78790	12407.78755		0.00035		0.00200	0.00000
11:	4 0 4 3 1 3						12407.87610	12407.87551		0.00059		0.00200	0.00000
12:	4 1 4 3 1 3						12437.25200	12437.25203		-0.00003		0.00200	0.00000
13:	4 0 4 3 0 3						12526.01360	12526.01341		0.00019		0.00200	0.00000
14:	4 1 4 3 0 3						12555.39010	12555.38992		0.00018		0.00200	0.00000
15:	2 2 0 1 1 1						12764.27460	12764.27091		0.00369		0.00200	0.00000
16:	3 2 1 2 2 0						12838.70030	12838.69922		0.00108		0.00200	0.00000
17:	4 1 3 3 2 2						13985.44220	13985.44452		-0.00232		0.00200	0.00000
18:	3 2 2 2 1 1						14032.48650	14032.48927		-0.00277		0.00200	0.00000
19:	5 0 5 4 1 4						15233.90810	15233.90818		-0.00008		0.00200	0.00000
20:	5 1 5 4 1 4						15240.47320	15240.47247		0.00073		0.00200	0.00000
21:	5 0 5 4 0 4						15263.28470	15263.28469		0.00001		0.00200	0.00000
22:	5 1 5 4 0 4						15269.84970	15269.84899		0.00071		0.00200	0.00000
23:	4 1 3 3 1 2						15610.14360	15610.14624		-0.00264		0.00200	0.00000

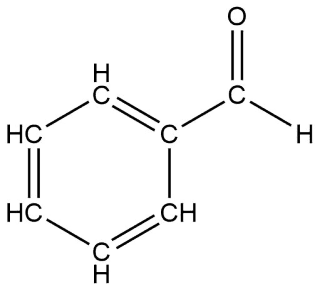
```
   24:   4  3  2  3  3  1                    15784.49960   15784.50039   -0.00079    0.00200   0.00000
   25:   4  2  3  3  1  2                    16330.49540   16330.49483    0.00057    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99832E-01    3   8.40159E-01    4   2.65524E-01    5   4.74148E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       3291.10524( 52)          0.00000
   2         20000          B      2392.970965(235)         0.000000
   3         30000          C      1386.396326(251)        -0.000000
   4           200    Delta_J          -0.0236( 59)E-03       0.0000E-03
   5          1100   Delta_JK           -0.307( 35)E-03       -0.000E-03
   6          2000    Delta_K     -2.266406368(  0)E-24 -0.000000000E-24
   7         40100     -del_J     -0.803383257(  0)E-24  0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =        0.000008 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001746 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.87301         0.87301
```

Molecule 184

IUPAC Name: benzaldehyde

Common name: benzaldehyde

SMILES: C1=CC=C(C=C1)C=O



184: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	3 0 3 2 0 2									8207.07400		8207.07363		0.00037	0.00200	0.00035
2:	3 1 2 2 1 1									8829.93920		8829.93807		0.00113	0.00200	0.00036
3:	4 1 4 3 1 3									10309.47580		10309.47589		-0.00009	0.00200	0.00042
4:	4 0 4 3 0 3									10831.40360		10831.40293		0.00067	0.00200	0.00041
5:	4 2 3 3 2 2									11056.21820		11056.21824		-0.00004	0.00200	0.00039
6:	4 2 2 3 2 1									11300.58270		11300.58329		-0.00059	0.00200	0.00041
7:	4 1 3 3 1 2									11741.23800		11741.23612		0.00188	0.00200	0.00041
8:	5 1 5 4 1 4									12846.70730		12846.70800		-0.00070	0.00200	0.00042
9:	5 0 5 4 0 4									13375.10690		13375.10676		0.00014	0.00200	0.00042
10:	5 2 4 4 2 3									13788.88050		13788.87894		0.00156	0.00200	0.00039
11:	5 2 3 4 2 2									14258.20010		14258.20121		-0.00111	0.00200	0.00042
12:	5 1 4 4 1 3									14621.72090		14621.71991		0.00099	0.00200	0.00042
13:	6 1 6 5 1 5									15362.45460		15362.45608		-0.00148	0.00200	0.00044
14:	6 0 6 5 0 5									15843.16360		15843.16428		-0.00068	0.00200	0.00043
15:	6 2 5 5 2 4									16500.89590		16500.89286		0.00304	0.00200	0.00035
16:	6 3 4 5 3 3									16723.11990		16723.11915		0.00075	0.00200	0.00055
17:	6 2 4 5 2 3									17269.97480		17269.97659		-0.00179	0.00200	0.00044
18:	6 1 5 5 1 4									17459.58900		17459.58700		0.00200	0.00200	0.00045
19:	7 0 7 6 0 6									18255.40590		18255.40591		-0.00001	0.00200	0.00057
20:	7 3 5 6 3 4									19528.43260		19528.43319		-0.00059	0.00200	0.00060
21:	7 3 4 6 3 3									19661.42360		19661.43008		-0.00648	0.00200	0.00061
22:	7 1 6 6 1 5									20240.93980		20240.93683		0.00297	0.00200	0.00057
23:	7 2 5 6 2 4									20311.08260		20311.08494		-0.00234	0.00200	0.00063
24:	8 1 8 7 1 7									20331.73460		20331.73639		-0.00179	0.00200	0.00106

```
  25:   8  1  7  7  1  6                  22950.90380   22950.90447   -0.00067    0.00200   0.00082
  26:   8  2  6  7  2  5                  23350.18870   23350.19424   -0.00554    0.00200   0.00107
  27:   9  1  8  8  1  7                  25576.68590   25576.67865    0.00725    0.00200   0.00120
  28:   2  1  2  1  0  1                   8848.40900    8848.40878    0.00022    0.00200   0.00035
  29:   4  2  2  4  1  3                  10171.45850   10171.46132   -0.00282    0.00200   0.00054
  30:   3  2  1  3  1  2                  10612.11240   10612.11414   -0.00174    0.00200   0.00057
  31:   5  0  5  4  1  4                  11016.18920   11016.18747    0.00173    0.00200   0.00055
  32:   2  2  0  2  1  1                  11035.40570   11035.40780   -0.00210    0.00200   0.00058
  33:   3  1  3  2  0  2                  11087.91900   11087.91996   -0.00096    0.00200   0.00046
  34:   2  2  1  2  1  2                  12089.02660   12089.02967   -0.00307    0.00200   0.00058
  35:   3  2  2  3  1  3                  12643.61560   12643.61440    0.00120    0.00200   0.00060
  36:   4  1  4  3  0  3                  13190.32070   13190.32222   -0.00152    0.00200   0.00054
  37:   4  2  3  4  1  4                  13390.35970   13390.35675    0.00295    0.00200   0.00068
  38:   6  0  6  5  1  5                  14012.64540   14012.64375    0.00165    0.00200   0.00055
  39:   5  1  5  4  0  4                  15205.62520   15205.62729   -0.00209    0.00200   0.00056
  40:   7  0  7  6  1  6                  16905.59480   16905.59357    0.00123    0.00200   0.00065
  41:   2  2  1  1  1  0                  16907.75820   16907.75815    0.00005    0.00200   0.00054
  42:   6  1  6  5  0  5                  17192.97440   17192.97662   -0.00222    0.00200   0.00054
  43:   2  2  0  1  1  1                  17292.49940   17292.49773    0.00167    0.00200   0.00053
  44:   4  3  1  4  2  2                  18969.70190   18969.70168    0.00022    0.00200   0.00071
  45:   3  3  0  3  2  1                  19140.74280   19140.74243    0.00037    0.00200   0.00082
  46:   7  1  7  6  0  6                  19206.72590   19206.72860   -0.00270    0.00200   0.00070
  47:   3  2  2  2  1  1                  19317.11650   19317.11560    0.00090    0.00200   0.00054
  48:   4  3  2  4  2  3                  19331.30320   19331.30668   -0.00348    0.00200   0.00070
  49:   3  2  1  2  1  2                  20520.82350   20520.82310    0.00040    0.00200   0.00055
  50:   8  1  8  7  0  7                  21283.05670   21283.05909   -0.00239    0.00200   0.00117
  51:   4  2  3  3  1  2                  21543.39560   21543.39577   -0.00017    0.00200   0.00058
  52:   5  2  4  4  1  3                  23591.03920   23591.03859    0.00061    0.00200   0.00064
  53:   4  2  2  3  1  3                  24069.13510   24069.13430    0.00080    0.00200   0.00067
  54:   6  2  5  5  1  4                  25470.21330   25470.21154    0.00176    0.00200   0.00072
  55:   7  2  6  6  1  5                  27199.26510   27199.26094    0.00416    0.00200   0.00089
  56:   3  3  1  2  2  0                  27546.28360   27546.28430   -0.00070    0.00200   0.00076
  57:   3  3  0  2  2  1                  27572.53870   27572.53587    0.00283    0.00200   0.00076
  58:   5  2  3  4  1  4                  28017.86060   28017.85962    0.00098    0.00200   0.00090
  59:   4  3  2  3  2  1                  30262.58780   30262.58832   -0.00052    0.00200   0.00067
  60:   4  3  1  3  2  2                  30395.22190   30395.22158    0.00032    0.00200   0.00067
  61:   6  2  4  5  1  5                  32441.12760   32441.12821   -0.00061    0.00200   0.00119
  62:   6  3  4  5  2  3                  35347.09680   35347.09769   -0.00089    0.00200   0.00084
  63:   6  3  3  5  2  4                  36276.71000   36276.71361   -0.00361    0.00200   0.00084
  64:   7  3  5  6  2  4                  37605.55820   37605.55428    0.00392    0.00200   0.00119
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.97476E-01    3   9.80884E-01    4   3.68351E-01    5   3.52868E-01    6   4.90684E-01
    7   5.12548E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                5234.364083(281)        -0.000000
   2         20000                1564.273324( 90)        -0.000000
   3         30000                1204.682629( 90)         0.000000
   4           200                   -0.06152( 74)E-03      0.00000E-03
```

