Supporting Information

Through-Space Effects of Substituents Dominate Molecular Electrostatic Potentials of Substituted Arenes

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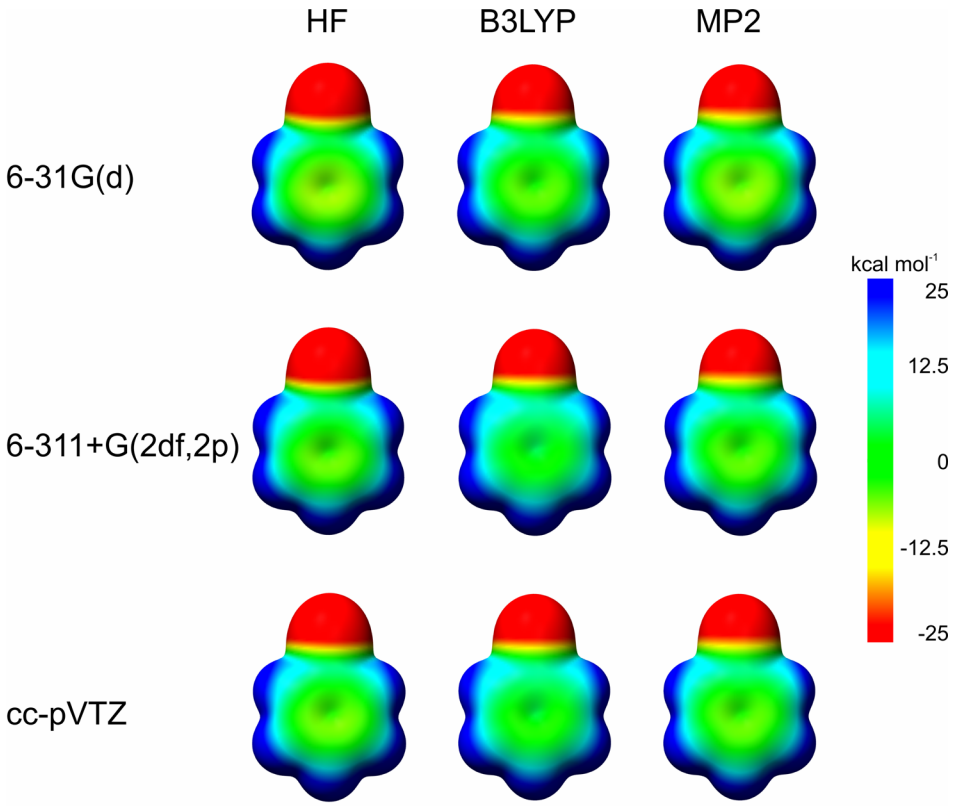

Figure S1. ESP plots for cyanobenzene at various levels of theory mapped onto the corresponding electron density isosurfaces (0.001 e/au^3).

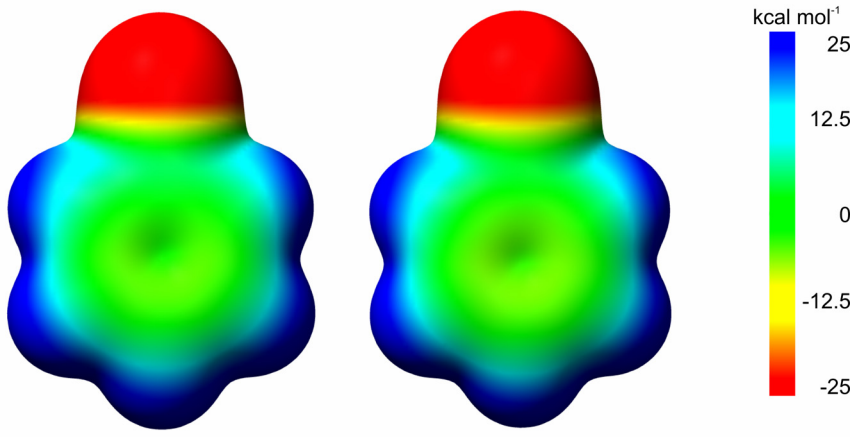

Figure S2. B3LYP/6-31G(d) ESP plots for cyanobenzene at the constrained geometry (left, carbons and hydrogens fixed at their corresponding positions in benzene) and the fully relaxed geometry (right), mapped onto the corresponding electron density isosurfaces (0.001 e/au^3).

Optimized Cartesian Coordinates (Angstrom)

