

# Topology Maps of a Bond Descriptor Based on the Kinetic Energy Density and the Essence of Chemical Bonding

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Supplementary Information

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Energies - Geometries - Frequencies

**C2H6 1**

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ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(3V)

Basis:

Carbon (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
C 0.000000 0.000000 -0.764738  
C 0.000000 0.000000 0.764896  
H -0.512113 0.887006 1.166463  
H -0.512113 -0.887006 1.166463  
H 1.024226 0.000000 1.166463  
H 0.512082 -0.886952 -1.166620  
H 0.512082 0.886952 -1.166620  
H -1.024163 0.000000 -1.166620  
-----

Net Charge: 0.00

Total Bonding Energy:

-1.484798649430184 hartree

-931.73 kcal/mol

-3898.34 kJ/mol

Zero-Point Energy : 190.26 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 234.02 J/mol-K

Internal Energy : 199.52 kJ/mol

Cv : 43.37 J/mol-K

Free Energy :-3766.12 kJ/mol

Frequencies (cm-1):

300.82 798.36 798.36 984.74 1176.58  
1176.58 1358.51 1371.73 1456.12 1456.12  
1456.62 1456.62 2958.58 2961.62 3012.07  
3012.07 3036.89 3036.89

Summary Geometry Optimization:

-----  
Energy Change : 0.000001

Gradient (Max): 0.000533

Gradient (RMS): 0.000135  
-----

Energies - Geometries - Frequencies

CNH5 2

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(S)

Basis:

Carbon (TZP)

Nitrogen (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
C -0.000016 -0.000016 0.000000  
N 1.469754 0.000319 0.000000  
H -0.476337 -0.998960 0.000000  
H -0.360116 0.545754 0.883301  
H -0.360116 0.545754 -0.883301  
H 1.816125 -0.510990 0.815025  
H 1.816125 -0.510990 -0.815025  
-----

Net Charge: 0.00

Total Bonding Energy:

-1.306505434557546 hartree

-819.84 kcal/mol

-3430.23 kJ/mol

Zero-Point Energy : 163.28 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 241.00 J/mol-K

Internal Energy : 172.38 kJ/mol

Cv : 40.82 J/mol-K

Free Energy : -3327.23 kJ/mol

Frequencies (cm-1):

294.45 822.05 949.30 1034.29 1135.95  
1309.13 1409.14 1451.10 1472.54 1612.87  
2898.55 2995.70 3034.19 3401.12 3478.40

Summary Geometry Optimization:

-----  
Energy Change : 0.000000

Gradient (Max): 0.000389

Gradient (RMS): 0.000105  
-----

Energies - Geometries - Frequencies

COH4 3

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEh

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(S)

Basis:

Carbon (TZP)

Oxygen (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
C 0.030051 -0.009198 0.000000  
O 1.461638 0.005453 0.000000  
H -0.293470 1.038892 0.000000  
H -0.382086 -0.499390 0.898573  
H -0.382086 -0.499390 -0.898573  
H 1.766155 -0.918464 0.000000  
-----

Net Charge: 0.00

Total Bonding Energy:

-1.106421479675394 hartree

-694.29 kcal/mol

-2904.91 kJ/mol

Zero-Point Energy : 130.43 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 239.04 J/mol-K

Internal Energy : 139.32 kJ/mol

Cv : 37.68 J/mol-K

Free Energy : -2834.38 kJ/mol

Frequencies (cm-1):

288.00 1009.50 1052.68 1130.92 1335.46

1428.48 1450.74 1462.41 2922.90 2973.03

3047.85 3705.24

Summary Geometry Optimization:

-----  
Energy Change : 0.000014

Gradient (Max): 0.000469

Gradient (RMS): 0.000167  
-----

Energies - Geometries - Frequencies

**CFH3 4**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEh

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(3V)

Basis:

Carbon (TZP)

Fluorine (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
C 0.000000 0.000000 0.039818  
F 0.000000 0.000000 1.443317  
H -0.520501 0.901534 -0.311315  
H -0.520501 -0.901534 -0.311315  
H 1.041002 0.000000 -0.311315  
-----

Net Charge: 0.00

Total Bonding Energy:

-0.878109518381149 hartree

-551.02 kcal/mol

-2305.48 kJ/mol

Zero-Point Energy : 99.80 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 223.02 J/mol-K

Internal Energy : 107.48 kJ/mol

Cv : 29.62 J/mol-K

Free Energy : -2262.01 kJ/mol

Frequencies (cm-1):

1019.38 1148.32 1148.32 1427.02 1444.24

1444.24 2960.35 3046.47 3046.47

Summary Geometry Optimization:

-----  
Energy Change : 0.000002

Gradient (Max): 0.000096

Gradient (RMS): 0.000048  
-----

Energies - Geometries - Frequencies

**C3H8 5**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: C(S)

Basis:  
Carbon (TZP)  
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
C -0.006474 -0.008423 0.000000  
C -1.536823 0.013241 0.000000  
C 0.571568 -1.427056 0.000000  
H 0.367930 0.539345 -0.880693  
H 0.367930 0.539345 0.880693  
H -1.940889 -0.498408 0.887707  
H -1.927382 1.041318 0.000000  
H -1.940889 -0.498408 -0.887707  
H 0.241851 -1.989148 0.887973  
H 1.671511 -1.417614 0.000000  
H 0.241851 -1.989148 -0.887973  
-----

Net Charge: 0.00

Total Bonding Energy:  
-2.090606796729378 hartree  
-1311.88 kcal/mol  
-5488.89 kJ/mol

Zero-Point Energy : 263.37 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 275.04 J/mol-K  
Internal Energy : 275.44 kJ/mol  
Cv : 63.73 J/mol-K

Free Energy :-5292.97 kJ/mol

Frequencies (cm-1):  
225.23 265.61 356.26 726.33 856.25  
880.43 900.06 1039.42 1138.45 1168.57  
1276.00 1316.70 1352.02 1369.08 1440.69  
1441.48 1448.16 1459.16 1463.31 2948.49  
2949.24 2952.37 2972.59 3011.80 3021.32  
3025.30 3028.54

Summary Geometry Optimization:

-----  
Energy Change : 0.000014  
Gradient (Max): 0.000977  
Gradient (RMS): 0.000256  
-----

Energies - Geometries - Frequencies

**C3H6 6**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: C(S)

Basis:  
Carbon (TZP)  
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
C 0.001837 0.000727 0.000000  
C 1.339503 0.004649 0.000000  
C 2.201415 1.232120 0.000000  
H -0.570489 0.932936 0.000000  
H -0.565626 -0.931713 0.000000  
H 1.868050 -0.956125 0.000000  
H 1.595322 2.148782 0.000000  
H 2.860543 1.251114 -0.882667  
H 2.860543 1.251114 0.882667  
-----

Net Charge: 0.00

Total Bonding Energy:  
-1.782806437610337 hartree  
-1118.73 kcal/mol  
-4680.76 kJ/mol

Zero-Point Energy : 202.66 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 265.49 J/mol-K  
Internal Energy : 213.56 kJ/mol  
Cv : 56.06 J/mol-K

Free Energy :-4543.87 kJ/mol

Frequencies (cm-1):  
203.86 412.91 569.78 895.85 907.64  
915.91 988.87 1027.46 1154.49 1284.90  
1354.80 1397.96 1430.46 1445.91 1656.08  
2950.16 3001.67 3033.39 3050.96 3057.06  
3141.41

Summary Geometry Optimization:

-----  
Energy Change : 0.000036  
Gradient (Max): 0.000662  
Gradient (RMS): 0.000188  
-----