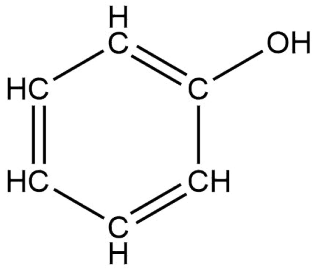
```
  5          2000                    -0.7204(264)E-03       0.0000E-03
  6          1100                    -0.1829( 61)E-03       0.0000E-03
  7         40100                    -0.01650( 53)E-03      0.00000E-03
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =       -0.000075 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002232 MHz, IR RMS =        0.00000
END OF ITERATION  2 OLD, NEW RMS ERROR=        1.11595         1.11595
```

Molecule 185

IUPAC Name: benzenol

Common name: phenol, hydroxybenzene

SMILES: C1=CC=C(C=C1)O

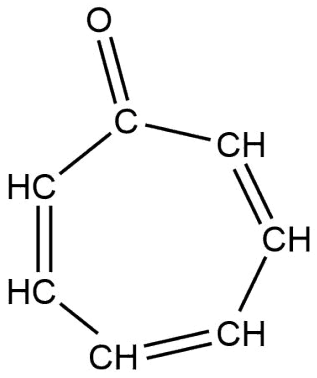


Molecule 186

IUPAC Name: 2,4,6-cycloheptatrien-1-one

Common name: tropone

SMILES: C1=CC=CC(=O)C=C1



186: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                     6498.20290    6498.20209    0.00081    0.00200   0.00000
    2:   2  1  1  1  1  0                     7396.11280    7396.10757    0.00523    0.00200   0.00000
    3:   3  1  3  2  1  2                     8847.59650    8847.59949   -0.00299    0.00200   0.00000
    4:   3  0  3  2  0  2                     9356.52630    9356.52577    0.00053    0.00200   0.00000
    5:   3  1  2  2  1  1                    10960.52110   10960.52077    0.00033    0.00200   0.00000
    6:   4  0  4  3  0  3                    11981.26560   11981.26570   -0.00010    0.00200   0.00000
    7:   4  2  3  3  2  2                    13218.19720   13218.19407    0.00313    0.00200   0.00000
    8:   4  1  3  3  1  2                    14324.20490   14324.20430    0.00060    0.00200   0.00000
    9:   5  1  5  4  1  4                    14362.50210   14362.50279   -0.00069    0.00200   0.00000
   10:   5  0  5  4  0  4                    14538.59660   14538.59723   -0.00063    0.00200   0.00000
   11:   4  2  2  3  2  1                    14595.90330   14595.90624   -0.00294    0.00200   0.00000
   12:   6  0  6  5  0  5                    17113.92320   17113.92239    0.00081    0.00200   0.00000
   13:   5  1  4  4  1  3                    17384.40050   17384.40287   -0.00237    0.00200   0.00000
   14:   7  0  7  6  0  6                    19714.38250   19714.38177    0.00073    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.47009E-01    3   2.90599E-01    4   6.74466E-01    5   1.00000E+00    6   2.81446E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                  3712.35671(316)         -0.00000
   2         20000                 2027.655158(314)         0.000000
   3         30000                 1313.144265(280)         0.000000
```

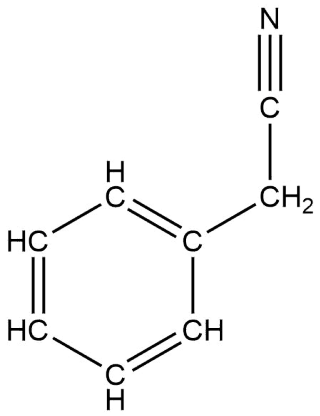
```
  4           200                    -0.0324( 39)E-03       0.0000E-03
  5          2000                -0.015738811(  0)E-18 -0.000000000E-18
  6          1100                     -0.282( 93)E-03       -0.000E-03
  7         40100                -0.047468413(  0)E-24 -0.000000000E-24
  8         50000                -0.328707538(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000175 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002134 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.06688         1.06688
```

Molecule 187

IUPAC Name: 2-phenylacetonitrile

Common name: benzylcyanide

SMILES: C1=CC=C(C=C1)CC#N



Molecule 188

IUPAC Name: 8-oxo-1,2,3,4,5,6,7-octaheptaenylidene

Common name: octacarbonmonoxide

SMILES: [C]=C=C=C=C=C=C=O

Molecule 189

IUPAC Name: 2,4,6,8-nonatetraynenitrile

Common name: cyanooctatetrayne

SMILES: C#CC#CC#CC#CC#N

Molecule 190

IUPAC Name: 9-oxo-1,2,3,4,5,6,7,8-nonaoctaenylidene

Common name: nonacarbonmonoxide

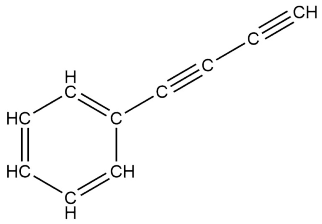
SMILES: [C]=C=C=C=C=C=C=C=O

Molecule 191

IUPAC Name: 1,3-butadiynylbenzene

Common name: phenyldiacetylene

SMILES: C#CC#CC1=CC=CC=C1



191: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-	AVG. CALC.FREQ.	-	DIFF.	-	WT.			
1:	3 1 2	2 1 1					3351.20000	3351.19091		0.00909		0.05000	0.00000		
2:	5 1 4	4 1 3					5584.00000	5583.95743		0.04257		0.05000	0.00000		
3:	6 0 6	5 0 5					6531.52000	6531.51933		0.00067		0.00200	0.00000		
4:	6 2 5	5 2 4					6543.72110	6543.72082		0.00028		0.00200	0.00000		
5:	6 2 4	5 2 3					6557.77420	6557.77387		0.00033		0.00200	0.00000		
6:	6 1 5	5 1 4					6699.61340	6699.61186		0.00154		0.00200	0.00000		
7:	7 1 7	6 1 6					7447.78680	7447.78629		0.00051		0.00200	0.00000		
8:	7 0 7	6 0 6					7614.05150	7614.05036		0.00114		0.00200	0.00000		
9:	7 2 6	6 2 5					7633.32430	7633.32306		0.00124		0.00200	0.00000		
10:	7 2 5	6 2 4					7655.77400	7655.77194		0.00206		0.00200	0.00000		
11:	7 1 6	6 1 5					7814.63050	7814.62830		0.00220		0.00200	0.00000		
12:	8 1 8	7 1 7					8509.84420	8509.84551		-0.00131		0.00200	0.00000		
13:	8 0 8	7 0 7					8693.83450	8693.83346		0.00104		0.00200	0.00000		
14:	8 2 7	7 2 6					8722.45760	8722.45577		0.00183		0.00200	0.00000		
15:	8 5 3	7 5 2					8729.04800	8729.04641		0.00159		0.00200	0.00000	8729.04641	0.00159
16:	8 5 4	7 5 3					8729.04800	8729.04641		0.00159		0.00200	0.00000	8729.04641	0.00159
17:	8 4 5	7 4 4					8730.02950	8730.02856		0.00094		0.00200	0.00000	8730.02983	-0.00033
18:	8 4 4	7 4 3					8730.02950	8730.03109		-0.00159		0.00200	0.00000	8730.02983	-0.00033
19:	8 3 6	7 3 5					8731.88930	8731.88858		0.00072		0.00200	0.00000		
20:	8 3 5	7 3 4					8732.37430	8732.37419		0.00011		0.00200	0.00000		
21:	8 2 6	7 2 5					8756.04680	8756.04685		-0.00005		0.00200	0.00000		
22:	8 1 7	7 1 6					8928.88920	8928.88548		0.00372		0.00200	0.00000		
23:	9 1 9	8 1 8					9571.17870	9571.17874		-0.00004		0.00200	0.00000		
24:	9 0 9	8 0 8					9770.52790	9770.52917		-0.00127		0.00200	0.00000		
25:	9 2 8	8 2 7					9811.05460	9811.05224		0.00236		0.00200	0.00000		
26:	9 4 6	8 4 5					9821.96590	9821.96251		0.00339		0.00200	0.00000	9821.96554	0.00036

27:	9	4	5	8	4	4	9821.96590	9821.96858	-0.00268	0.00200	0.00000	9821.96554	0.00036
28:	9	3	7	8	3	6	9824.48750	9824.48548	0.00202	0.00200	0.00000		
29:	9	2	7	8	2	6	9858.86970	9858.87030	-0.00060	0.00200	0.00000		
30:	9	1	8	8	1	7	10042.25830	10042.25518	0.00312	0.00200	0.00000		
31:	10	1	10	9	1	9	10631.71820	10631.71852	-0.00032	0.00200	0.00000		
32:	10	0	10	9	0	9	10843.83530	10843.83604	-0.00074	0.00200	0.00000		
33:	10	2	9	9	2	8	10899.04810	10899.04598	0.00212	0.00200	0.00000		
34:	10	5	6	9	5	5	10912.30590	10912.30882	-0.00292	0.00200	0.00000	10912.30884	-0.00294
35:	10	5	5	9	5	4	10912.30590	10912.30887	-0.00297	0.00200	0.00000	10912.30884	-0.00294
36:	10	4	7	9	4	6	10914.14230	10914.13557	0.00673	0.00200	0.00000	10914.14215	0.00015
37:	10	4	6	9	4	5	10914.14230	10914.14872	-0.00642	0.00200	0.00000	10914.14215	0.00015
38:	10	3	8	9	3	7	10917.42230	10917.42168	0.00062	0.00200	0.00000		
39:	10	3	7	9	3	6	10918.94490	10918.94601	-0.00111	0.00200	0.00000		
40:	10	2	8	9	2	7	10964.47430	10964.47558	-0.00128	0.00200	0.00000		
41:	10	1	9	9	1	8	11154.60260	11154.60114	0.00146	0.00200	0.00000		
42:	11	1	11	10	1	10	11691.40520	11691.40513	0.00007	0.00200	0.00000		
43:	11	0	11	10	0	10	11913.50260	11913.50371	-0.00111	0.00200	0.00000		
44:	11	2	10	10	2	9	11986.37660	11986.37092	0.00568	0.00200	0.00000		
45:	11	5	7	10	5	6	12004.18690	12004.18195	0.00495	0.00200	0.00000	12004.18202	0.00488
46:	11	5	6	10	5	5	12004.18690	12004.18209	0.00481	0.00200	0.00000	12004.18202	0.00488
47:	11	4	8	10	4	7	12006.57770	12006.57342	0.00428	0.00200	0.00000		
48:	11	4	7	10	4	6	12006.59320	12006.59972	-0.00652	0.00200	0.00000		
49:	11	3	9	10	3	8	12010.70650	12010.70642	0.00008	0.00200	0.00000		
50:	11	3	8	10	3	7	12013.18080	12013.18100	-0.00020	0.00200	0.00000		
51:	11	2	9	10	2	8	12073.04420	12073.04435	-0.00015	0.00200	0.00000		
52:	11	1	10	10	1	9	12265.77820	12265.77811	0.00009	0.00200	0.00000		
53:	12	1	12	11	1	11	12750.18610	12750.18711	-0.00101	0.00200	0.00000		
54:	12	0	12	11	0	11	12979.34640	12979.34670	-0.00030	0.00200	0.00000		
55:	12	2	11	11	2	10	13072.96490	13072.96150	0.00340	0.00200	0.00000		
56:	12	5	8	11	5	7	13096.23920	13096.23866	0.00054	0.00200	0.00000	13096.23881	0.00039
57:	12	5	7	11	5	6	13096.23920	13096.23897	0.00023	0.00200	0.00000	13096.23881	0.00039
58:	12	3	10	11	3	9	13104.34110	13104.34064	0.00046	0.00200	0.00000		
59:	12	2	10	11	2	9	13184.68880	13184.69264	-0.00384	0.00200	0.00000		
60:	12	1	11	11	1	10	13375.63180	13375.63086	0.00094	0.00200	0.00000		
61:	13	1	13	12	1	12	13808.02760	13808.02173	0.00587	0.00200	0.00000		
62:	13	0	13	12	0	12	14041.25590	14041.25741	-0.00151	0.00200	0.00000		
63:	13	2	12	12	2	11	14158.75720	14158.75283	0.00437	0.00200	0.00000		
64:	13	4	10	12	4	9	14192.33840	14192.34334	-0.00494	0.00200	0.00000		
65:	13	3	11	12	3	10	14198.31690	14198.31655	0.00035	0.00200	0.00000		
66:	14	0	14	13	0	13	15099.21410	15099.21657	-0.00247	0.00200	0.00000		
67:	14	4	11	13	4	10	15285.73220	15285.72337	0.00883	0.00200	0.00000		
68:	14	4	10	13	4	9	15285.86950	15285.87221	-0.00271	0.00200	0.00000		