Monosubstituted Benzenes

```
14
C6H5BF2
C         0.0000000         1.3937980         0.0000000
C         1.2070640         0.6968990         0.0000000
C        -1.2070640         0.6968990         0.0000000
C         0.0000000        -1.3937980         0.0000000
C        -1.2070640        -0.6968990         0.0000000
C         1.2070640        -0.6968990         0.0000000
H         2.1451990         1.2385310         0.0000000
H         2.1451990        -1.2385310         0.0000000
H         0.0000000        -2.4770620         0.0000000
H        -2.1451990        -1.2385310         0.0000000
H        -2.1451990         1.2385310         0.0000000
B         0.0000000         2.9418060        -0.0001520
F         1.1325220         3.6403670        -0.0003410
F        -1.1325220         3.6403670        -0.0003410

4
HBF2 as in C6H5BF2
H         0.0000000         1.7539420         0.0001180
B         0.0000000         2.9418060        -0.0001520
F         1.1325220         3.6403670        -0.0003410
F        -1.1325220         3.6403670        -0.0003410

14
C6H5CCH
C         0.0000000         1.3937980         0.0000000
C         1.2070640         0.6968990         0.0000000
C        -1.2070640         0.6968990         0.0000000
C         0.0000000        -1.3937980         0.0000000
C        -1.2070640        -0.6968990         0.0000000
C         1.2070640        -0.6968990         0.0000000
H         2.1451990         1.2385310         0.0000000
H         2.1451990        -1.2385310         0.0000000
H         0.0000000        -2.4770620         0.0000000
H        -2.1451990        -1.2385310         0.0000000
H        -2.1451990         1.2385310         0.0000000
C         0.0000000         2.8271110         0.0000000
C         0.0000000         4.0368540         0.0000000
H         0.0000000         5.1031920         0.0000000

5
HCCH as in C6H5CCH
H         0.0000000         1.7602190         0.0000000
C         0.0000000         2.8271110         0.0000000
C         0.0000000         4.0368540         0.0000000
H         0.0000000         5.1031920         0.0000000

15
C6H5CF3
C         0.0000000         1.3937980         0.0000000
C         1.2070640         0.6968990         0.0000000
C        -1.2070640         0.6968990         0.0000000
C         0.0000000        -1.3937980         0.0000000
C        -1.2070640        -0.6968990         0.0000000
C         1.2070640        -0.6968990         0.0000000
H         2.1451990         1.2385310         0.0000000
H         2.1451990        -1.2385310         0.0000000
H         0.0000000        -2.4770620         0.0000000
H        -2.1451990        -1.2385310         0.0000000
H        -2.1451990         1.2385310         0.0000000
C        -0.0000070         2.8970100         0.0637840
F        -1.0902960         3.4276100        -0.5346890
F         0.0000000         3.3435180         1.3418350
F         1.0903280         3.4276270        -0.5347240

5
HCF3 as in C6H5CF3
H         0.0000130         1.8073230         0.0132430
C        -0.0000070         2.8970100         0.0637840
F        -1.0902960         3.4276100        -0.5346890
F         0.0000000         3.3435180         1.3418350
F         1.0903280         3.4276270        -0.5347240
```

16
C6H5CH2OH
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
C 0.0047160 2.9130060 0.0327040
H 0.1143770 3.2707700 1.0636620
H -0.9612540 3.2951270 -0.3352670
O 1.0942290 3.4977510 -0.6706660
H 1.0576040 3.1662940 -1.5821600

6
HCH2OH as in C6H5CH2OH
H 0.0080630 1.8141870 0.0194620
C 0.0047160 2.9130060 0.0327040
H 0.1143770 3.2707700 1.0636620
H -0.9612540 3.2951270 -0.3352670
O 1.0942290 3.4977510 -0.6706660
H 1.0576040 3.1662940 -1.5821600

15
C6H5CH3
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
C -0.0000260 2.9088660 0.0321440
H -0.8849560 3.3221760 -0.4640200
H -0.0019270 3.2848340 1.0643490
H 0.8867330 3.3221300 -0.4607670

5
HCH3 as in C6H5CH3
H -0.0000050 1.8181880 0.0058740
C -0.0000260 2.9088660 0.0321440
H -0.8849560 3.3221760 -0.4640200
H -0.0019270 3.2848340 1.0643490
H 0.8867330 3.3221300 -0.4607670

14
C6H5CHO
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
C -0.0064860 2.8750990 0.0000000
O 0.9884610 3.5737970 0.0000000
H -1.0220320 3.3328560 0.0000000

4
HCHO as in C6H5CHO
H 0.0375800 1.7673310 0.0000000
C -0.0064860 2.8750990 0.0000000
O 0.9884610 3.5737970 0.0000000
H -1.0220320 3.3328560 0.0000000

```
13
C6H5CN
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
C        0.0000000        2.8298550        0.0000000
N        0.0000000        3.9930500        0.0000000

3
HCN as in C6H5CN
H        0.0000000        1.7591240        0.0000000
C        0.0000000        2.8298550        0.0000000
N        0.0000000        3.9930500        0.0000000

17
C6H5COCH3
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
C        0.0602610        2.8952860        0.0000000
O        1.1353560        3.4752140       -0.0000230
C       -1.2391440        3.6864090       -0.0000250
H       -1.8456580        3.4528640       -0.8834060
H       -1.8456710        3.4528970        0.8833560
H       -0.9974190        4.7505440       -0.0000420

7
HCOCH3 as in C6H5COCH3
H       -0.0076280        1.7874280        0.0000440
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O        1.1353560        3.4752140       -0.0000230
C       -1.2391440        3.6864090       -0.0000250
H       -1.8456580        3.4528640       -0.8834060
H       -1.8456710        3.4528970        0.8833560
H       -0.9974190        4.7505440       -0.0000420

18
C6H5COOCH3
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
C        0.0608800        2.8843640       -0.0000070
O        1.0891290        3.5324730        0.0000200
O       -1.1679300        3.4531140       -0.0000180
C       -1.1770370        4.8882740        0.0001080
H       -0.6734640        5.2764120       -0.8893690
H       -2.2296180        5.1733740        0.0004750
H       -0.6728530        5.2762750        0.8892920

8
HCOOCH3 as in C6H5COOCH3
H       -0.0265620        1.7900100        0.0000180
C        0.0608800        2.8843640       -0.0000070
O        1.0891290        3.5324730        0.0000200
O       -1.1679300        3.4531140       -0.0000180
C       -1.1770370        4.8882740        0.0001080
H       -0.6734640        5.2764120       -0.8893690
H       -2.2296180        5.1733740        0.0004750
H       -0.6728530        5.2762750        0.8892920

15
C6H5COOH
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
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H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
C        0.0561190        2.8802480       -0.0000240
O        1.0766480        3.5395660        0.0005630
O       -1.1727430        3.4605160       -0.0008360
H       -1.0073640        4.4213910       -0.0009240

5
HCOOH as in C6H5COOH
H       -0.0260310        1.7865490        0.0001220
C        0.0561190        2.8802480       -0.0000240
O        1.0766480        3.5395660        0.0005630
O       -1.1727430        3.4605160       -0.0008360
H       -1.0073640        4.4213910       -0.0009240


12
C6H5F
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
F        0.0000000        2.7401870        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000

2
HF as in C6H5F
F        0.0000000        2.7401870        0.0000000
H        0.0000000        1.8996520        0.0000000

20
C6H5NCH3_2
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
N       -0.0000990        2.7966770       -0.0247350
C       -1.2417630        3.5106360        0.2150510
H       -1.0495560        4.5847550        0.1736570
H       -1.9857750        3.2834960       -0.5584130
H       -1.6920130        3.2800190        1.1951200
C        1.2418460        3.5109540        0.2125110
H        1.6932550        3.2821060        1.1924950
H        1.9848870        3.2823680       -0.5614010
H        1.0496580        4.5850100        0.1693120

10
HNCH3_2 as in C6H5NCH3_2
H        0.0004740        1.8787230        0.4019420
N       -0.0000990        2.7966770       -0.0247350
C       -1.2417630        3.5106360        0.2150510
H       -1.0495560        4.5847550        0.1736570
H       -1.9857750        3.2834960       -0.5584130
H       -1.6920130        3.2800190        1.1951200
C        1.2418460        3.5109540        0.2125110
H        1.6932550        3.2821060        1.1924950
H        1.9848870        3.2823680       -0.5614010
H        1.0496580        4.5850100        0.1693120
```