Energies - Geometries - Frequencies

**C3H4 7**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: C(3V)

Basis:  
Carbon (TZP)  
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
C 0.000000 0.000000 0.048327  
C 0.000000 0.000000 1.503658  
C 0.000000 0.000000 2.715878  
H 0.000000 0.000000 3.786232  
H 0.513314 0.889086 -0.345712  
H -1.026628 0.000000 -0.345712  
H 0.513314 -0.889086 -0.345712  
-----

Net Charge: 0.00

Total Bonding Energy:  
-1.456747449905545 hartree  
-914.12 kcal/mol  
-3824.69 kJ/mol

Zero-Point Energy : 141.41 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 248.68 J/mol-K  
Internal Energy : 152.05 kJ/mol  
Cv : 53.17 J/mol-K

Free Energy : -3744.30 kJ/mol

Frequencies (cm-1):  
325.39 325.39 614.66 614.66 933.05  
1014.54 1014.54 1362.29 1432.18 1432.18  
2151.70 2964.14 3029.28 3029.28 3398.31

Summary Geometry Optimization:

-----  
Energy Change : 0.000002  
Gradient (Max): 0.000937  
Gradient (RMS): 0.000250  
-----



Energies - Geometries - Frequencies

CH4 8

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEh  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: T(D)

Basis:  
Carbon (TZP)  
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
C 0.000000 0.000000 0.000000  
H 0.633164 0.633164 0.633164  
H -0.633164 -0.633164 0.633164  
H 0.633164 -0.633164 -0.633164  
H -0.633164 0.633164 -0.633164  
-----

Net Charge: 0.00

Total Bonding Energy:  
-0.881456586720729 hartree  
-553.12 kcal/mol  
-2314.26 kJ/mol

Zero-Point Energy : 114.20 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 186.30 J/mol-K  
Internal Energy : 121.75 kJ/mol  
Cv : 27.48 J/mol-K

Free Energy :-2245.58 kJ/mol

Frequencies (cm-1):  
1287.94 1287.94 1287.94 1514.05 1514.05  
2964.03 3078.68 3078.68 3078.68

Summary Geometry Optimization:  
-----  
Energy Change : 0.000000  
Gradient (Max): 0.000014  
Gradient (RMS): 0.000013  
-----

Energies - Geometries - Frequencies

**SiH4 9**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEh

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: T(D)

Basis:

Silicon (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
Si 0.000000 0.000000 0.000000  
H 0.862147 0.862147 0.862147  
H -0.862147 -0.862147 0.862147  
H -0.862147 0.862147 -0.862147  
H 0.862147 -0.862147 -0.862147  
-----

Net Charge: 0.00

Total Bonding Energy:

-0.693742291881820 hartree

-435.33 kcal/mol

-1821.42 kJ/mol

Zero-Point Energy : 79.30 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 205.10 J/mol-K

Internal Energy : 87.45 kJ/mol

Cv : 35.46 J/mol-K

Free Energy :-1792.64 kJ/mol

Frequencies (cm-1):

873.46 873.46 873.46 946.59 946.59

2172.91 2190.29 2190.29 2190.29

Summary Geometry Optimization:

-----  
Energy Change : 0.000003

Gradient (Max): 0.000131

Gradient (RMS): 0.000117  
-----

Energies - Geometries - Frequencies

**GeH4 10**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: T(D)

Basis:  
Germanium (TZP)  
Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
Ge 0.000000 0.000000 0.000000  
H 0.890133 0.890133 0.890133  
H -0.890133 -0.890133 0.890133  
H -0.890133 0.890133 -0.890133  
H 0.890133 -0.890133 -0.890133  
-----

Net Charge: 0.00

Total Bonding Energy:  
-0.648026014724808 hartree  
-406.64 kcal/mol  
-1701.39 kJ/mol

Zero-Point Energy : 75.12 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 217.97 J/mol-K  
Internal Energy : 83.48 kJ/mol  
Cv : 37.68 J/mol-K

Free Energy :-1680.42 kJ/mol

Frequencies (cm-1):  
788.18 788.18 788.18 900.06 900.06  
2087.58 2101.98 2101.98 2101.98

Summary Geometry Optimization:  
-----  
Energy Change : 0.000052  
Gradient (Max): 0.000229  
Gradient (RMS): 0.000205  
-----

Energies - Geometries - Frequencies

CF4 11

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEh  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: T(D)

Basis:  
Carbon (TZP)  
Fluorine (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
C 0.000000 0.000000 0.000000  
F 0.774050 0.774050 0.774050  
F -0.774050 -0.774050 0.774050  
F 0.774050 -0.774050 -0.774050  
F -0.774050 0.774050 -0.774050  
-----

Net Charge: 0.00

Total Bonding Energy:  
-0.935628695657962 hartree  
-587.12 kcal/mol  
-2456.49 kJ/mol

Zero-Point Energy : 42.07 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 263.60 J/mol-K  
Internal Energy : 52.69 kJ/mol  
Cv : 55.22 J/mol-K

Free Energy :-2479.92 kJ/mol

Frequencies (cm-1):  
405.77 405.77 592.66 592.66 592.66  
864.97 1192.76 1192.76 1192.76

Summary Geometry Optimization:  
-----  
Energy Change : 0.000077  
Gradient (Max): 0.000131  
Gradient (RMS): 0.000117  
-----

Energies - Geometries - Frequencies

PF3 12

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(3V)

Basis:

Phosphorus (TZP)

Fluorine (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
P 0.000000 0.000000 -0.194008  
F 1.399964 0.000000 0.605282  
F -0.699982 -1.212405 0.605282  
F -0.699982 1.212405 0.605282  
-----

Net Charge: 0.00

Total Bonding Energy:

-0.725409988075226 hartree

-455.20 kcal/mol

-1904.56 kJ/mol

Zero-Point Energy : 20.68 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 276.18 J/mol-K

Internal Energy : 31.59 kJ/mol

Cv : 52.77 J/mol-K

Free Energy :-1952.84 kJ/mol

Frequencies (cm-1):

311.67 311.67 437.11 787.50 787.50  
821.90

Summary Geometry Optimization:

-----  
Energy Change : 0.000000

Gradient (Max): 0.000573

Gradient (RMS): 0.000205  
-----

Energies - Geometries - Frequencies

**SF2 13**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(2V)

Basis:

Sulphur (TZP)

Fluorine (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
S 0.000000 0.000000 -0.104527  
F 0.000000 -1.256057 -1.155051  
F 0.000000 1.256057 -1.155051  
-----

Net Charge: 0.00

Total Bonding Energy:

-0.382339480596118 hartree

-239.92 kcal/mol

-1003.83 kJ/mol

Zero-Point Energy : 11.06 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 259.61 J/mol-K

Internal Energy : 20.02 kJ/mol

Cv : 37.75 J/mol-K

Free Energy :-1058.73 kJ/mol

Frequencies (cm-1):

309.63 758.33 780.61

Summary Geometry Optimization:

-----  
Energy Change : 0.000001

Gradient (Max): 0.000018

Gradient (RMS): 0.000009  
-----

Energies - Geometries - Frequencies

**ClF3 14**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: C(2V)

Basis:  
Chlorine (TZP)  
Fluorine (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
Cl 0.000000 0.000000 0.098858  
F 0.000000 0.000000 -1.577642  
F 1.756627 0.000000 0.085300  
F -1.756627 0.000000 0.085300  
-----

Net Charge: 0.00

Total Bonding Energy:  
-0.338223610980255 hartree  
-212.24 kcal/mol  
-888.01 kJ/mol

Zero-Point Energy : 16.60 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 287.71 J/mol-K  
Internal Energy : 28.56 kJ/mol  
Cv : 58.29 J/mol-K

Free Energy : -942.75 kJ/mol

Frequencies (cm-1):  
248.04 310.74 347.91 498.04 673.54  
696.88

Summary Geometry Optimization:

-----  
Energy Change : 0.000008  
Gradient (Max): 0.000407  
Gradient (RMS): 0.000136  
-----

Energies - Geometries - Frequencies

PF5 15

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: C(3V)

Basis:  
Phosphorus (TZP)  
Fluorine (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
P 0.000000 0.000000 0.000570  
F 0.787878 -1.364645 0.000526  
F 0.787878 1.364645 0.000526  
F -1.575756 0.000000 0.000526  
F 0.000000 0.000000 -1.610666  
F 0.000000 0.000000 1.611770  
-----

Net Charge: 0.00

Total Bonding Energy:  
-1.071404319649902 hartree  
-672.32 kcal/mol  
-2812.97 kJ/mol

Zero-Point Energy : 41.16 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 312.88 J/mol-K  
Internal Energy : 56.07 kJ/mol  
Cv : 80.74 J/mol-K

Free Energy : -2847.70 kJ/mol

Frequencies (cm-1):  
150.84 150.84 469.11 469.11 489.90  
489.90 530.68 599.95 740.97 896.22  
946.91 946.91

Summary Geometry Optimization:  
-----  
Energy Change : 0.000010  
Gradient (Max): 0.000196  
Gradient (RMS): 0.000075  
-----



Energies - Geometries - Frequencies

**SF4 16**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)  
Density Functional: VWN PBEc PBEEx  
Relativistic Corrections: ---  
General Accuracy: 5.00  
Symmetry: C(2V)

Basis:  
Sulphur (TZP)  
Fluorine (TZP)

Final Geometry (x,y,z in Angstrom)  
-----  
S 0.000000 0.000000 0.378901  
F 0.000000 1.697347 0.306960  
F 1.235894 0.000000 -0.644158  
F 0.000000 -1.697347 0.306960  
F -1.235894 0.000000 -0.644158  
-----

Net Charge: 0.00

Total Bonding Energy:  
-0.692846378442915 hartree  
-434.77 kcal/mol  
-1819.07 kJ/mol

Zero-Point Energy : 27.51 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:  
Entropy : 300.96 J/mol-K  
Internal Energy : 40.98 kJ/mol  
Cv : 71.29 J/mol-K

Free Energy :-1865.34 kJ/mol

Frequencies (cm-1):  
201.55 299.77 397.20 453.54 459.87  
509.28 705.14 768.63 803.85

Summary Geometry Optimization:  
-----  
Energy Change : 0.000003  
Gradient (Max): 0.000388  
Gradient (RMS): 0.000187  
-----

Energies - Geometries - Frequencies

**NH3 18**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(3V)

Basis:

Nitrogen (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
N 0.000000 0.000000 0.117476  
H -0.471152 0.816060 -0.281879  
H 0.942305 0.000000 -0.281879  
H -0.471152 -0.816060 -0.281879  
-----

Net Charge: 0.00

Total Bonding Energy:

-0.715449207708494 hartree

-448.95 kcal/mol

-1878.41 kJ/mol

Zero-Point Energy : 87.65 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 192.59 J/mol-K

Internal Energy : 95.18 kJ/mol

Cv : 26.77 J/mol-K

Free Energy :-1838.17 kJ/mol

Frequencies (cm-1):

1035.01 1626.01 1626.01 3374.40 3495.98  
3495.98

Summary Geometry Optimization:

-----  
Energy Change : 0.000010

Gradient (Max): 0.000205

Gradient (RMS): 0.000070  
-----

Energies - Geometries - Frequencies

**BH3 17**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: D(3H)

Basis:

Boron (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
B 0.000000 0.000000 0.000000  
H -0.599891 1.039042 0.000000  
H -0.599891 -1.039042 0.000000  
H 1.199782 0.000000 0.000000  
-----

Net Charge: 0.00

Total Bonding Energy:

-0.581902182204788 hartree

-365.15 kcal/mol

-1527.78 kJ/mol

Zero-Point Energy : 66.81 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 188.55 J/mol-K

Internal Energy : 74.42 kJ/mol

Cv : 28.05 J/mol-K

Free Energy :-1507.10 kJ/mol

Frequencies (cm-1):

1117.26 1155.19 1155.19 2493.19 2624.64  
2624.64

Summary Geometry Optimization:

-----  
Energy Change : 0.000000

Gradient (Max): 0.000002

Gradient (RMS): 0.000001  
-----

Energies - Geometries - Frequencies

**H3NBH3 19**

=====  
ADF - Version 2008.01

GEOMETRY OPTIMIZATION (Threshold met)

Density Functional: VWN PBEc PBEEx

Relativistic Corrections: ---

General Accuracy: 5.00

Symmetry: C(3V)

Basis:

Boron (TZP)

Nitrogen (TZP)

Hydrogen (TZP)

Final Geometry (x,y,z in Angstrom)

-----  
B 0.000000 0.000000 -0.835476  
N 0.000000 0.000000 0.813283  
H -0.476483 0.825293 1.186179  
H -0.476483 -0.825293 1.186179  
H 0.952967 0.000000 1.186179  
H 0.587855 -1.018194 -1.152852  
H 0.587855 1.018194 -1.152852  
H -1.175709 0.000000 -1.152852  
-----

Net Charge: 0.00

Total Bonding Energy:

-1.352029545315899 hartree

-848.41 kcal/mol

-3549.75 kJ/mol

Zero-Point Energy : 178.32 kJ/mol

Thermochemistry at 298.15 K and 1.00 atm:

Entropy : 240.40 J/mol-K

Internal Energy : 188.50 kJ/mol

Cv : 51.19 J/mol-K

Free Energy :-3430.45 kJ/mol

Frequencies (cm-1):

253.16 627.23 627.23 664.49 1038.08  
1038.08 1140.61 1140.61 1144.29 1295.14  
1621.92 1621.92 2388.07 2444.73 2444.73  
3371.73 3475.32 3475.32

Summary Geometry Optimization:

-----  
Energy Change : 0.000040

Gradient (Max): 0.000745

Gradient (RMS): 0.000259  
-----

**C2H6 1**

Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	-0.378760	-0.656030	1.058540	0.912790
Xa	-0.378760	0.656030	1.058540	0.912790
Xa	0.757520	0.000000	1.058540	0.912790
Xa	0.378740	-0.656000	-1.058590	0.912780
Xa	0.378740	0.656000	-1.058590	0.912780
Xa	-0.757480	0.000000	-1.058590	0.912780
Xa	0.000000	0.000000	0.000060	0.819190
Xa	0.001630	0.000000	-0.764180	0.794140
Xa	0.000820	0.001420	0.764330	0.794110
Xb	0.491290	0.000000	-1.107530	0.507470
Xb	-0.245650	-0.425470	-1.107530	0.507470
Xb	-0.245650	0.425470	-1.107530	0.507470
Xb	0.245660	0.425490	1.107630	0.507450
Xb	0.245660	-0.425490	1.107630	0.507450
Xb	-0.491310	0.000000	1.107630	0.507450
Xb	-0.244660	0.423760	0.423460	0.500770
Xb	-0.244660	-0.423760	0.423460	0.500770
Xb	0.489320	0.000000	0.423460	0.500770
Xb	-0.489350	0.000000	-0.423380	0.500750
Xb	0.244680	-0.423790	-0.423380	0.500750
Xb	0.244680	0.423790	-0.423380	0.500750
Xb	-0.125040	-0.216570	0.847660	0.170400
Xb	-0.125040	0.216570	0.847660	0.170400
Xb	0.250070	0.000000	0.847660	0.170400
Xb	0.125030	-0.216560	-0.847530	0.170390
Xb	0.125030	0.216560	-0.847530	0.170390
Xb	-0.250060	0.000000	-0.847530	0.170390
Xb	0.000000	0.000000	-0.498390	0.165420
Xb	0.000000	0.000000	0.498550	0.165420
Xc	0.543940	0.000000	-0.570430	0.418320
Xc	-0.271970	0.471070	-0.570430	0.418320
Xc	-0.271970	-0.471070	-0.570430	0.418320
Xc	0.271960	0.471050	0.570540	0.418310
Xc	0.271960	-0.471050	0.570540	0.418310
Xc	-0.543920	0.000000	0.570540	0.418310
Xc	0.000000	0.000000	1.343380	0.410430
Xc	0.000000	0.000000	-1.343240	0.410430
Xc	0.115910	0.200760	0.905550	0.160330
Xc	0.115910	-0.200760	0.905550	0.160330
Xc	-0.231820	0.000000	0.905550	0.160330
Xc	0.231810	0.000000	-0.905410	0.160320
Xc	-0.115900	0.200750	-0.905410	0.160320
Xc	-0.115900	-0.200750	-0.905410	0.160320
Xc	0.207300	0.000000	0.588350	0.158850
Xc	-0.103650	0.179530	0.588350	0.158850
Xc	-0.103650	-0.179530	0.588350	0.158850
Xc	0.103670	-0.179570	-0.588250	0.158850
Xc	0.103670	0.179570	-0.588250	0.158850
Xc	-0.207350	0.000000	-0.588250	0.158850
Xd	0.127160	-0.220240	0.653440	0.152320
Xd	0.127160	0.220240	0.653440	0.152320
Xd	-0.254310	0.000000	0.653440	0.152320
Xd	0.254330	0.000000	-0.653320	0.152320
Xd	-0.127170	-0.220260	-0.653320	0.152320
Xd	-0.127170	0.220260	-0.653320	0.152320
Xd	0.000000	0.000000	1.043240	0.149890
Xd	0.000000	0.000000	-1.043080	0.149890

CNH5 2

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	-0.261140	0.400380	0.651440	0.918510
Xa	-0.261140	0.400380	-0.651440	0.918510
Xa	-0.345450	-0.735850	0.000000	0.913540
Xa	1.744980	-0.416470	-0.656150	0.900330
Xa	1.744980	-0.416470	0.656150	0.900330
Xa	1.470150	0.001070	0.000000	0.797700
Xa	0.003170	-0.000300	0.000000	0.790850
Xa	0.696190	-0.023930	0.000000	0.768870
Xa	1.625630	0.450250	0.000000	0.628340
Xb	1.750120	0.171880	0.371770	0.564590
Xb	1.750120	0.171880	-0.371770	0.564590
Xb	1.137670	0.375420	0.000000	0.560130
Xb	1.570720	-0.494460	0.000000	0.518550
Xb	-0.294620	0.516810	0.000000	0.515500
Xb	1.191620	-0.362950	-0.214360	0.513840
Xb	1.191620	-0.362950	0.214360	0.513840
Xb	-0.324300	-0.233270	-0.439130	0.511080
Xb	-0.324300	-0.233270	0.439130	0.511080
Xb	0.328770	-0.492030	0.000000	0.480100
Xb	0.368920	0.203480	0.411960	0.478570
Xb	0.368920	0.203480	-0.411960	0.478570
Xb	1.534520	0.198160	0.000000	0.204660
Xb	1.407400	-0.212350	0.000000	0.189870
Xb	-0.063070	0.128030	0.219400	0.173390
Xb	-0.063070	0.128030	-0.219400	0.173390
Xb	-0.083210	-0.249050	0.000000	0.171870
Xb	0.270070	-0.024130	0.000000	0.156970
Xc	1.276960	-0.452890	0.000000	0.508010
Xc	1.226040	0.074920	0.425900	0.470070
Xc	1.226040	0.074920	-0.425900	0.470070
Xc	1.938350	-0.160520	0.000000	0.466070
Xc	0.223610	-0.277930	-0.450280	0.413880
Xc	0.223610	-0.277930	0.450280	0.413880
Xc	0.260420	0.509640	0.000000	0.400590
Xc	-0.576190	0.031360	0.000000	0.391860
Xc	1.554760	-0.038640	0.201570	0.172010
Xc	1.554760	-0.038640	-0.201570	0.172010
Xc	1.250690	0.051260	0.000000	0.166870
Xc	-0.101680	0.249920	0.000000	0.162200
Xc	-0.110640	-0.124390	-0.212850	0.161870
Xc	-0.110640	-0.124390	0.212850	0.161870
Xc	0.208920	-0.178610	0.000000	0.154570
Xc	0.224360	0.052340	-0.149840	0.154280
Xc	0.224360	0.052340	0.149840	0.154280
Xd	1.324870	0.027690	-0.173800	0.163340
Xd	1.324870	0.027690	0.173800	0.163340
Xd	1.681120	-0.085270	0.000000	0.161320
Xd	0.163980	-0.123620	-0.187930	0.151380
Xd	0.163980	-0.123620	0.187930	0.151380
Xd	0.178410	0.215270	0.000000	0.149360
Xd	-0.280460	0.010820	0.000000	0.143720

**COH4 3**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	-0.203300	0.759160	0.000000	0.924680
Xa	-0.267290	-0.370350	-0.658490	0.919390
Xa	-0.267290	-0.370350	0.658490	0.919390
Xa	1.713440	-0.778230	0.000000	0.880220
Xa	1.460830	0.004340	0.000000	0.798400
Xa	0.034900	-0.009890	0.000000	0.786940
Xa	0.688040	-0.028490	0.000000	0.708000
Xa	1.553950	0.154060	0.368710	0.601730
Xa	1.553950	0.154060	-0.368710	0.601730
Xb	1.689300	0.348190	0.000000	0.580220
Xb	1.584790	-0.277860	0.307670	0.555680
Xb	1.584790	-0.277860	-0.307670	0.555680
Xb	1.115120	0.038830	0.281340	0.548500
Xb	1.115120	0.038830	-0.281340	0.548500
Xb	-0.252210	0.258620	-0.442260	0.517310
Xb	-0.252210	0.258620	0.442260	0.517310
Xb	-0.271950	-0.514570	0.000000	0.515010
Xb	0.398030	-0.262550	0.383090	0.461170
Xb	0.398030	-0.262550	-0.383090	0.461170
Xb	0.426510	0.418390	0.000000	0.455450
Xb	1.473890	0.025950	-0.176730	0.217510
Xb	1.473890	0.025950	0.176730	0.217510
Xb	-0.019600	0.246130	0.000000	0.176340
Xb	-0.034320	-0.136900	0.218390	0.174670
Xb	-0.034320	-0.136900	-0.218390	0.174670
Xb	0.304100	-0.048350	0.000000	0.147720
Xc	1.191230	0.339100	0.000000	0.505910
Xc	1.872800	-0.110810	0.000000	0.502900
Xc	1.184860	-0.347290	0.000000	0.498480
Xc	0.290660	-0.519310	0.000000	0.408230
Xc	0.314250	0.227610	0.434770	0.395110
Xc	0.314250	0.227610	-0.434770	0.395110
Xc	-0.546330	0.013710	0.000000	0.374950
Xc	1.555170	0.160160	0.000000	0.199140
Xc	1.392840	-0.174530	0.000000	0.183570
Xc	-0.058870	-0.263330	0.000000	0.163870
Xc	-0.054890	0.114750	0.223140	0.163750
Xc	-0.054890	0.114750	-0.223140	0.163750
Xc	0.287460	-0.092910	0.063130	0.147520
Xc	0.287460	-0.092910	-0.063130	0.147520
Xc	0.292970	0.081790	0.000000	0.146990
Xd	1.620260	-0.102960	0.000000	0.172150
Xd	1.282850	0.079340	0.000000	0.170840
Xd	0.264030	-0.161910	0.000000	0.147190
Xd	0.257850	0.064220	-0.147120	0.145670
Xd	0.257850	0.064220	0.147120	0.145670
Xd	-0.252980	-0.001510	0.000000	0.137640