69:	14	3	12	13	3	11	15292.61760	15292.61731	0.00029	0.00200	0.00000		
70:	14	3	11	13	3	10	15300.97150	15300.97308	-0.00158	0.00200	0.00000		
71:	15	0	15	14	0	14	16153.29660	16153.29945	-0.00285	0.00200	0.00000		
72:	15	3	13	14	3	12	16387.21690	16387.21689	0.00001	0.00200	0.00000		
73:	15	3	12	14	3	11	16399.02240	16399.02290	-0.00050	0.00200	0.00000		
74:	16	0	16	15	0	15	17203.66950	17203.67594	-0.00644	0.00200	0.00000		
75:	16	3	14	15	3	13	17482.07930	17482.08005	-0.00075	0.00200	0.00000		

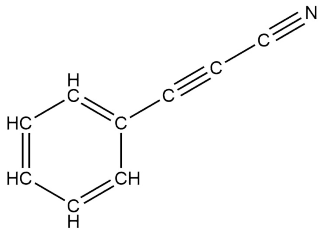
```
   76:  16  3 13 15  3 12                    17498.36870   17498.37361   -0.00491    0.00200   0.00000
   77:  17  0 17 16  0 16                    18250.60200   18250.60392   -0.00192    0.00200   0.00000
   78:  17  3 15 16  3 14                    18577.16090   18577.16248   -0.00158    0.00200   0.00000
   79:  17  3 14 16  3 13                    18599.18100   18599.18765   -0.00665    0.00200   0.00000
   80:  18  0 18 17  0 17                    19294.41340   19294.41572   -0.00232    0.00200   0.00000
   81:  19  0 19 18  0 18                    20335.49550   20335.49904   -0.00354    0.00200   0.00000
   82:  21  0 21 20  0 20                    22411.17040   22411.17151   -0.00111    0.00200   0.00000
   83:  22  0 22 21  0 21                    23446.60970   23446.60805    0.00165    0.00200   0.00000
   84:  23  0 23 22  0 22                    24480.97360   24480.97141    0.00219    0.00200   0.00000
   85:  25  0 25 24  0 24                    26547.81630   26547.80651    0.00979    0.00200   0.00000
   86:  26  0 26 25  0 25                    27580.80990   27580.81403   -0.00413    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   6.18432E-01    3   2.24542E-01    4   4.01413E-01    5   1.00000E+00    6   9.99980E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    5672.6028(311)           0.0000
   2         20000                   571.684990( 56)         0.000000
   3         30000                   519.244290( 61)        -0.000000
   4           200                      -3.502( 40)E-06       -0.000E-06
   5          2000                  0.518826831(  0)E-21 -0.000000000E-21
   6          1100                     -0.86852(190)E-03      0.00000E-03
   7         40100                  -5.36425720( 28)E-30  -0.00000000E-30
   8         41000                  -4.95790905( 40)E-30  -0.00000000E-30
 MICROWAVE AVG =        0.000803 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005692 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.45378         1.45378
```

Molecule 192

IUPAC Name: 3-phenyl-2-propynenitrile

Common name: 3-phenylpropiolonitrile

SMILES: C1=CC=C(C=C1)C#CC#N



Molecule 193

IUPAC Name: 2,4,6,8,10-undecapentaynenitrile

Common name: cyanodecapentayne

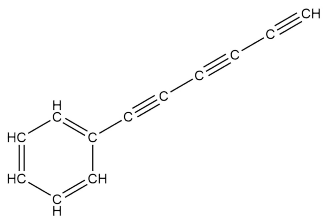
SMILES: C#CC#CC#CC#CC#N

Molecule 194

IUPAC Name: 1,3,5-hexatriynylbenzene

Common name: phenyltriacetylene

SMILES: C#CC#CC#CC1=CC=CC=C1



194: Fit file

EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.
1:	16 1 15 15 1 14							8678.48880		8678.48665		0.00215		0.00200 0.00000
2:	15 1 15 14 1 14							7945.97210		7945.97114		0.00096		0.00200 0.00000
3:	16 1 16 15 1 15							8475.26060		8475.26099		-0.00039		0.00200 0.00000
4:	17 1 17 16 1 16							9004.47000		9004.46897		0.00103		0.00200 0.00000
5:	18 1 18 17 1 17							9533.59090		9533.59106		-0.00016		0.00200 0.00000
6:	19 1 19 18 1 18							10062.61560		10062.62346		-0.00786		0.00200 0.00000
7:	20 1 20 19 1 19							10591.56410		10591.56254		0.00156		0.00200 0.00000
8:	21 1 21 20 1 20							11120.40850		11120.40490		0.00360		0.00200 0.00000
9:	22 1 22 21 1 21							11649.14820		11649.14733		0.00087		0.00200 0.00000
10:	14 0 14 13 0 13							7497.89510		7497.89517		-0.00007		0.00200 0.00000
11:	15 0 15 14 0 14							8031.84780		8031.84630		0.00150		0.00200 0.00000
12:	16 0 16 15 0 15							8565.46990		8565.46931		0.00059		0.00200 0.00000
13:	17 0 17 16 0 16							9098.74570		9098.74509		0.00061		0.00200 0.00000
14:	18 0 18 17 0 17							9631.65650		9631.65542		0.00108		0.00200 0.00000
15:	19 0 19 18 0 18							10164.18270		10164.18312		-0.00042		0.00200 0.00000
16:	20 0 20 19 0 19							10696.31070		10696.31228		-0.00158		0.00200 0.00000
17:	21 0 21 20 0 20							11228.02540		11228.02837		-0.00297		0.00200 0.00000
18:	22 0 22 21 0 21							11759.32030		11759.31848		0.00182		0.00200 0.00000
19:	13 0 13 12 0 12							6963.63430		6963.63583		-0.00153		0.00200 0.00000
20:	13 1 12 12 1 11							7052.38390		7052.38161		0.00229		0.00200 0.00000
21:	16 1 15 15 1 14							8678.48790		8678.48665		0.00125		0.00200 0.00000
22:	18 1 17 17 1 16							9762.07000		9762.07490		-0.00490		0.00200 0.00000
23:	20 1 19 19 1 18							10845.20870		10845.20851		0.00019		0.00200 0.00000
24:	23 0 23 22 0 22							12290.17240		12290.17145		0.00095		0.00200 0.00000

NORMALIZED DIAGONAL:

1 1.00000E+00 2 4.66512E-01 3 2.71777E-01 4 1.16739E-01 5 1.00000E+00 6 9.52721E-01
7 1.00000E+00 8 1.00000E+00

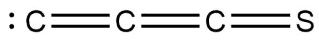
```
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000                    5669.33( 90)             0.00
   2         20000                  274.503470( 70)        -0.000000
   3         30000                  261.788609( 66)        -0.000000
   4           200                     -0.833(130)E-06       -0.000E-06
   5          2000                -1.640706907(100)E-30  0.000000000E-30
   6          1100                     -0.419( 88)E-03        0.000E-03
   7         40100                 -5.36425720( 28)E-30   0.00000000E-30
   8         41000                 -4.95790905( 40)E-30  -0.00000000E-30
 MICROWAVE AVG =        0.000024 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002397 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.19847         1.19847
```

Molecule 195

IUPAC Name: 3-thioxo-1,2-propadien-1-ylidene

Common name: tricarbon monosulfide

SMILES: [C]=C=C=S

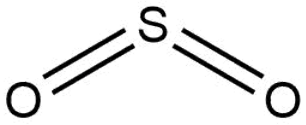


Molecule 196

IUPAC Name: sulfur dioxide

Common name: sulfur dioxide

SMILES: O=S=O

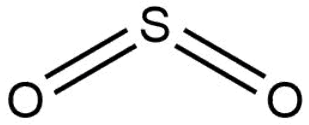


Molecule 197

IUPAC Name: sulfur dioxide (1v2)

Common name: sulfur dioxide (1v2)

SMILES: O=S=O

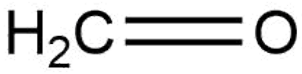


Molecule 198

IUPAC Name: formaldehyde

Common name: formaldehyde

SMILES: C=O

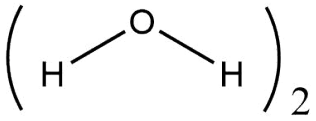


Molecule 199

IUPAC Name: water dimer

Common name: water dimer

SMILES: O.O



Molecule 200

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

200: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   6  1  6  5  1  5                     6433.13070    6433.13143   -0.00073    0.00200   0.00000
    2:   6  0  6  5  0  5                     6568.03040    6568.02945    0.00095    0.00200   0.00000
    3:   7  1  7  6  1  6                     7503.80310    7503.80301    0.00009    0.00200   0.00000
    4:   7  0  7  6  0  6                     7656.44470    7656.44257    0.00213    0.00200   0.00000
    5:   7  1  6  6  1  5                     7844.57550    7844.57519    0.00031    0.00200   0.00000
    6:   8  1  8  7  1  7                     8573.80400    8573.80477   -0.00077    0.00200   0.00000
    7:   8  0  8  7  0  7                     8742.02980    8742.02719    0.00261    0.00200   0.00000
    8:   8  1  7  7  1  6                     8963.01830    8963.01903   -0.00073    0.00200   0.00000
    9:   9  1  9  8  1  8                     9643.06210    9643.06227   -0.00017    0.00200   0.00000
   10:   9  0  9  8  0  8                     9824.44020    9824.44679   -0.00659    0.00200   0.00000
   11:   9  1  8  8  1  7                    10080.53260   10080.53262   -0.00002    0.00200   0.00000
   12:  10  1 10  9  1  9                    10711.50920   10711.50912    0.00008    0.00200   0.00000
   13:  10  0 10  9  0  9                    10903.41510   10903.41252    0.00258    0.00200   0.00000
   14:  11  1 11 10  1 10                    11779.08830   11779.08769    0.00061    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   7.08458E-01    3   5.93162E-01    4   2.74539E-01    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A         4825.520(147)            0.000
   2         20000          B       572.909000(130)         0.000000
   3         30000          C       524.187274(152)         0.000000
   4           200    Delta_J         -0.01482( 71)E-03     -0.00000E-03
   5          2000    Delta_K      1.242615019(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK      0.019681979(  0)E-21  0.000000000E-21
   7         40100     -del_J      0.104038237(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
 MICROWAVE AVG =        0.000023 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.002146 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.07322         1.07322
```