14
C6H5NH2
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
N 0.0000000 2.7976610 -0.0588810
H 0.8336820 3.2322300 0.3182530
H -0.8336820 3.2322300 0.3182530

4
HNH2 as in C6H5NH2
H -0.0002590 1.8367180 0.2770250
N 0.0000000 2.7976610 -0.0588810
H 0.8336820 3.2322300 0.3182530
H -0.8336820 3.2322300 0.3182530

17
C6H5NHCH3
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
N 0.0339140 2.7922180 -0.0403440
C -1.1311950 3.5896290 0.2919470
H -0.8416910 4.6439050 0.2989390
H -1.9115290 3.4695810 -0.4686980
H -1.5721160 3.3414250 1.2720450
H 0.9054540 3.1811640 0.2936200

7
HNHCH3 as in C6H5NHCH3
H -0.0389010 1.8449270 0.3164510
N 0.0339140 2.7922180 -0.0403440
C -1.1311950 3.5896290 0.2919470
H -0.8416910 4.6439050 0.2989390
H -1.9115290 3.4695810 -0.4686980
H -1.5721160 3.3414250 1.2720450
H 0.9054540 3.1811640 0.2936200

15
C6H5NHOH
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
N 0.0415130 2.8101550 -0.0956680
O -1.1194670 3.4331810 0.4618720
H -1.4859330 3.9134550 -0.2981910
H 0.8259380 3.1848810 0.4348330

5
HNHOH as in C6H5NHOH
H -0.0432910 1.8361330 0.2018810
N 0.0415130 2.8101550 -0.0956680
O -1.1194670 3.4331810 0.4618720
H -1.4859330 3.9134550 -0.2981910
H 0.8259380 3.1848810 0.4348330

13
C6H5NO
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
N -0.1036370 2.8317190 0.0000000
O 0.9664440 3.4222230 0.0000000
3
HNO as in C6H5NO
H 0.0998230 1.7842180 0.0000000
N -0.1036370 2.8317190 0.0000000
O 0.9664440 3.4222230 0.0000000

14
C6H5NO2
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
N 0.0000000 2.8605710 0.0000000
O 1.0905650 3.4308910 -0.0000340
O -1.0905650 3.4308910 -0.0000340

4
HNO2 as in C6H5NO2
H 0.0000000 1.8193500 0.0000250
N 0.0000000 2.8605710 0.0000000
O 1.0905650 3.4308910 -0.0000340
O -1.0905650 3.4308910 -0.0000340

16
C6H5OCF3
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
O -0.1063000 2.7871980 -0.0489780
C 0.8125120 3.5691230 0.5669640
F 1.9975300 3.5892690 -0.0839780
F 0.3336560 4.8127590 0.5832710
F 1.0608170 3.1803640 1.8296660

6
HOCF3 as in C6H5OCF3
H 0.2235870 1.8734660 -0.0675810
O -0.1063000 2.7871980 -0.0489780
C 0.8125120 3.5691230 0.5669640
F 1.9975300 3.5892690 -0.0839780
F 0.3336560 4.8127590 0.5832710
F 1.0608170 3.1803640 1.8296660

13
C6H5OH
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
O -0.0622570 2.7623200 0.0000000
H 0.8405920 3.1165350 0.0000000

3
HOH as in C6H5OH
H 0.0690340 1.8025590 0.0000000
O -0.0622570 2.7623200 0.0000000
H 0.8405920 3.1165350 0.0000000

16
C6H5OMe
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
O -0.1061940 2.7585350 0.0000010
C 1.0846720 3.5268560 -0.0000020
H 1.6923950 3.3343950 -0.8945140
H 0.7670250 4.5713810 -0.0000150
H 1.6923850 3.3344150 0.8945220

6
HOMe as in C6H5OMe
H 0.1452590 1.8234540 0.0000050
O -0.1061940 2.7585350 0.0000010
C 1.0846720 3.5268560 -0.0000020
H 1.6923950 3.3343950 -0.8945140
H 0.7670250 4.5713810 -0.0000150
H 1.6923850 3.3344150 0.8945220