**CFH3 4**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	-0.380420	-0.658910	-0.212980	0.926880
Xa	-0.380420	0.658910	-0.212980	0.926880
Xa	0.760850	0.000000	-0.212980	0.926880
Xa	-0.000040	-0.000070	0.039150	0.796260
Xa	-0.008860	0.000000	1.443510	0.771190
Xa	0.000000	0.000000	0.677280	0.642470
Xa	0.176660	-0.305980	1.512440	0.578950
Xa	-0.353320	0.000000	1.512440	0.578950
Xa	0.176660	0.305980	1.512440	0.578950
Xb	0.352740	0.000000	1.514120	0.578210
Xb	-0.176370	0.305480	1.514120	0.578210
Xb	-0.176370	-0.305480	1.514120	0.578210
Xb	-0.207780	0.000000	1.092880	0.524800
Xb	0.103890	-0.179940	1.092880	0.524800
Xb	0.103890	0.179940	1.092880	0.524800
Xb	-0.522030	0.000000	-0.220350	0.520440
Xb	0.261010	0.452090	-0.220350	0.520440
Xb	0.261010	-0.452090	-0.220350	0.520440
Xb	-0.211110	-0.365650	0.446520	0.438280
Xb	0.422210	0.000000	0.446520	0.438280
Xb	-0.211110	0.365650	0.446520	0.438280
Xb	0.077640	0.134480	1.452250	0.222730
Xb	0.077640	-0.134480	1.452250	0.222730
Xb	-0.155280	0.000000	1.452250	0.222730
Xb	0.254510	0.000000	-0.009360	0.178080
Xb	-0.127250	0.220410	-0.009360	0.178080
Xb	-0.127250	-0.220410	-0.009360	0.178080
Xc	0.208870	0.000000	1.094700	0.524480
Xc	-0.104440	0.180890	1.094700	0.524480
Xc	-0.104440	-0.180890	1.094700	0.524480
Xc	0.000000	0.000000	1.810660	0.520170
Xc	-0.472400	0.000000	0.361090	0.387320
Xc	0.236200	-0.409110	0.361090	0.387320
Xc	0.236200	0.409110	0.361090	0.387320
Xc	0.000000	0.000000	-0.537220	0.357400
Xc	-0.077650	-0.134490	1.452280	0.222680
Xc	-0.077650	0.134500	1.452280	0.222680
Xc	0.155300	0.000000	1.452280	0.222680
Xc	0.129520	-0.224330	-0.028620	0.166060
Xc	0.129520	0.224330	-0.028620	0.166060
Xc	-0.259030	0.000000	-0.028620	0.166060
Xd	0.000000	0.000000	1.605150	0.190530
Xd	0.000000	0.000000	1.274560	0.180920
Xd	0.000000	0.000000	0.323660	0.136110
Xd	0.000000	0.000000	-0.246180	0.130810



**C3H8 5**

Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	0.268450	0.393830	-0.651600	0.912890
Xa	0.268450	0.393830	0.651600	0.912890
Xa	-1.822950	0.773980	0.000000	0.912790
Xa	1.384380	-1.417310	0.000000	0.912780
Xa	0.326820	-1.840070	-0.656990	0.911980
Xa	0.326820	-1.840070	0.656990	0.911980
Xa	-1.832800	-0.365000	-0.656840	0.911970
Xa	-1.832800	-0.365000	0.656840	0.911970
Xa	-0.771610	-0.002990	0.000000	0.819430
Xa	0.277680	-0.719640	0.000000	0.819340
Xa	-0.006720	-0.008790	-0.000440	0.796750
Xa	0.572250	-1.428670	0.000000	0.794040
Xa	-1.538830	0.013290	0.000000	0.793440
Xb	0.331640	0.486460	0.000000	0.508030
Xb	0.926270	-1.655020	-0.425440	0.506650
Xb	0.926270	-1.655020	0.425440	0.506650
Xb	-1.878250	0.260760	0.425370	0.506630
Xb	-1.878250	0.260760	-0.425370	0.506630
Xb	-1.883880	-0.475800	0.000000	0.506350
Xb	0.242040	-1.928050	0.000000	0.506310
Xb	0.217420	-1.204170	0.423720	0.503610
Xb	0.217420	-1.204170	-0.423720	0.503610
Xb	-1.200660	-0.235650	-0.423810	0.503590
Xb	-1.200660	-0.235650	0.423810	0.503590
Xb	-0.352570	0.228250	-0.425280	0.503190
Xb	-0.352570	0.228250	0.425280	0.503190
Xb	0.340210	-0.244870	0.425080	0.503180
Xb	0.340210	-0.244870	-0.425080	0.503180
Xb	-1.190630	0.497480	0.000000	0.500330
Xb	0.896610	-0.928360	0.000000	0.500270
Xb	-0.342120	-0.500640	0.000000	0.496620
Xb	0.076110	0.112330	0.218660	0.170860
Xb	0.076110	0.112330	-0.218660	0.170860
Xb	-1.619130	0.263610	0.000000	0.170060
Xb	0.834730	-1.412590	0.000000	0.170040
Xb	-1.620470	-0.111010	0.216970	0.169900
Xb	-1.620470	-0.111010	-0.216970	0.169900
Xb	0.486210	-1.550050	0.217020	0.169900
Xb	0.486210	-1.550050	-0.217020	0.169900
Xb	-1.271320	0.006290	0.000000	0.166400
Xb	0.468570	-1.182180	0.000000	0.166310
Xb	-0.272220	-0.017980	0.000000	0.166110
Xb	0.081540	-0.259440	0.000000	0.166010
Xc	-0.003980	-1.454240	0.000000	0.420330
Xc	-1.352990	-0.532800	0.000000	0.420260
Xc	0.754130	-1.147520	0.471150	0.419380
Xc	0.754130	-1.147520	-0.471150	0.419380
Xc	-1.343020	0.284910	0.471240	0.419320
Xc	-1.343020	0.284910	-0.471240	0.419320
Xc	-0.195590	-0.285860	-0.469530	0.417650
Xc	-0.195590	-0.285860	0.469530	0.417650
Xc	0.571540	0.001010	0.000000	0.411840
Xc	-0.207890	0.533420	0.000000	0.411760
Xc	-2.115320	0.017130	0.000000	0.410920
Xc	0.785440	-1.964600	0.000000	0.410890
Xc	-1.679360	0.128810	0.199860	0.160050
Xc	-1.679360	0.128810	-0.199860	0.160050
Xc	0.731100	-1.517560	0.199940	0.160040
Xc	0.731100	-1.517560	-0.199940	0.160040
Xc	0.146590	0.215290	0.000000	0.159850
Xc	-1.680920	-0.216780	0.000000	0.159840
Xc	0.409520	-1.644800	0.000000	0.159830
Xc	-1.367660	-0.096910	0.181920	0.159430