Molecule 201

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

201: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   6  1  6  5  1  5                     6935.22990    6935.22991   -0.00001    0.00200   0.00000
    2:   6  0  6  5  0  5                     7035.92750    7035.92775   -0.00025    0.00200   0.00000
    3:   6  1  5  5  1  4                     7153.90250    7153.90263   -0.00013    0.00200   0.00000
    4:   7  1  7  6  1  6                     8089.90420    8089.90382    0.00038    0.00200   0.00000
    5:   7  2  6  6  2  5                     8219.20910    8219.20904    0.00006    0.00200   0.00000
    6:   7  2  5  6  2  4                     8237.05270    8237.05317   -0.00047    0.00200   0.00000
    7:   7  0  7  6  0  6                     8203.74380    8203.74305    0.00075    0.00200   0.00000
    8:   7  1  6  6  1  5                     8344.92300    8344.92311   -0.00011    0.00200   0.00000
    9:   8  1  8  7  1  7                     9244.04880    9244.04877    0.00003    0.00200   0.00000
   10:   8  0  8  7  0  7                     9369.37300    9369.37307   -0.00007    0.00200   0.00000
   11:   8  2  7  7  2  6                     9392.27260    9392.27194    0.00066    0.00200   0.00000
   12:   8  2  6  7  2  5                     9418.95310    9418.95366   -0.00056    0.00200   0.00000
   13:   8  1  7  7  1  6                     9535.32040    9535.32000    0.00040    0.00200   0.00000
   14:   9  1  9  8  1  8                    10397.60590   10397.60589    0.00001    0.00200   0.00000
   15:   9  0  9  8  0  8                    10532.55990   10532.56000   -0.00010    0.00200   0.00000
   16:   9  1  8  8  1  7                    10724.98610   10724.98608    0.00002    0.00200   0.00000
   17:  10  1 10  9  1  9                    11550.52260   11550.52263   -0.00003    0.00200   0.00000
   18:  10  0 10  9  0  9                    11693.08420   11693.08440   -0.00020    0.00200   0.00000
   19:  10  1  9  9  1  8                    11913.80710   11913.80682    0.00028    0.00200   0.00000
   20:  11  1 11 10  1 10                    12702.75340   12702.75328    0.00012    0.00200   0.00000
   21:  11  0 11 10  0 10                    12850.77700   12850.77761   -0.00061    0.00200   0.00000
   22:  11  1 10 10  1  9                    13101.65940   13101.65946   -0.00006    0.00200   0.00000
   23:  12  0 12 11  0 11                    14005.53300   14005.53393   -0.00093    0.00200   0.00000
   24:  13  0 13 12  0 12                    15157.32180   15157.32090    0.00090    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.06527E-01    3   2.01313E-01    4   2.24153E-01    5   1.00000E+00    6   9.96291E-01
    7   8.29446E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
```