16
C6H5SCH3
C 0.0000000 1.3937980 0.0000000
C 1.2070640 0.6968990 0.0000000
C -1.2070640 0.6968990 0.0000000
C 0.0000000 -1.3937980 0.0000000
C -1.2070640 -0.6968990 0.0000000
C 1.2070640 -0.6968990 0.0000000
H 2.1451990 1.2385310 0.0000000
H 2.1451990 -1.2385310 0.0000000
H 0.0000000 -2.4770620 0.0000000
H -2.1451990 -1.2385310 0.0000000
H -2.1451990 1.2385310 0.0000000
S -0.1259000 3.1792430 0.0000130
C 1.6087750 3.7378810 -0.0001190
H 2.1410460 3.4069510 -0.8963770
H 1.5654100 4.8300000 -0.0001600
H 2.1411630 3.4070230 0.8960950

6
HSCH3 as in C6H5SCH3
H 0.1216980 1.8513030 -0.0000520
S -0.1259000 3.1792430 0.0000130
C 1.6087750 3.7378810 -0.0001190
H 2.1410460 3.4069510 -0.8963770
H 1.5654100 4.8300000 -0.0001600
H 2.1411630 3.4070230 0.8960950

```
13
C6H5SH
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
S       -0.0800220        3.1837070        0.0000000
H        1.2502400        3.4061270        0.0000000

3
HSH as in C6H5SH
H        0.0777910        1.8432860        0.0000000
S       -0.0800220        3.1837070        0.0000000
H        1.2502400        3.4061270        0.0000000

15
C6H5SiF3
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
Si       -0.0000140        3.2319900        0.0276110
F       -1.2988550        3.8001710       -0.7058820
F        0.0003510        3.8578250        1.4975450
F        1.2984330        3.8002370       -0.7065240

5
HSiF3 as in C6H5SiF3
H        0.0000250        1.7675610        0.0527750
Si       -0.0000140        3.2319900        0.0276110
F       -1.2988550        3.8001710       -0.7058820
F        0.0003510        3.8578250        1.4975450
F        1.2984330        3.8002370       -0.7065240

15
C6H5SiH3
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        2.1451990       -1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1451990       -1.2385310        0.0000000
H       -2.1451990        1.2385310        0.0000000
Si        0.0001490        3.2772270        0.0358490
H       -1.2136080        3.8014840       -0.6485020
H        0.0001980        3.8116970        1.4274900
H        1.2140780        3.8011390       -0.6484680

5
HSiH3 as in C6H5SiH3
H       -0.0000590        1.7926330        0.0394350
Si        0.0001490        3.2772270        0.0358490
H       -1.2136080        3.8014840       -0.6485020
H        0.0001980        3.8116970        1.4274900
H        1.2140780        3.8011390       -0.6484680
```

Polysubstituted Benzenes

```
24
hexaaminobenzene
C        0.0000000        1.3937980       -0.0641980
C       -1.2070640        0.6968990       -0.0641980
C        1.2070640        0.6968990       -0.0641980
C        0.0000000       -1.3937980       -0.0641980
C        1.2070640       -0.6968990       -0.0641980
C       -1.2070640       -0.6968990       -0.0641980
N        0.0000000        2.8637980       -0.0641980
H       -0.8164970        3.1971310        0.4072070
H        0.8164970        3.1971310        0.4072070
N       -2.4801220        1.4318980       -0.0641980
H       -3.1770450        0.8914580        0.4072070
H       -2.4113350        2.3120300        0.4374470
N       -2.4801220       -1.4318980       -0.0641980
H       -2.4113350       -2.3120300        0.4374470
H       -3.1770450       -0.8914580        0.4072070
N        0.0000000       -2.8637980       -0.0641980
H        0.8164970       -3.1971310        0.4072070
H       -0.8164970       -3.1971310        0.4072070
N        2.4801220       -1.4318980       -0.0641980
H        3.1770450       -0.8914580        0.4072070
H        2.4113350       -2.3120300        0.4374470
N        2.4801220        1.4318980       -0.0641980
H        2.4113350        2.3120300        0.4374470
H        3.1770450        0.8914580        0.4072070

24
6 HNH2 as in hexaaminobenzene
H        0.0000000        1.8508490        0.0337050
N        0.0000000        2.8637980       -0.0641980
H       -0.8164970        3.1971310        0.4072070
H        0.8164970        3.1971310        0.4072070
H       -1.5952670        0.9508160        0.0890810
N       -2.4801220        1.4318980       -0.0641980
H       -3.1770450        0.8914580        0.4072070
H       -2.4113350        2.3120300        0.4374470
H       -1.5950280       -0.9511110        0.0887440
N       -2.4801220       -1.4318980       -0.0641980
H       -2.4113350       -2.3120300        0.4374470
H       -3.1770450       -0.8914580        0.4072070
H        0.0000000       -1.8508490        0.0337050
N        0.0000000       -2.8637980       -0.0641980
H        0.8164970       -3.1971310        0.4072070
H       -0.8164970       -3.1971310        0.4072070
H        1.5952670       -0.9508160        0.0890810
N        2.4801220       -1.4318980       -0.0641980
H        3.1770450       -0.8914580        0.4072070
H        2.4113350       -2.3120300        0.4374470
H        1.5950280        0.9511110        0.0887440
N        2.4801220        1.4318980       -0.0641980
H        2.4113350        2.3120300        0.4374470
H        3.1770450        0.8914580        0.4072070

15
tricyanobenzene
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
H        2.1451990        1.2385310        0.0000000
H        0.0000000       -2.4770620        0.0000000
H       -2.1462430        1.2391560        0.0000000
C        0.0000190        2.8293840        0.0000000
N        0.0000370        3.9915530        0.0000000
C       -2.4503500       -1.4146550        0.0000000
N       -3.4569280       -1.9955470        0.0000000
C        2.4503600       -1.4146380        0.0000000
N        3.4569470       -1.9955140        0.0000000

9
3 HCN as in tricyanobenzene
H        0.0000030        1.7586860        0.0000000
C        0.0000190        2.8293840        0.0000000
N        0.0000370        3.9915530        0.0000000
H       -1.5229970       -0.8794800        0.0000000
C       -2.4503500       -1.4146550        0.0000000
N       -3.4569280       -1.9955470        0.0000000
H        1.5229990       -0.8794770        0.0000000
C        2.4503600       -1.4146380        0.0000000
N        3.4569470       -1.9955140        0.0000000

12
hexafluorobenzene
C        0.0000000        1.3937980        0.0000000
C        1.2070640        0.6968990        0.0000000
C       -1.2070640        0.6968990        0.0000000
C        0.0000000       -1.3937980        0.0000000
C       -1.2070640       -0.6968990        0.0000000
C        1.2070640       -0.6968990        0.0000000
F        0.0000000        2.7294300        0.0000000
F        2.3637560        1.3647150        0.0000000
F        2.3637560       -1.3647150        0.0000000
F        0.0000000       -2.7294300        0.0000000
F       -2.3637560       -1.3647150        0.0000000
F       -2.3637560        1.3647150        0.0000000
```

```
12
6 HF as in hexafluorobenzene
H         0.0000000         1.7956700         0.0000000
F         0.0000000         2.7294300         0.0000000
H         1.5185600         0.9677960         0.0000000
F         2.3637560         1.3647150         0.0000000
H         1.5185600        -0.9677960         0.0000000
F         2.3637560        -1.3647150         0.0000000
H         0.0000000        -1.7956700         0.0000000
F         0.0000000        -2.7294300         0.0000000
H        -1.5185600        -0.9677960         0.0000000
F        -2.3637560        -1.3647150         0.0000000
H        -1.5185600         0.9677960         0.0000000
F        -2.3637560         1.3647150         0.0000000
```