LOL Topologies

Xc	-1.367660	-0.096910	-0.181920	0.159430
Xc	0.407490	-1.309050	-0.181680	0.159400
Xc	0.407490	-1.309050	0.181680	0.159400
Xc	-0.182550	0.076240	0.189240	0.159010
Xc	-0.182550	0.076240	-0.189240	0.159010
Xc	0.136710	-0.142040	0.188790	0.158970
Xc	0.136710	-0.142040	-0.188790	0.158970
Xc	-1.363070	0.222640	0.000000	0.158900
Xc	0.703100	-1.188830	0.000000	0.158870
Xc	-0.160000	-0.234380	0.000000	0.157680
Xd	-1.437120	-0.245410	0.000000	0.152720
Xd	0.294360	-1.427830	0.000000	0.152700
Xd	-1.429590	0.141650	-0.221400	0.152310
Xd	-1.429590	0.141650	0.221400	0.152310
Xd	0.652040	-1.280170	-0.221260	0.152300
Xd	0.652040	-1.280170	0.221260	0.152300
Xd	-0.105840	-0.154710	-0.214460	0.152090
Xd	-0.105840	-0.154710	0.214460	0.152090
Xd	-1.815220	0.014040	0.000000	0.150090
Xd	0.673570	-1.686110	0.000000	0.150060
Xd	0.271780	-0.018930	0.000000	0.149870
Xd	-0.117180	0.247080	0.000000	0.149840

**C3H6 6**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	1.730310	-0.699380	0.000000	0.920820
Xa	-0.416420	-0.685330	0.000000	0.920020
Xa	-0.419860	0.686050	0.000000	0.919180
Xa	1.752420	1.907790	0.000000	0.915440
Xa	2.688420	1.243830	0.653230	0.911780
Xa	2.688420	1.243830	-0.653230	0.911780
Xa	1.761200	0.613920	0.000000	0.822340
Xa	2.201310	1.231830	0.000000	0.797470
Xa	0.002610	0.000730	0.000000	0.796450
Xa	1.340450	0.004700	0.000000	0.796310
Xa	0.673120	0.010350	0.000000	0.775970
Xb	2.801220	1.225250	0.000000	0.513420
Xb	2.206480	1.651280	-0.426490	0.504930
Xb	2.206480	1.651280	0.426490	0.504930
Xb	2.199540	0.819970	0.434760	0.503680
Xb	2.199540	0.819970	-0.434760	0.503680
Xb	1.609240	1.238330	0.000000	0.500570
Xb	1.920740	-0.021000	0.000000	0.488270
Xb	-0.581550	0.000440	0.000000	0.483700
Xb	0.149410	0.403140	-0.408720	0.468670
Xb	0.149410	0.403140	0.408720	0.468670
Xb	0.144730	-0.390710	-0.422630	0.468440
Xb	0.144730	-0.390710	0.422630	0.468440
Xb	1.157640	-0.416090	-0.372810	0.466100
Xb	1.157640	-0.416090	0.372810	0.466100
Xb	1.193500	0.415310	0.399660	0.463650
Xb	1.193500	0.415310	-0.399660	0.463650
Xb	1.083520	0.014070	0.000000	0.181490
Xb	0.258830	0.004590	0.000000	0.180000
Xb	1.490730	-0.209290	0.000000	0.173380
Xb	-0.149660	-0.213550	0.000000	0.172440
Xb	-0.150090	0.215010	0.000000	0.171940
Xb	2.044740	1.443340	0.000000	0.171010
Xb	1.506800	0.208460	0.000000	0.170700
Xb	2.358620	1.225380	0.211560	0.170030
Xb	2.358620	1.225380	-0.211560	0.170030
Xb	2.043200	1.019240	0.000000	0.167060
Xc	1.057890	-0.498660	0.000000	0.455340
Xc	0.269340	0.511900	0.000000	0.454300
Xc	0.276500	-0.506790	0.000000	0.450610
Xc	1.085550	0.520780	0.000000	0.449780
Xc	-0.218310	0.002610	-0.550100	0.426340
Xc	-0.218310	0.002610	0.550100	0.426340
Xc	1.872610	1.239360	0.475400	0.420480
Xc	1.872610	1.239360	-0.475400	0.420480
Xc	2.524430	0.754530	0.000000	0.416260
Xc	1.533310	-0.009920	-0.560550	0.415930
Xc	1.533310	-0.009920	0.560550	0.415930
Xc	2.535560	1.703740	0.000000	0.412780
Xc	1.610720	0.006510	0.000000	0.163140
Xc	-0.269940	0.002360	0.000000	0.161930
Xc	2.471470	1.214710	0.000000	0.161430
Xc	1.930570	1.214660	0.000000	0.160240
Xc	2.196700	1.413170	0.202050	0.159940
Xc	2.196700	1.413170	-0.202050	0.159940
Xc	2.189970	1.033840	-0.185830	0.159200
Xc	2.189970	1.033840	0.185830	0.159200
Xc	0.106450	0.252080	0.000000	0.158690
Xc	1.226020	-0.242640	0.000000	0.158080
Xc	0.112400	-0.248530	0.000000	0.158060
Xc	1.249880	0.262490	0.000000	0.157840
Xd	2.042890	1.221600	-0.227270	0.152670
Xd	2.042890	1.221600	0.227270	0.152670

## LOL Topologies

Xd	2.342780	0.993260	0.000000	0.152580
Xd	2.360590	1.460070	0.000000	0.150600
Xd	-0.054250	0.002010	-0.275600	0.144240
Xd	-0.054250	0.002010	0.275600	0.144240
Xd	1.390650	0.005670	-0.278340	0.141160
Xd	1.390650	0.005670	0.278340	0.141160

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XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	0.000000	0.000000	3.509100	0.926930
Xa	0.379930	-0.658060	-0.241450	0.915420
Xa	0.379930	0.658060	-0.241450	0.915420
Xa	-0.759870	0.000000	-0.241450	0.915420
Xa	0.000000	0.000000	0.793850	0.815660
Xa	0.000000	0.000000	2.716690	0.796720
Xa	-0.000040	0.000000	0.049730	0.794980
Xa	0.000000	0.000000	1.507220	0.789900
Xa	-0.085790	0.148600	2.106970	0.694200
Xa	0.171580	0.000000	2.106970	0.694200
Xa	-0.085790	-0.148600	2.106970	0.694200
Xb	-0.245440	-0.425110	-0.289250	0.511610
Xb	0.490880	0.000000	-0.289250	0.511610
Xb	-0.245440	0.425110	-0.289250	0.511610
Xb	0.247240	0.428240	0.390320	0.498430
Xb	-0.494490	0.000000	0.390320	0.498430
Xb	0.247240	-0.428240	0.390320	0.498430
Xb	0.576790	0.000000	2.849000	0.450530
Xb	-0.288390	0.499510	2.849000	0.450530
Xb	-0.288390	-0.499510	2.849000	0.450530
Xb	-0.288660	-0.499970	1.379640	0.445310
Xb	-0.288660	0.499970	1.379640	0.445310
Xb	0.577320	0.000000	1.379640	0.445310
Xb	0.000000	0.000000	1.757050	0.184340
Xb	0.000000	0.000000	2.461690	0.183630
Xb	0.000000	0.000000	2.976990	0.176800
Xb	0.000000	0.000000	1.242330	0.176750
Xb	-0.250340	0.000000	-0.030870	0.172010
Xb	0.125170	0.216800	-0.030870	0.172010
Xb	0.125170	-0.216800	-0.030870	0.172010
Xb	0.000000	0.000000	0.315740	0.163690
Xc	0.000000	0.000000	2.107430	0.691470
Xc	-0.576870	0.000000	2.848390	0.450210
Xc	0.288440	0.499590	2.848390	0.450210
Xc	0.288440	-0.499590	2.848390	0.450210
Xc	0.288690	-0.500020	1.382470	0.443580
Xc	0.288690	0.500020	1.382470	0.443580
Xc	-0.577380	0.000000	1.382470	0.443580
Xc	-0.270740	0.468940	0.250950	0.416440
Xc	-0.270740	-0.468940	0.250950	0.416440
Xc	0.541480	0.000000	0.250950	0.416440
Xc	0.000000	0.000000	-0.527610	0.411530
Xc	0.236620	0.000000	-0.082090	0.161800
Xc	-0.118310	0.204920	-0.082090	0.161800
Xc	-0.118310	-0.204920	-0.082090	0.161800
Xc	-0.195810	0.000000	0.238320	0.158380
Xc	0.097900	-0.169570	0.238320	0.158380
Xc	0.097900	0.169570	0.238320	0.158380
Xc	-0.136530	-0.236490	2.768820	0.149770
Xc	0.273070	0.000000	2.768820	0.149770
Xc	0.273850	0.000000	1.451250	0.148430
Xd	-0.122870	-0.212820	0.177820	0.152730
Xd	-0.122870	0.212820	0.177820	0.152730
Xd	0.245750	0.000000	0.177820	0.152730
Xd	0.136560	0.236520	2.768720	0.149740
Xd	0.136550	-0.236520	2.768720	0.149740
Xd	-0.273110	0.000000	2.768720	0.149740
Xd	0.000000	0.000000	-0.229480	0.149430
Xd	0.137030	-0.237340	1.451720	0.148270
Xd	-0.274050	0.000000	1.451720	0.148270
Xd	0.137030	0.237340	1.451720	0.148270