```
  1         10000          A         3702.002(105)            0.000
  2         20000          B       605.494559(247)        -0.000000
  3         30000          C       569.035714(189)         0.000000
  4           200    Delta_J         -0.09021( 50)E-03     -0.00000E-03
  5          2000    Delta_K      1.242615019(  0)E-27 -0.000000000E-27
  6          1100   Delta_JK           1.9682(288)E-03       0.0000E-03
  7         40100     -del_J          0.01040( 55)E-03      0.00000E-03
  8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
MICROWAVE AVG =        0.000004 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000415 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.20729         0.20729
```

Molecule 202

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

202: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.-	EST.ERR.-	AVG. CALC.FREQ.	-	DIFF.	-	WT.	
1:	4	0	4	3	1	3			7287.91730		7287.91888		-0.00158	0.00200	0.00000
2:	4	1	4	3	1	3			7741.84240		7741.84349		-0.00109	0.00200	0.00000
3:	4	0	4	3	0	3			8059.26080		8059.26134		-0.00054	0.00200	0.00000
4:	4	1	4	3	0	3			8513.18610		8513.18595		0.00015	0.00200	0.00000
5:	4	2	3	3	2	2			8628.58780		8628.58682		0.00098	0.00200	0.00000
6:	5	0	5	4	0	4			9800.07340		9800.07389		-0.00049	0.00200	0.00000
7:	5	1	5	4	0	4			10040.49670		10040.49778		-0.00108	0.00200	0.00000
8:	6	0	6	5	1	5			11281.12660		11281.12849		-0.00189	0.00200	0.00000
9:	6	0	6	5	0	5			11521.55110		11521.55239		-0.00129	0.00200	0.00000
10:	6	1	6	5	0	5			11639.78710		11639.78752		-0.00042	0.00200	0.00000
11:	3	1	3	2	0	2			7005.88010		7005.87682		0.00328	0.00200	0.00000
12:	3	1	2	2	1	1			7078.08010		7078.07830		0.00180	0.00200	0.00000
13:	2	2	1	1	1	0			9204.17380		9204.17241		0.00139	0.00200	0.00000
14:	4	2	2	3	2	1			9254.88900		9254.88732		0.00168	0.00200	0.00000
15:	4	1	3	3	1	2			9330.41650		9330.41656		-0.00006	0.00200	0.00000
16:	5	0	5	4	1	4			9346.15030		9346.14928		0.00102	0.00200	0.00000
17:	5	1	5	4	1	4			9586.57060		9586.57317		-0.00257	0.00200	0.00000
18:	2	2	0	1	1	1			9687.40390		9687.40468		-0.00078	0.00200	0.00000
19:	5	2	4	4	2	3			10694.65170		10694.65075		0.00095	0.00200	0.00000
20:	3	2	2	2	1	1			10966.22660		10966.22255		0.00405	0.00200	0.00000
21:	5	3	3	4	3	2			11035.40230		11035.40150		0.00080	0.00200	0.00000
22:	5	3	2	4	3	1			11200.63090		11200.63059		0.00031	0.00200	0.00000
23:	6	1	6	5	1	5			11399.36290		11399.36363		-0.00073	0.00200	0.00000
24:	5	1	4	4	1	3			11468.97010		11468.96905		0.00105	0.00200	0.00000
25:	5	2	3	4	2	2			11746.20490		11746.20552		-0.00062	0.00200	0.00000
26:	4	2	3	3	1	2			12516.72950		12516.73107		-0.00157	0.00200	0.00000
27:	6	2	5	5	2	4			12705.20740		12705.20623		0.00117	0.00200	0.00000
28:	7	0	7	6	1	6			13134.51310		13134.51492		-0.00182	0.00200	0.00000
29:	7	1	7	6	1	6			13189.77980		13189.78031		-0.00051	0.00200	0.00000

```
  30:   6  3  4  5  3  3                  13244.34410   13244.34214    0.00196    0.00200   0.00000
  31:   7  0  7  6  0  6                  13252.74900   13252.75005   -0.00105    0.00200   0.00000
  32:   6  1  5  5  1  4                  13454.85360   13454.85266    0.00094    0.00200   0.00000
  33:   6  3  3  5  3  2                  13645.40220   13645.40165    0.00055    0.00200   0.00000
  34:   5  2  4  4  1  3                  13880.96940   13880.96527    0.00413    0.00200   0.00000
  35:   6  2  4  5  2  3                  14185.47320   14185.47218    0.00102    0.00200   0.00000
  36:   8  0  8  7  0  7                  14996.75050   14996.75140   -0.00090    0.00200   0.00000
  37:   7  1  6  6  1  5                  15281.96390   15281.96386    0.00004    0.00200   0.00000
  38:   7  3  4  6  3  3                  16191.15410   16191.15856   -0.00446    0.00200   0.00000
  39:   8  2  7  7  2  6                  16554.24390   16554.24151    0.00239    0.00200   0.00000
  40:   9  1  9  8  1  8                  16735.38730   16735.38609    0.00121    0.00200   0.00000
  41:   9  0  9  8  0  8                  16749.36440   16749.36422    0.00018    0.00200   0.00000
  42:   4  3  2  3  2  1                  16943.35530   16943.35787   -0.00257    0.00200   0.00000
  43:   8  1  7  7  1  6                  16999.72990   16999.72885    0.00105    0.00200   0.00000
  44:   4  3  1  3  2  2                  17355.32450   17355.32535   -0.00085    0.00200   0.00000
  45:   5  3  3  4  2  2                  18723.87000   18723.87205   -0.00205    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.99697E-01    3   3.92865E-01    4   2.37980E-01    5   1.00000E+00    6   1.00000E+00
    7   9.92515E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A      2774.382429(196)        -0.000000
   2         20000          B      1290.566578(174)        -0.000000
   3         30000          C       881.025985( 97)        -0.000000
   4           200    Delta_J         -0.02804(120)E-03      0.00000E-03
   5          2000    Delta_K      7.004783594(  0)E-24 -0.000000000E-24
   6          1100   Delta_JK     -0.633405052(  0)E-24  0.000000000E-24
   7         40100     -del_J            -9.38( 77)E-06         0.00E-06
   8         41000     -del_K     -0.012129138(  0)E-21 -0.000000000E-21
 MICROWAVE AVG =        0.000070 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001707 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.85335         0.85335
```

Molecule 203

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

203: Fit file

	EXP.FREQ.			CALC.FREQ.			DIFF.		EXP.ERR.	EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.	
1:	3	0	3	2	2	0	2	1			8521.51620	8521.51814	-0.00194	0.00200	0.00000
2:	3	0	3	4	2	0	2	3			8521.70140	8521.70279	-0.00139	0.00200	0.00000
3:	3	0	3	3	2	0	2	2			8521.71910	8521.71669	0.00241	0.00200	0.00000
4:	4	0	4	3	3	0	3	2			11261.61510	11261.61405	0.00105	0.00200	0.00000
5:	4	0	4	5	3	0	3	4			11261.70430	11261.70422	0.00008	0.00200	0.00000
6:	4	0	4	4	3	0	3	3			11261.74210	11261.74322	-0.00112	0.00200	0.00000
7:	5	0	5	4	4	0	4	3			13931.32350	13931.32358	-0.00008	0.00200	0.00000
8:	5	0	5	6	4	0	4	5			13931.37790	13931.37775	0.00015	0.00200	0.00000
9:	5	0	5	5	4	0	4	4			13931.42980	13931.42966	0.00014	0.00200	0.00000
10:	6	0	6	5	5	0	5	4			16538.58630	16538.58511	0.00119	0.00200	0.00000
11:	6	0	6	7	5	0	5	6			16538.62160	16538.62101	0.00059	0.00200	0.00000
12:	6	0	6	6	5	0	5	5			16538.67370	16538.67448	-0.00078	0.00200	0.00000
13:	7	0	7	8	6	0	6	7			19103.85590	19103.85529	0.00061	0.00200	0.00000
14:	7	0	7	7	6	0	6	6			19103.90100	19103.90263	-0.00163	0.00200	0.00000
15:	3	1	3	3	2	1	2	2			8152.14320	8152.14394	-0.00074	0.00200	0.00000
16:	3	1	3	4	2	1	2	3			8152.37700	8152.37618	0.00082	0.00200	0.00000
17:	3	1	3	2	2	1	2	1			8152.41760	8152.41843	-0.00083	0.00200	0.00000
18:	3	1	2	3	2	1	1	2			9043.93970	9043.94038	-0.00068	0.00200	0.00000
19:	3	1	2	2	2	1	1	1			9044.13100	9044.13136	-0.00036	0.00200	0.00000
20:	3	1	2	4	2	1	1	3			9044.18970	9044.19089	-0.00119	0.00200	0.00000
21:	4	1	4	4	3	1	3	3			10845.33480	10845.33243	0.00237	0.00200	0.00000
22:	4	1	4	3	3	1	3	2			10845.40740	10845.40886	-0.00146	0.00200	0.00000
23:	4	1	4	5	3	1	3	4			10845.42390	10845.42440	-0.00050	0.00200	0.00000
24:	4	1	3	4	3	1	2	3			12029.24680	12029.24396	0.00284	0.00200	0.00000
25:	4	1	3	3	3	1	2	2			12029.27750	12029.28048	-0.00298	0.00200	0.00000
26:	4	1	3	5	3	1	2	4			12029.34640	12029.34441	0.00199	0.00200	0.00000
27:	5	1	5	5	4	1	4	4			13520.63610	13520.63601	0.00009	0.00200	0.00000
28:	5	1	5	4	4	1	4	3			13520.65670	13520.65722	-0.00052	0.00200	0.00000
29:	5	1	5	6	4	1	4	5			13520.67740	13520.67644	0.00096	0.00200	0.00000