Cryptolepines

```
31
Cryptolepine
C       -4.0851940        1.2487790       -0.1301040
C       -2.7175120        1.4555950       -0.0971380
C       -1.8543350        0.3385730        0.0008640
C       -2.4314150       -0.9679670        0.0244100
C       -3.8119100       -1.1744780       -0.0061530
C       -4.6265910       -0.0530260       -0.0765670
C       -0.4322550        0.1279040        0.0388840
C       -0.2028990       -1.2897590        0.0517690
N       -1.4269230       -1.9151230        0.0619400
N        0.6239160        0.9771390        0.0790010
C        1.9308300        0.4985970        0.0094550
C        2.1610100       -0.9170230        0.0154660
C        1.0670690       -1.8105380        0.0595290
C        3.0366260        1.3749130       -0.0751600
C        4.3195320        0.8660990       -0.1244720
C        4.5591950       -0.5254180       -0.0894660
C        3.4979590       -1.3962420       -0.0250280
C        0.3784200        2.4221370        0.2426520
H       -4.7526310        2.1005230       -0.2070780
H       -2.3363630        2.4663150       -0.1716310
H       -4.2303890       -2.1756420        0.0180040
H       -5.7042680       -0.1813870       -0.1031630
H       -1.5686250       -2.9148030        0.0518010
H        1.2451770       -2.8817260        0.0843220
H        2.8973130        2.4463000       -0.1333130
H        5.1564190        1.5532890       -0.1992910
H        5.5765310       -0.9008160       -0.1239700
H        3.6602270       -2.4699370       -0.0113610
H        1.1719620        2.8577600        0.8464580
H       -0.5575910        2.5555230        0.7785000
H        0.3321070        2.9216120       -0.7295000
```

```
35
7,9-dinitrocryptolepine
C       -4.0851940        1.2487790       -0.1301040
C       -2.7175120        1.4555950       -0.0971380
C       -1.8543350        0.3385730        0.0008640
C       -2.4314150       -0.9679670        0.0244100
C       -3.8119100       -1.1744780       -0.0061530
C       -4.6265910       -0.0530260       -0.0765670
C       -0.4322550        0.1279040        0.0388840
C       -0.2028990       -1.2897590        0.0517690
N       -1.4269230       -1.9151230        0.0619400
N        0.6239160        0.9771390        0.0790010
C        1.9308300        0.4985970        0.0094550
C        2.1610100       -0.9170230        0.0154660
C        1.0670690       -1.8105380        0.0595290
C        3.0366260        1.3749130       -0.0751600
C        4.3195320        0.8660990       -0.1244720
C        4.5591950       -0.5254180       -0.0894660
C        3.4979590       -1.3962420       -0.0250280
C        0.3784200        2.4221370        0.2426520
H       -2.3363630        2.4663150       -0.1716310
H       -5.7042680       -0.1813870       -0.1031630
H       -1.5686250       -2.9148030        0.0518010
H        1.2451770       -2.8817260        0.0843220
H        2.8973130        2.4463000       -0.1333130
H        5.1564190        1.5532890       -0.1992910
H        5.5765310       -0.9008160       -0.1239700
H        3.6602270       -2.4699370       -0.0113610
H        1.1719620        2.8577600        0.8464580
H       -0.5575910        2.5555230        0.7785000
H        0.3321070        2.9216120       -0.7295000
N       -4.4006470       -2.5125350        0.0223250
O       -3.6100730       -3.4640800        0.0538300
O       -5.6173340       -2.6014560        0.0127730
N       -4.9900390        2.4069760       -0.2327380
O       -4.4624490        3.5146470       -0.2899590
O       -6.1920440        2.1749510       -0.2520070

8
2 HNO2 as in 7,9-dinitrocryptolepine
H       -3.9859750       -1.5565220        0.0022130
N       -4.4006470       -2.5125350        0.0223250
O       -3.6100730       -3.4640800        0.0538300
O       -5.6173340       -2.6014560        0.0127730
H       -4.3512610        1.5859850       -0.1604170
N       -4.9900390        2.4069760       -0.2327380
O       -4.4624490        3.5146470       -0.2899590
O       -6.1920440        2.1749510       -0.2520070
```