**CH4 8**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	-0.468170	-0.468170	0.468170	0.913070
Xa	0.468170	0.468170	0.468170	0.913070
Xa	-0.468170	0.468170	-0.468170	0.913070
Xa	0.468170	-0.468170	-0.468170	0.913070
Xa	0.000540	0.000540	-0.000540	0.795930
Xb	-0.598580	0.000000	0.000000	0.505590
Xb	0.000000	-0.598580	0.000000	0.505590
Xb	0.000000	0.000000	-0.598580	0.505590
Xb	0.598580	0.000000	0.000000	0.505590
Xb	0.000000	0.000000	0.598580	0.505590
Xb	0.000000	0.598580	0.000000	0.505590
Xb	-0.152250	0.152250	-0.152250	0.169970
Xb	0.152250	-0.152250	-0.152250	0.169970
Xb	-0.152250	-0.152250	0.152250	0.169970
Xb	0.152250	0.152250	0.152250	0.169970
Xc	-0.333810	0.333810	0.333810	0.418150
Xc	0.333810	0.333810	-0.333810	0.418150
Xc	-0.333810	-0.333810	-0.333810	0.418150
Xc	0.333810	-0.333810	0.333810	0.418150
Xc	0.000000	0.000000	-0.271330	0.160400
Xc	0.000000	-0.271330	0.000000	0.160400
Xc	0.271330	0.000000	0.000000	0.160400
Xc	0.000000	0.271330	0.000000	0.160400
Xc	0.000000	0.000000	0.271330	0.160400
Xc	-0.271330	0.000000	0.000000	0.160400
Xd	-0.160160	0.160160	0.160160	0.152630
Xd	0.160160	0.160160	-0.160160	0.152630
Xd	0.160160	-0.160160	0.160160	0.152630
Xd	-0.160160	-0.160160	-0.160160	0.152630

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Xa	-0.611410	-0.611410	0.611410	0.870550
Xa	0.611410	0.611410	0.611410	0.870550
Xa	-0.611410	0.611410	-0.611410	0.870550
Xa	0.611410	-0.611410	-0.611410	0.870550
Xa	-0.856810	0.856810	-0.856970	0.822820
Xa	-0.856980	-0.856980	0.856620	0.822780
Xa	0.856510	-0.856070	-0.856070	0.822720
Xa	0.856560	0.856560	0.858430	0.821480
Xa	-0.008420	-0.008420	-0.008420	0.712530
Xa	-0.118140	0.118140	0.118140	0.571320
Xa	0.118140	0.118140	-0.118140	0.571320
Xa	-0.118140	-0.118140	-0.118140	0.571320
Xa	0.118140	-0.118140	0.118140	0.571320
Xb	-0.831200	-0.831200	0.831200	0.821810
Xb	-0.831200	0.831200	-0.831200	0.821810
Xb	0.831200	-0.831200	-0.831200	0.821810
Xb	0.831200	0.831200	0.831200	0.821810
Xb	0.000000	-0.204360	0.000000	0.570010
Xb	0.204360	0.000000	0.000000	0.570010
Xb	0.000000	0.204360	0.000000	0.570010
Xb	0.000000	0.000000	0.204360	0.570010
Xb	0.000000	0.000000	-0.204360	0.570010
Xb	-0.204360	0.000000	0.000000	0.570010
Xb	-0.990820	0.000000	0.000000	0.409720
Xb	0.000000	0.000000	-0.990820	0.409720
Xb	0.000000	-0.990820	0.000000	0.409720
Xb	0.000000	0.000000	0.990820	0.409720
Xb	0.990820	0.000000	0.000000	0.409720
Xb	0.000000	0.990820	0.000000	0.409720
Xb	-0.052080	-0.052080	-0.052080	0.265990
Xb	0.052080	-0.052080	0.052080	0.265990
Xb	0.052080	0.052080	-0.052080	0.265990
Xb	-0.052080	0.052080	0.052080	0.265990
Xb	-0.315100	-0.315100	0.315100	0.178270
Xb	0.315100	-0.315100	-0.315100	0.178270
Xb	-0.315100	0.315100	-0.315100	0.178270
Xb	0.315100	0.315100	0.315100	0.178270
Xc	0.117830	0.117830	0.117830	0.568660
Xc	0.117830	-0.117830	-0.117830	0.568660
Xc	-0.117830	-0.117830	0.117830	0.568660
Xc	-0.117830	0.117830	-0.117830	0.568660
Xc	-0.570870	-0.570870	-0.570870	0.269830
Xc	0.570870	0.570870	-0.570870	0.269830
Xc	0.570870	-0.570870	0.570870	0.269830
Xc	-0.570870	0.570870	0.570870	0.269830
Xc	0.090230	0.000000	0.000000	0.265910
Xc	0.000000	0.000000	0.090230	0.265910
Xc	-0.090230	0.000000	0.000000	0.265910
Xc	0.000000	0.090230	0.000000	0.265910
Xc	0.000000	0.000000	-0.090230	0.265910
Xc	0.000000	-0.090230	0.000000	0.265910
Xc	0.588100	0.000000	0.000000	0.147460
Xc	0.000000	0.588100	0.000000	0.147460
Xc	0.000000	-0.588100	0.000000	0.147460
Xc	0.000000	0.000000	-0.588100	0.147460
Xc	-0.588100	0.000000	0.000000	0.147460
Xc	0.000000	0.000000	0.588100	0.147460
Xd	0.052110	0.052110	0.052110	0.265820
Xd	0.052110	-0.052110	-0.052110	0.265820
Xd	-0.052110	0.052110	-0.052110	0.265820
Xd	-0.052110	-0.052110	0.052110	0.265820
Xd	-0.358990	-0.358990	-0.358990	0.125930
Xd	-0.358990	0.358990	0.358990	0.125930
Xd	0.358990	-0.358990	0.358990	0.125930
Xd	0.358990	0.358990	-0.358990	0.125930