```
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   8.60956E-01    3   2.78927E-01    4   9.49876E-02    5   5.10601E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00    9   8.45618E-01   10   9.97840E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                                NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A        4325.1802(281)          -0.0000
   2         20000          B      1584.254078(266)         0.000000
   3         30000          C      1286.619053(204)         0.000000
   4           200    Delta_J          -0.4433( 74)E-03       0.0000E-03
   5          1100   Delta_JK            3.521(311)E-03       -0.000E-03
   6          2000    Delta_K     -1.573881133(  0)E-27  0.000000000E-27
   7         40100     -del_J     -0.803383257(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24  0.000000000E-24
   9     110010000     chi_aa          -2.8150(162)           0.0000
  10     110020000     chi_bb           2.2269(159)           0.0000
 MICROWAVE AVG =       -0.000031 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.001355 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.67774         0.67774
```

Molecule 204

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

204: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  0  3  2  1  2                     8150.78180    8150.77927    0.00253    0.00200   0.00161
    2:   4  1  4  3  0  3                    12060.31430   12060.31531   -0.00101    0.00200   0.00121
    3:   5  0  5  4  1  4                    14085.39880   14085.40736   -0.00856    0.00200   0.00152
    4:   3  1  3  2  0  2                     9734.68130    9734.67936    0.00194    0.00200   0.00145
    5:   4  0  4  3  1  3                    11221.37510   11221.37681   -0.00171    0.00200   0.00117
    6:   2  2  1  1  1  0                    11554.66190   11554.66503   -0.00313    0.00200   0.00125
    7:   2  2  0  1  1  1                    12336.55090   12336.54403    0.00687    0.00200   0.00135
    8:   3  2  2  2  1  1                    14179.62530   14179.63132   -0.00602    0.00200   0.00183
    9:   5  1  5  4  0  4                    14469.59930   14469.58926    0.01004    0.00200   0.00147
   10:   4  0  4  3  0  3                    11790.40000   11790.42587   -0.02587    0.05000   0.00099
   11:   2  1  1  1  0  1                     9220.18000    9220.11547    0.06453    0.05000   0.00171
   12:   2  2  0  1  1  0                    11713.67630   11713.67603    0.00027    0.00200   0.00111
   13:   2  2  1  1  1  1                    12177.51000   12177.53302   -0.02302    0.05000   0.00120
   14:   3  1  2  2  0  2                    13445.51000   13445.50061    0.00939    0.05000   0.00376
   15:   3  2  1  2  1  1                    14916.53000   14916.51014    0.01986    0.05000   0.00279
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.92664E-01    3   8.54287E-01    4   2.82461E-01    5   2.19904E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       3414.05880(123)          0.00000
   2         20000          B       1935.35307( 62)          0.00000
   3         30000          C       1312.48508( 43)         -0.00000
   4           200    Delta_J          -0.1512( 89)E-03       0.0000E-03
   5          1100   Delta_JK            0.381(137)E-03       -0.000E-03
   6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   7         40100     -del_J     -0.803383257(  0)E-24  0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =        0.003075 MHz, IR AVG =        0.00000
```

```
MICROWAVE RMS =        0.020213 MHz, IR RMS =        0.00000
END OF ITERATION  2 OLD, NEW RMS ERROR=        2.20163         2.20163
```

Molecule 205

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

205: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                      7104.55580    7104.55276    0.00304    0.00200   0.00000
    2:   3  1  3  2  1  2                      9974.37180    9974.36989    0.00191    0.00200   0.00000
    3:   3  0  3  2  0  2                     10445.78640   10445.78581    0.00059    0.00200   0.00000
    4:   3  1  2  2  1  1                     11497.72960   11497.72595    0.00365    0.00200   0.00000
    5:   3  2  2  2  2  1                     10794.19220   10794.19028    0.00192    0.00200   0.00000
    6:   4  1  4  3  1  3                     13213.66900   13213.66804    0.00096    0.00200   0.00000
    7:   4  0  4  3  0  3                     13611.97260   13611.97371   -0.00111    0.00200   0.00000
    8:   4  2  3  3  2  2                     14320.42740   14320.42842   -0.00102    0.00200   0.00000
    9:   4  1  3  3  1  2                     15197.40640   15197.41419   -0.00779    0.00200   0.00000
   10:   5  0  5  4  0  4                     16672.78550   16672.78488    0.00062    0.00200   0.00000
   11:   6  0  6  5  0  5                     19708.79210   19708.79146    0.00064    0.00200   0.00000
   12:   3  1  3  2  0  2                     11417.13180   11417.13489   -0.00309    0.00200   0.00000
   13:   2  1  1  1  0  1                     10081.12820   10081.12424    0.00396    0.00200   0.00000
   14:   2  2  0  1  1  0                     13386.32600   13386.32563    0.00037    0.00200   0.00000
   15:   2  2  1  1  1  1                     13806.02710   13806.02585    0.00125    0.00200   0.00000
   16:   2  1  2  1  0  1                      8547.31460    8547.31776   -0.00316    0.00200   0.00000
   17:   4  1  4  3  0  3                     14185.01570   14185.01711   -0.00141    0.00200   0.00000
   18:   5  0  5  4  1  4                     16099.74090   16099.74148   -0.00058    0.00200   0.00000
   19:   3  2  2  2  1  1                     16381.55130   16381.55241   -0.00111    0.00200   0.00000
   20:   5  1  5  4  0  4                     16977.11330   16977.11033    0.00297    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   9.91145E-01    3   3.35638E-01    4   8.67259E-01    5   2.66621E-01    6   4.50975E-01
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       3917.12838(144)         -0.00000
   2         20000          B      2054.667419(247)         0.000000
   3         30000          C      1543.398595(273)         0.000000
   4           200    Delta_J          -0.3332( 47)E-03       0.0000E-03
```

```
  5          2000    Delta_K           -2.795(286)E-03        0.000E-03
  6          1100   Delta_JK            1.176( 56)E-03       -0.000E-03
  7         40100     -del_J      1.879755191(  0)E-24  0.000000000E-24
  8         41000     -del_K      0.084021739(  0)E-21  0.000000000E-21
MICROWAVE AVG =        0.000131 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.002685 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.34255         1.34255
```

Molecule 206

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

206: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  0  3  2  1  2                     6487.54760    6487.54771   -0.00011    0.00200   0.00000
    2:   2  1  1  2  0  2                     7077.93800    7077.93754    0.00046    0.00200   0.00000
    3:   2  1  2  1  1  1                     7669.98290    7669.98263    0.00027    0.00200   0.00000
    4:   2  0  2  1  0  1                     8124.68400    8124.68423   -0.00023    0.00200   0.00000
    5:   2  1  1  1  1  0                     8634.48100    8634.47973    0.00127    0.00200   0.00000
    6:   3  1  3  2  1  2                    11488.19680   11488.19765   -0.00085    0.00200   0.00000
    7:   3  0  3  2  0  2                    12118.73500   12118.73544   -0.00044    0.00200   0.00000
    8:   3  1  2  2  1  1                    12933.93800   12933.93774    0.00026    0.00200   0.00000
    9:   4  1  4  3  1  3                    15287.62910   15287.62961   -0.00051    0.00200   0.00000
   10:   4  0  4  3  0  3                    16034.19940   16034.19997   -0.00057    0.00200   0.00000
   11:   4  1  3  3  1  2                    17210.66100   17210.66160   -0.00060    0.00200   0.00000
   12:   5  1  5  4  1  4                    19064.17030   19064.16971    0.00059    0.00200   0.00000
   13:   5  0  5  4  0  4                    19854.77650   19854.77660   -0.00010    0.00200   0.00000
   14:   5  1  4  4  1  3                    21454.72490   21454.72484    0.00006    0.00200   0.00000
   15:   1  1  0  1  0  1                     6568.14260    6568.14204    0.00056    0.00200   0.00000
   16:   3  1  2  3  0  3                     7893.13750    7893.13983   -0.00233    0.00200   0.00000
   17:   4  1  3  4  0  4                     9069.60250    9069.60146    0.00104    0.00200   0.00000
   18:   1  1  1  0  0  0                    10162.00850   10162.00872   -0.00022    0.00200   0.00000
   19:   4  0  4  3  1  3                    11033.55060   11033.55003    0.00057    0.00200   0.00000
   20:   2  1  2  1  0  1                    13755.87220   13755.87196    0.00024    0.00200   0.00000
   21:   3  1  3  2  0  2                    17119.38610   17119.38538    0.00072    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   4.92794E-01    4   3.75883E-01    5   5.34787E-01    6   1.00000E+00
    7   9.31251E-01    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A       8365.07232(113)         -0.00000
   2         20000          B      2279.188121(299)         0.000000
   3         30000          C      1796.934019(247)         0.000000
```

```
  4           200    Delta_J          -0.6863( 51)E-03      -0.0000E-03
  5          1100   Delta_JK            2.215(105)E-03       -0.000E-03
  6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
  7         40100     -del_J          -0.1735( 40)E-03      -0.0000E-03
  8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
MICROWAVE AVG =        0.000005 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.000757 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.37868         0.37868
```