Klärner Guest Molecules

```
24
AQ
C       -3.6951200       -0.6999450       -0.0000010
C       -2.4906630       -1.3980760       -0.0000020
C       -1.2748940       -0.7043870        0.0000030
C       -1.2748940        0.7043870        0.0000060
C       -2.4906630        1.3980760        0.0000070
C       -3.6951200        0.6999450        0.0000050
C        0.0000000       -1.4785380        0.0000050
C        0.0000000        1.4785380       -0.0000030
C        1.2748940        0.7043870        0.0000000
C        1.2748940       -0.7043870       -0.0000030
C        2.4906630       -1.3980760       -0.0000030
H        2.4645020       -2.4827730       -0.0000070
C        3.6951200       -0.6999450        0.0000030
C        3.6951200        0.6999450        0.0000050
C        2.4906630        1.3980760        0.0000040
H       -4.6361860       -1.2430060       -0.0000020
H       -2.4645020       -2.4827730       -0.0000080
H       -2.4645020        2.4827730        0.0000090
H       -4.6361860        1.2430060        0.0000050
H        4.6361860       -1.2430060        0.0000090
H        4.6361860        1.2430060        0.0000050
H        2.4645020        2.4827730        0.0000040
O        0.0000000        2.7050370       -0.0000150
O        0.0000000       -2.7050370       -0.0000060
```

```
28
1,5-DNAQ
C       -3.6951200       -0.6999450       -0.0000010
C       -2.4906630       -1.3980760       -0.0000020
C       -1.2748940       -0.7043870        0.0000030
C       -1.2748940        0.7043870        0.0000060
C       -2.4906630        1.3980760        0.0000070
C       -3.6951200        0.6999450        0.0000050
C        0.0000000       -1.4785380        0.0000050
C        0.0000000        1.4785380       -0.0000030
C        1.2748940        0.7043870        0.0000000
C        1.2748940       -0.7043870       -0.0000030
C        2.4906630       -1.3980760       -0.0000030
C        3.6951200       -0.6999450        0.0000030
C        3.6951200        0.6999450        0.0000050
C        2.4906630        1.3980760        0.0000040
H       -4.6361860       -1.2430060       -0.0000020
H       -2.4645020       -2.4827730       -0.0000080
H       -4.6361860        1.2430060        0.0000050
H        4.6361860       -1.2430060        0.0000090
H        4.6361860        1.2430060        0.0000050
H        2.4645020        2.4827730        0.0000040
O        0.0000000        2.7050370       -0.0000150
O        0.0000000       -2.7050370       -0.0000060
N       -2.5918730        2.8734850       -0.0004490
O       -2.6772980        3.4139190       -1.0953680
O       -2.6787400        3.4144920        1.0941290
N        2.5918770       -2.8734780       -0.0000660
O        2.6777980       -3.4141570       -1.0948430
O        2.6781970       -3.4142470        1.0946560
```

```
8
2 HNO2 as in 1,5-DNAQ
H       -2.4288760        1.8426530       -0.0000620
N       -2.5918730        2.8734850       -0.0004490
O       -2.6772980        3.4139190       -1.0953680
O       -2.6787400        3.4144920        1.0941290
H        2.4289280       -1.8426390        0.0000100
N        2.5918770       -2.8734780       -0.0000660
O        2.6777980       -3.4141570       -1.0948430
O        2.6781970       -3.4142470        1.0946560
```

28
1,8-DNAQ

C	-3.6951200	-0.6999450	-0.0000010
C	-2.4906630	-1.3980760	-0.0000020
C	-1.2748940	-0.7043870	0.0000030
C	-1.2748940	0.7043870	0.0000060
C	-2.4906630	1.3980760	0.0000070
C	-3.6951200	0.6999450	0.0000050
C	0.0000000	-1.4785380	0.0000050
C	0.0000000	1.4785380	-0.0000030
C	1.2748940	0.7043870	0.0000000
C	1.2748940	-0.7043870	-0.0000030
C	2.4906630	-1.3980760	-0.0000030
C	3.6951200	-0.6999450	0.0000030
C	3.6951200	0.6999450	0.0000050
C	2.4906630	1.3980760	0.0000040
H	-4.6361860	-1.2430060	-0.0000020
H	-2.4645020	2.4827730	0.0000090
H	-4.6361860	1.2430060	0.0000050
H	4.6361860	-1.2430060	0.0000090
H	4.6361860	1.2430060	0.0000050
H	2.4645020	2.4827730	0.0000040
O	0.0000000	2.7050370	-0.0000150
O	0.0000000	-2.7050370	-0.0000060
N	-2.5947380	-2.8735390	-0.0000040
N	2.5947380	-2.8735390	-0.0000050
O	-2.6828410	-3.4127020	-1.0950640
O	2.6828110	-3.4127090	1.0950540
O	-2.6828860	-3.4127010	1.0950530
O	2.6828480	-3.4127020	-1.0950650