Molecule 207

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

207: Fit file

```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   2  0  2  1  0  1                    10044.87260   10044.87303   -0.00043    0.00200   0.00000
    2:   3  1  3  2  1  2                    14789.99730   14789.99743   -0.00013    0.00200   0.00000
    3:   3  0  3  2  0  2                    15065.32330   15065.32561   -0.00231    0.00200   0.00000
    4:   3  1  2  2  1  1                    15346.40790   15346.40789    0.00001    0.00200   0.00000
    5:   4  1  4  3  1  3                    19719.28810   19719.28800    0.00010    0.00200   0.00000
    6:   4  0  4  3  0  3                    20083.39560   20083.39819   -0.00259    0.00200   0.00000
    7:   5  0  5  4  0  4                    25098.29840   25098.29970   -0.00130    0.00200   0.00000
    8:   6  0  6  5  0  5                    30109.25370   30109.24326    0.01044    0.00200   0.00000
    9:   7  0  7  6  0  6                    35115.44450   35115.44993   -0.00543    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.35781E-01    3   3.07619E-01    4   2.89488E-02    5   9.99215E-01    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                               NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            32719( 34)               0
   2         20000          B       2604.14711( 48)         0.00000
   3         30000          C       2418.67614( 56)        -0.00000
   4           200    Delta_J            2.519( 40)E-03        0.000E-03
   5          1100   Delta_JK            -0.89( 73)E-03        -0.00E-03
   6          2000    Delta_K     -1.573881133(  0)E-27 -0.000000000E-27
   7         40100     -del_J     -0.803383257(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
 MICROWAVE AVG =       -0.000181 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.004115 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        2.05765         2.05765
```