8
2 HNO2 as in 1,8-DNAQ

H	-2.4275040	-1.8432920	-0.0000010
N	-2.5947380	-2.8735390	-0.0000040
O	-2.6828410	-3.4127020	-1.0950640
O	-2.6828860	-3.4127010	1.0950530
H	4.587438	-3.483298	-0.000009
N	4.903344	-5.430202	-0.000009
O	5.069778	-6.449085	2.069352
O	5.069848	-6.449072	-2.069373

26
dicyanomethylenefluorene

C	-3.0084510	-2.2791450	0.0000010
C	-1.6371320	-2.5650480	0.0000000
C	-0.7347360	-1.5101490	-0.0000010
C	-1.1854220	-0.1662590	-0.0000020
C	-2.5546170	0.1100920	0.0000000
C	-3.4593580	-0.9579810	0.0000010
H	-3.7266330	-3.0943210	0.0000030
H	-2.9299840	1.1255280	-0.0000010
C	0.7347570	-1.5101390	-0.0000010
C	1.6371660	-2.5650270	0.0000000
C	1.1854250	-0.1662440	-0.0000020
C	3.0084800	-2.2791080	0.0000010
H	1.2912990	-3.5949720	0.0000010
C	2.5546170	0.1101240	0.0000000
C	3.4593710	-0.9579370	0.0000010
H	3.7266730	-3.0942740	0.0000030
H	2.9299720	1.1255650	-0.0000010
C	-0.0000040	0.7196190	-0.0000040
C	-0.0000140	2.0942990	-0.0000030
C	-1.1965140	2.8790730	-0.0000010
C	1.1964750	2.8790910	-0.0000010
N	-2.1521950	3.5440190	0.0000030
N	2.1521460	3.5440510	0.0000030
H	-4.5251380	-0.7503250	0.0000020
H	-1.2912520	-3.5949880	0.0000010
H	4.5251480	-0.7502680	0.0000020

```
32
TNF
C       -3.0084510       -2.2791450        0.0000010
C       -1.6371320       -2.5650480        0.0000000
C       -0.7347360       -1.5101490       -0.0000010
C       -1.1854220       -0.1662590       -0.0000020
C       -2.5546170        0.1100920        0.0000000
C       -3.4593580       -0.9579810        0.0000010
H       -3.7266330       -3.0943210        0.0000030
H       -2.9299840        1.1255280       -0.0000010
C        0.7347570       -1.5101390       -0.0000010
C        1.6371660       -2.5650270        0.0000000
C        1.1854250       -0.1662440       -0.0000020
C        3.0084800       -2.2791080        0.0000010
H        1.2912990       -3.5949720        0.0000010
C        2.5546170        0.1101240        0.0000000
C        3.4593710       -0.9579370        0.0000010
H        3.7266730       -3.0942740        0.0000030
H        2.9299720        1.1255650       -0.0000010
C       -0.0000040        0.7196190       -0.0000040
C       -0.0000140        2.0942990       -0.0000030
C       -1.1965140        2.8790730       -0.0000010
C        1.1964750        2.8790910       -0.0000010
N       -2.1521950        3.5440190        0.0000030
N        2.1521460        3.5440510        0.0000030
N       -4.9061000       -0.6903450        0.0086310
O       -5.2570680        0.4854540       -0.0133760
O       -5.6566790       -1.6623160        0.0370050
N       -1.2987370       -3.9955730        0.0635060
O       -0.4607670       -4.3479080        0.8916720
O       -1.9222990       -4.7405630       -0.6832700
N        4.9044340       -0.6797510        0.0014410
O        5.2522340        0.4980270       -0.0012060
O        5.6627760       -1.6469320        0.0037160

12
3 HNO2 as in TNF
H       -3.8814950       -0.8809970        0.0026250
N       -4.9061000       -0.6903450        0.0086310
O       -5.2570680        0.4854540       -0.0133760
O       -5.6566790       -1.6623160        0.0370050
H       -1.4952280       -2.9745670       -0.0071440
N       -1.2987370       -3.9955730        0.0635060
O       -0.4607670       -4.3479080        0.8916720
O       -1.9222990       -4.7405630       -0.6832700
H        3.8810200       -0.8759160        0.0010000
N        4.9044340       -0.6797510        0.0014410
O        5.2522340        0.4980270       -0.0012060
O        5.6627760       -1.6469320        0.0037160
```

Supramolecular Synthons

```
48
1,3,5-trisphenethynylbenzene
C        1.2214360         0.7051960         0.0000000
C        0.0000000         1.4008080         0.0000000
C       -1.2214360         0.7051960         0.0000000
C       -1.2131350        -0.7004040         0.0000000
C        0.0000000        -1.4103920         0.0000000
C        1.2131350        -0.7004040         0.0000000
H        0.0000000         2.4851080         0.0000000
H       -2.1521670        -1.2425540         0.0000000
H        2.1521670        -1.2425540         0.0000000
C       -2.4556780         1.4177860         0.0000000
C       -3.5087850         2.0257980         0.0000000
C        2.4556780         1.4177860         0.0000000
C        3.5087850         2.0257980         0.0000000
C        0.0000000        -2.8355730         0.0000000
C        0.0000000        -4.0515960         0.0000000
C        0.0000000        -5.4768070         0.0000000
C        1.2135770        -6.1935190         0.0000000
C       -1.2135770        -6.1935190         0.0000000
H       -2.1509090        -5.6456910         0.0000000
C       -1.2087730        -7.5857460         0.0000000
C        1.2087730        -7.5857460         0.0000000
H        2.1510910        -8.1270370         0.0000000
C        0.0000000        -8.2866830         0.0000000
H        0.0000000        -9.3731680         0.0000000
H        2.1509090        -5.6456910         0.0000000
H       -2.1510910        -8.1270370         0.0000000
C        4.7430540         2.7384030         0.0000000
C        4.7569560         4.1477480         0.0000000
H        3.8138570         4.6855870         0.0000000
C        5.9650620         4.8397010         0.0000000
C        5.9705330         2.0457710         0.0000000
C        7.1738350         2.7460450         0.0000000
H        8.1137660         2.2006190         0.0000000
C       -4.7430540         2.7384030         0.0000000
C       -5.9705330         2.0457710         0.0000000
H       -5.9647660         0.9601030         0.0000000
C       -7.1738350         2.7460450         0.0000000
C       -7.1764780         4.1433410         0.0000000
H       -8.1174020         4.6865840         0.0000000
C       -5.9650620         4.8397010         0.0000000
H       -5.9626750         5.9264180         0.0000000
C       -4.7569560         4.1477480         0.0000000
C        7.1764780         4.1433410         0.0000000
H        8.1174020         4.6865840         0.0000000
H        5.9647660         0.9601030         0.0000000
H        5.9626750         5.9264180         0.0000000
H       -3.8138570         4.6855870         0.0000000
H       -8.1137660         2.2006190         0.0000000
```

```
48
1,3,5-tris(perfluorophenethynyl)benzene
C        1.2214360         0.7051960         0.0000000
C        0.0000000         1.4008080         0.0000000
C       -1.2214360         0.7051960         0.0000000
C       -1.2131350        -0.7004040         0.0000000
C        0.0000000        -1.4103920         0.0000000
C        1.2131350        -0.7004040         0.0000000
H        0.0000000         2.4851080         0.0000000
H       -2.1521670        -1.2425540         0.0000000
H        2.1521670        -1.2425540         0.0000000
C       -2.4556780         1.4177860         0.0000000
C       -3.5087850         2.0257980         0.0000000
C        2.4556780         1.4177860         0.0000000
C        3.5087850         2.0257980         0.0000000
C        0.0000000        -2.8355730         0.0000000
C        0.0000000        -4.0515960         0.0000000
C        0.0000000        -5.4768070         0.0000000
C        1.2135770        -6.1935190         0.0000000
C       -1.2135770        -6.1935190         0.0000000
C       -1.2087730        -7.5857460         0.0000000
C        1.2087730        -7.5857460         0.0000000
C        0.0000000        -8.2866830         0.0000000
C        4.7430540         2.7384030         0.0000000
C        4.7569560         4.1477480         0.0000000
C        5.9650620         4.8397010         0.0000000
C        5.9705330         2.0457710         0.0000000
C        7.1738350         2.7460450         0.0000000
C       -4.7430540         2.7384030         0.0000000
C       -5.9705330         2.0457710         0.0000000
C       -7.1738350         2.7460450         0.0000000
C       -7.1764780         4.1433410         0.0000000
C       -5.9650620         4.8397010         0.0000000
C       -4.7569560         4.1477480         0.0000000
C        7.1764780         4.1433410         0.0000000
F       -2.3774360        -5.5431240         0.0000000
F        2.3621150        -8.2634150         0.0000000
F        0.0000000        -9.6193530         0.0000000
F        2.3774360        -5.5431240         0.0000000
F       -2.3621150        -8.2634150         0.0000000
F        3.6114280         4.8299370         0.0000000
F        8.3380430         2.0872430         0.0000000
F       -5.9888690         0.7125960         0.0000000
F       -8.3308700         4.8090200         0.0000000
F       -5.9759560         6.1774380         0.0000000
F        8.3308700         4.8090200         0.0000000
F        5.9888690         0.7125960         0.0000000
F        5.9759560         6.1774380         0.0000000
F       -3.6114280         4.8299370         0.0000000
F       -8.3380430         2.0872430         0.0000000
```

```
30
15 HF as in 1,3,5-tris(perfluorophenethynyl)benzene
H        5.9791210         1.6462090         0.0000000
F        5.9888690         0.7125960         0.0000000
H       -5.9791210         1.6462090         0.0000000
F       -5.9888690         0.7125960         0.0000000
H        1.5536710        -7.7960850         0.0000000
F        2.3621150        -8.2634150         0.0000000
H       -7.5086320         4.3672340         0.0000000
F       -8.3308700         4.8090200         0.0000000
H       -5.9684500         5.2436670         0.0000000
F       -5.9759560         6.1774380         0.0000000
H       -4.4157330         4.3557860         0.0000000
F       -3.6114280         4.8299370         0.0000000
H        1.5586040        -5.9917360         0.0000000
F        2.3774360        -5.5431240         0.0000000
H       -7.5211460         2.5396380         0.0000000
F       -8.3380430         2.0872430         0.0000000
H        0.0000000        -8.6859510         0.0000000
F        0.0000000        -9.6193530         0.0000000
H       -1.5536710        -7.7960850         0.0000000
F       -2.3621150        -8.2634150         0.0000000
H       -1.5586040        -5.9917360         0.0000000
F       -2.3774360        -5.5431240         0.0000000
H        4.4157330         4.3557860         0.0000000
F        3.6114280         4.8299370         0.0000000
H        5.9684500         5.2436670         0.0000000
F        5.9759560         6.1774380         0.0000000
H        7.5086320         4.3672340         0.0000000
F        8.3308700         4.8090200         0.0000000
H        7.5211460         2.5396380         0.0000000
F        8.3380430         2.0872430         0.0000000
```