Molecule 208

IUPAC Name: Unknown

Common name: Unknown

SMILES: -

Unknown

208: Fit file

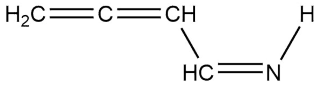
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   1  0  1  0  0  0                     6750.89870    6750.89912   -0.00042    0.00200   0.00000
    2:   2  0  2  1  0  1                    13501.26940   13501.26927    0.00013    0.00200   0.00000
    3:   3  0  3  2  0  2                    20250.58120   20250.58149   -0.00029    0.00200   0.00000
    4:   4  0  4  3  0  3                    26998.30750   26998.30699    0.00051    0.00200   0.00000
    5:   5  0  5  4  0  4                    33743.91710   33743.91730   -0.00020    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   1.00000E+00    3   1.33413E-02    4   1.00000E+00    5   1.00000E+00    6   1.00000E+00
    7   1.00000E+00    8   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A  59000.000000029(  0)      0.000000000
   2         20000          B        3474.4847(205)           0.0000
   3         30000          C        3276.4144(199)          -0.0000
   4           200    Delta_J     -3.332331220(  0)E-24 -0.000000000E-24
   5          2000    Delta_K     -0.027950456(  0)E-21  0.000000000E-21
   6          1100   Delta_JK      0.011760147(  0)E-21  0.000000000E-21
   7         40100     -del_J      1.879755191(  0)E-24 -0.000000000E-24
   8         41000     -del_K      0.084021739(  0)E-21  0.000000000E-21
 MICROWAVE AVG =       -0.000054 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.000342 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.17118         0.17118
```

Molecule 209

IUPAC Name: 2,3-butadien-1-imine (syn)

Common name: 2,3-butadien-1-imine (syn)

SMILES: C=C=CC=N



209: Fit file

	EXP.FREQ.	-	CALC.FREQ.	-	DIFF.	-	EXP.ERR.	-	EST.ERR.	-	AVG. CALC.FREQ.	-	DIFF.	-	WT.			
1:	2	0	2	1	1	0	1	1			9231.51900		9231.51795		0.00105	0.00200	0.00000	
2:	2	0	2	3	1	0	1	2			9231.74550		9231.74661		-0.00111	0.00200	0.00000	
3:	2	0	2	2	1	0	1	1			9231.75490		9231.75349		0.00141	0.00200	0.00000	
4:	2	0	2	1	1	0	1	0			9231.87930		9231.87930		0.00000	0.00200	0.00000	
5:	2	0	2	2	1	0	1	2			9231.89700		9231.89803		-0.00103	0.00200	0.00000	
6:	3	0	3	2	2	0	2	2			13846.68630		13846.68588		0.00042	0.00200	0.00000	
7:	3	0	3	4	2	0	2	3			13846.89040		13846.89039		0.00001	0.00200	0.00000	13846.89049	-0.00009
8:	3	0	3	3	2	0	2	2			13846.89040		13846.89064		-0.00024	0.00200	0.00000	13846.89049	-0.00009
9:	3	0	3	2	2	0	2	1			13846.92020		13846.92142		-0.00122	0.00200	0.00000	
10:	4	0	4	5	3	0	3	4			18461.14490		18461.14423		0.00067	0.00200	0.00000	
11:	4	0	4	4	3	0	3	3			18461.13930		18461.14037		-0.00107	0.00200	0.00000	
12:	4	0	4	3	3	0	3	2			18461.16070		18461.15931		0.00139	0.00200	0.00000	
13:	5	0	5	6	4	0	4	5			23074.21400		23074.21416		-0.00016	0.00200	0.00000	
14:	5	0	5	5	4	0	4	4			23074.20510		23074.20716		-0.00206	0.00200	0.00000	
15:	5	0	5	4	4	0	4	3			23074.22780		23074.22348		0.00432	0.00200	0.00000	
16:	6	0	6	7	5	0	5	6			27685.80700		27685.80561		0.00139	0.00200	0.00000	
17:	6	0	6	5	5	0	5	4			27685.81400		27685.81215		0.00185	0.00200	0.00000	
18:	6	0	6	6	5	0	5	5			27685.78870		27685.79593		-0.00723	0.00200	0.00000	
19:	7	0	7	8	6	0	6	7			32295.63240		32295.62458		0.00782	0.00500	0.00000	
20:	7	0	7	7	6	0	6	6			32295.61200		32295.61246		-0.00046	0.00500	0.00000	
21:	7	0	7	6	6	0	6	5			32295.63240		32295.62955		0.00285	0.00500	0.00000	
22:	3	1	2	4	2	1	1	3			14017.36190		14017.36104		0.00086	0.00200	0.00000	
23:	3	1	2	3	2	1	1	2			14017.44270		14017.44067		0.00203	0.00200	0.00000	
24:	3	1	2	2	2	1	1	1			14017.56140		14017.55841		0.00299	0.00200	0.00000	
25:	3	1	3	2	2	1	2	1			13678.54020		13678.54265		-0.00245	0.00200	0.00000	
26:	3	1	3	4	2	1	2	3			13678.73590		13678.73758		-0.00168	0.00200	0.00000	13678.73968	-0.00378
27:	3	1	3	3	2	1	2	2			13678.73590		13678.74177		-0.00587	0.00200	0.00000	13678.73968	-0.00378
28:	2	1	2	3	1	1	1	2			9119.30910		9119.31525		-0.00615	0.00200	0.00000	
29:	2	1	2	2	1	1	1	1			9119.39280		9119.39710		-0.00430	0.00200	0.00000	
30:	2	1	1	3	1	1	0	2			9344.98230		9344.97903		0.00327	0.00200	0.00000	

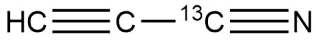
```
   31:   2  1  1  2  1  1  0  1              9345.20440    9345.19669    0.00771    0.00200   0.00000
   32:   4  1  4  3  3  1  3  2             18237.84350   18237.83816    0.00534    0.00200   0.00000
   33:   4  1  4  4  3  1  3  3             18237.91770   18237.91687    0.00083    0.00200   0.00000
   34:   4  1  4  5  3  1  3  4             18237.92720   18237.92347    0.00373    0.00200   0.00000
   35:   4  1  3  5  3  1  2  4             18689.46730   18689.47187   -0.00457    0.00200   0.00000
   36:   4  1  3  4  3  1  2  3             18689.50920   18689.51327   -0.00407    0.00200   0.00000
   37:   4  1  3  3  3  1  2  2             18689.56910   18689.57036   -0.00126    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   4.33106E-01    3   4.19484E-01    4   7.39306E-02    5   1.00000E+00    6   9.98227E-01
    7   1.00000E+00    8   1.00000E+00    9   9.94764E-01   10   9.99999E-01
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1         10000          A            35689( 36)               0
   2         20000          B      2364.463682(213)         0.000000
   3         30000          C      2251.563902(214)        -0.000000
   4           200    Delta_J          -0.3945(126)E-03      -0.0000E-03
   5          2000    Delta_K      1.242615019(  0)E-27 -0.000000000E-27
   6          1100   Delta_JK         0.033462(293)         0.000000
   7         40100     -del_J      0.104038237(  0)E-24 -0.000000000E-24
   8         41000     -del_K     -1.443000706(  0)E-24 -0.000000000E-24
   9     110010000     chi_aa          0.48182(236)         -0.00000
  10     110020000     chi_bb          -3.4092(245)           0.0000
 MICROWAVE AVG =        0.000255 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.003395 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.56968         1.56968
```

Molecule 210

IUPAC Name: 2-propynenitrile (13C1)

Common name: cyanoacetylene, propiolonitrile (13C1)

SMILES: C#CC#N

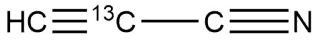


Molecule 211

IUPAC Name: 2-propynenitrile (13C2)

Common name: cyanoacetylene, propiolonitrile (13C2)

SMILES: C#CC#N

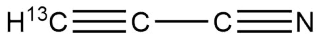


Molecule 212

IUPAC Name: 2-propynenitrile (13C3)

Common name: cyanoacetylene, propiolonitrile (13C3)

SMILES: C#CC#N

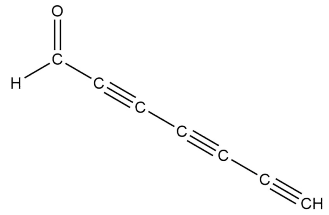


Molecule 213

IUPAC Name: 2,4,6-heptatriynal

Common name: 2,4,6-helptatriynal

SMILES: C#CC#CC#CC=O

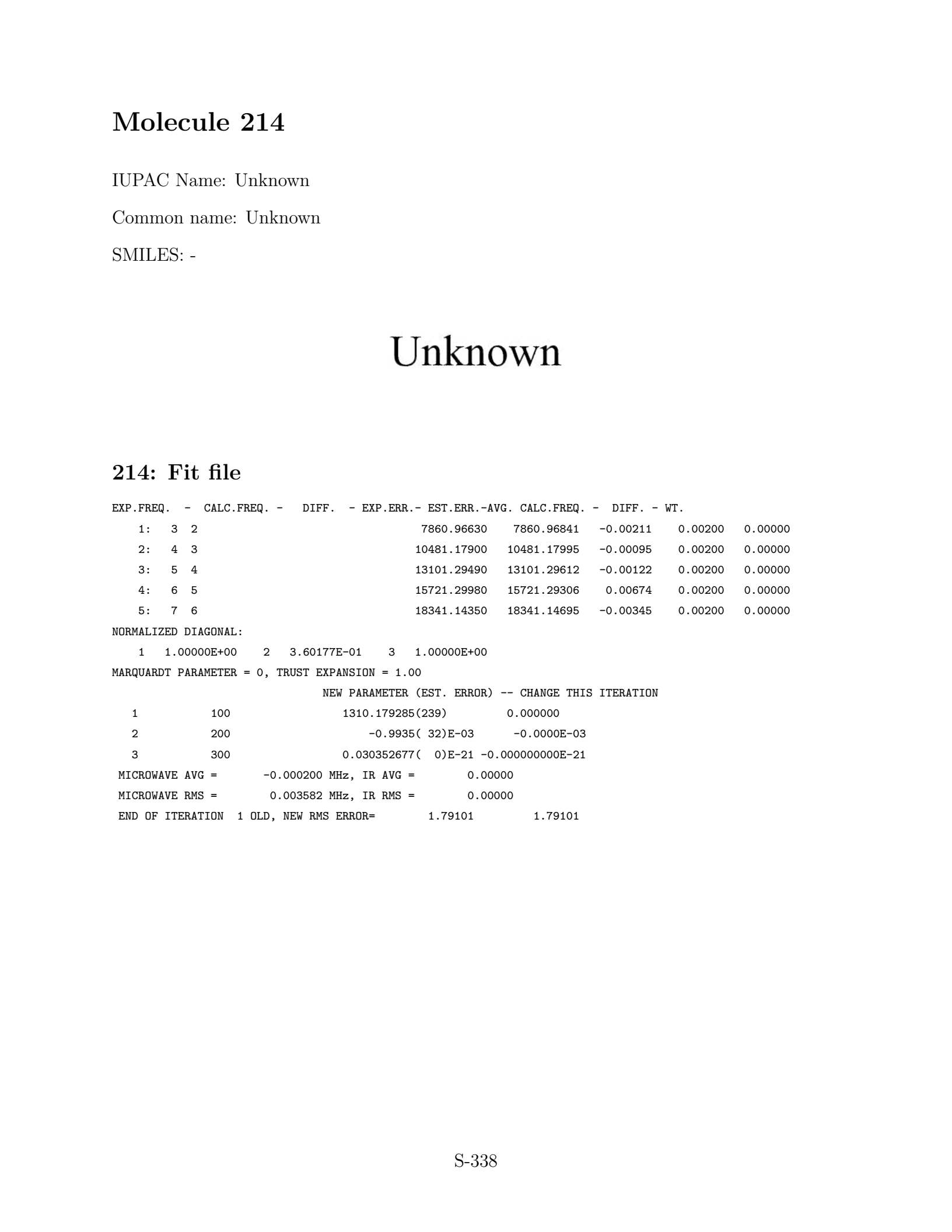


Molecule 214

IUPAC Name: Unknown

Common name: Unknown

SMILES: -



214: Fit file

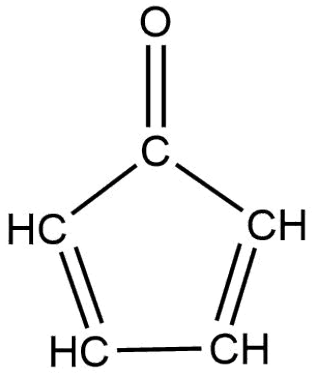
```
EXP.FREQ.  -  CALC.FREQ. -   DIFF.  - EXP.ERR.- EST.ERR.-AVG. CALC.FREQ. -  DIFF. - WT.
    1:   3  2                                  7860.96630    7860.96841   -0.00211    0.00200   0.00000
    2:   4  3                                 10481.17900   10481.17995   -0.00095    0.00200   0.00000
    3:   5  4                                 13101.29490   13101.29612   -0.00122    0.00200   0.00000
    4:   6  5                                 15721.29980   15721.29306    0.00674    0.00200   0.00000
    5:   7  6                                 18341.14350   18341.14695   -0.00345    0.00200   0.00000
NORMALIZED DIAGONAL:
    1   1.00000E+00    2   3.60177E-01    3   1.00000E+00
MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00
                              NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION
   1           100                1310.179285(239)         0.000000
   2           200                    -0.9935( 32)E-03      -0.0000E-03
   3           300                0.030352677(  0)E-21 -0.000000000E-21
 MICROWAVE AVG =       -0.000200 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.003582 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.79101         1.79101
```

Molecule 215

IUPAC Name: 2,4-cyclopentadien-1-one (ve2)

Common name: cyclopentadienone (ve2)

SMILES: C1=CC(=O)C=C1



215: Line file

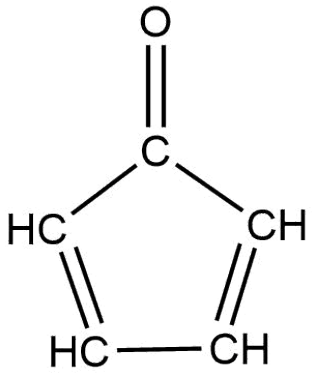
```
cyclopentadienone (ve2)
  2  0  2  1  0  1                    12936.6602     0.0020  /2-455268
  3  0  3  2  0  2                    18834.2320     0.0020  /2-455268
```

Molecule 216

IUPAC Name: 2,4-cyclopentadien-1-one (ve3)

Common name: cyclopentadienone (ve3)

SMILES: C1=CC(=O)C=C1



216: Line file

```
cyclopentadienone (ve3)
  2  0  2  1  0  1                    12947.5136     0.0020  /2-455270
  3  0  3  2  0  2                    18850.5687     0.0020  /2-455038
```

Molecule 217

IUPAC Name: but-2-enedinitrile (Z)

Common name: maleonitrile

SMILES: N#CC=CC#N