**GeH4 10**

Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	-0.885560	-0.885560	0.885670	0.821370
Xa	0.884430	0.884430	0.884590	0.821190
Xa	0.884370	-0.884370	-0.884710	0.821170
Xa	-0.884590	0.884600	-0.884260	0.821170
Xa	-0.722640	-0.722640	0.722640	0.820440
Xa	-0.722640	0.722640	-0.722640	0.820440
Xa	0.722640	-0.722640	-0.722640	0.820440
Xa	0.722640	0.722640	0.722640	0.820440
Xa	0.162310	0.162310	0.162310	0.571270
Xa	-0.162310	-0.162310	0.162310	0.571270
Xa	-0.162310	0.162310	-0.162310	0.571270
Xa	0.162310	-0.162310	-0.162310	0.571270
Xa	0.043380	-0.043380	0.043380	0.562590
Xa	-0.043380	-0.043380	-0.043380	0.562590
Xa	0.043380	0.043380	-0.043380	0.562590
Xa	-0.043380	0.043380	0.043380	0.562590
Xa	0.017500	0.017500	0.017500	0.332260
Xb	-0.817090	-0.817090	0.817090	0.815870
Xb	-0.817090	0.817090	-0.817090	0.815870
Xb	0.817090	-0.817090	-0.817090	0.815870
Xb	0.817090	0.817090	0.817090	0.815870
Xb	0.282220	0.000000	0.000000	0.568090
Xb	0.000000	-0.282220	0.000000	0.568090
Xb	-0.282220	0.000000	0.000000	0.568090
Xb	0.000000	0.282220	0.000000	0.568090
Xb	0.000000	0.000000	-0.282220	0.568090
Xb	0.000000	0.000000	0.282220	0.568090
Xb	0.000000	-0.075110	0.000000	0.561920
Xb	0.075110	0.000000	0.000000	0.561920
Xb	0.000000	0.075110	0.000000	0.561920
Xb	0.000000	0.000000	0.075110	0.561920
Xb	0.000000	0.000000	-0.075110	0.561920
Xb	-0.075110	0.000000	0.000000	0.561920
Xb	-1.107750	0.000000	0.000000	0.328980
Xb	0.000000	0.000000	-1.107750	0.328980
Xb	0.000000	0.000000	1.107750	0.328980
Xb	0.000000	1.107750	0.000000	0.328980
Xb	1.107750	0.000000	0.000000	0.328980
Xb	0.000000	-1.107750	0.000000	0.328980
Xb	-0.020140	-0.020140	-0.020140	0.319750
Xb	-0.020140	0.020140	0.020140	0.319750
Xb	0.020140	-0.020140	0.020140	0.319750
Xb	0.020140	0.020140	-0.020140	0.319750
Xb	0.089500	-0.089500	-0.089500	0.312500
Xb	-0.089500	-0.089500	0.089500	0.312500
Xb	-0.089500	0.089500	-0.089500	0.312500
Xb	0.089500	0.089500	0.089500	0.312500
Xb	-0.377730	-0.377730	0.377730	0.226980
Xb	0.377730	-0.377730	-0.377730	0.226980
Xb	-0.377730	0.377730	-0.377730	0.226980
Xb	0.377730	0.377730	0.377730	0.226980
Xc	-0.163450	-0.163450	-0.163450	0.565380
Xc	0.163450	0.163450	-0.163450	0.565380
Xc	0.163450	-0.163450	0.163450	0.565380
Xc	-0.163450	0.163450	0.163450	0.565380
Xc	-0.043360	-0.043360	0.043360	0.561330
Xc	-0.043360	0.043360	-0.043360	0.561330
Xc	0.043360	0.043360	0.043360	0.561330
Xc	0.043360	-0.043360	-0.043360	0.561330
Xc	-0.034900	0.000000	0.000000	0.319660
Xc	0.000000	-0.034900	0.000000	0.319660
Xc	0.000000	0.000000	-0.034900	0.319660
Xc	0.034900	0.000000	0.000000	0.319660



LOL Topologies

Xc	0.000000	0.000000	0.034900	0.319660
Xc	0.000000	0.034900	0.000000	0.319660
Xc	0.000000	0.155520	0.000000	0.310570
Xc	0.155520	0.000000	0.000000	0.310570
Xc	0.000000	-0.155520	0.000000	0.310570
Xc	-0.155520	0.000000	0.000000	0.310570
Xc	0.000000	0.000000	0.155520	0.310570
Xc	0.000000	0.000000	-0.155520	0.310570
Xc	-0.608140	-0.608140	-0.608140	0.253140
Xc	-0.608140	0.608140	0.608140	0.253140
Xc	0.608140	0.608140	-0.608140	0.253140
Xc	0.608140	-0.608140	0.608140	0.253140
Xc	-0.707200	0.000000	0.000000	0.209550
Xc	0.000000	0.000000	0.707200	0.209550
Xc	0.000000	0.707200	0.000000	0.209550
Xc	0.707200	0.000000	0.000000	0.209550
Xc	0.000000	0.000000	-0.707200	0.209550
Xc	0.000000	-0.707200	0.000000	0.209550
Xd	-0.020150	0.020150	-0.020150	0.319570
Xd	0.020150	0.020150	0.020150	0.319570
Xd	0.020150	-0.020150	-0.020150	0.319570
Xd	-0.020150	-0.020150	0.020150	0.319570
Xd	0.090040	-0.090040	0.090040	0.309250
Xd	-0.090040	-0.090040	-0.090040	0.309250
Xd	-0.090040	0.090040	0.090040	0.309250
Xd	0.090040	0.090040	-0.090040	0.309250
Xd	-0.426560	-0.426560	-0.426560	0.203790
Xd	-0.426560	0.426560	0.426560	0.203790
Xd	0.426560	-0.426560	0.426560	0.203790
Xd	0.426560	0.426560	-0.426560	0.203790

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Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	0.000510	0.000510	-0.000510	0.796170
Xa	-0.766250	0.783550	-0.766250	0.748520
Xa	0.783550	0.766250	0.766250	0.748520
Xa	-0.766250	-0.783550	0.766250	0.748520
Xa	0.766250	-0.766250	-0.783550	0.748520
Xa	-0.341660	-0.341660	0.341660	0.664480
Xa	-0.341660	0.341660	-0.341660	0.664480
Xa	0.341660	-0.341660	-0.341660	0.664480
Xa	0.341660	0.341660	0.341660	0.664480
Xa	-0.957380	-0.525790	0.957380	0.577770
Xa	0.957380	0.525790	0.957380	0.577770
Xa	0.525790	0.957380	0.957380	0.577770
Xa	0.957380	0.957380	0.525790	0.577770
Xa	-0.525790	0.957380	-0.957380	0.577770
Xa	-0.957380	-0.957380	0.525790	0.577770
Xa	-0.957380	0.525790	-0.957380	0.577770
Xa	-0.525790	-0.957380	0.957380	0.577770
Xa	0.525790	-0.957380	-0.957380	0.577770
Xa	-0.957380	0.957380	-0.525790	0.577770
Xa	0.957380	-0.525790	-0.957380	0.577770
Xa	0.957380	-0.957380	-0.525790	0.577770
Xb	0.672080	0.672080	1.102340	0.576380
Xb	-0.672080	-1.102340	0.672080	0.576380
Xb	-0.672080	-0.672080	1.102340	0.576380
Xb	-1.102340	-0.672080	0.672080	0.576380
Xb	1.102340	0.672080	0.672080	0.576380
Xb	0.672080	1.102340	0.672080	0.576380
Xb	0.672080	-1.102340	-0.672080	0.576380
Xb	1.102340	-0.672080	-0.672080	0.576380
Xb	0.672080	-0.672080	-1.102340	0.576380
Xb	-0.672080	1.102340	-0.672080	0.576380
Xb	-1.102340	0.672080	-0.672080	0.576380
Xb	-0.672080	0.672080	-1.102340	0.576380
Xb	-0.395280	-0.674830	0.674830	0.531770
Xb	0.674830	0.395280	0.674830	0.531770
Xb	0.674830	-0.674830	-0.395280	0.531770
Xb	-0.395280	0.674830	-0.674830	0.531770
Xb	0.395280	-0.674830	-0.674830	0.531770
Xb	0.674830	-0.395280	-0.674830	0.531770
Xb	-0.674830	-0.674830	0.395280	0.531770
Xb	-0.674830	0.674830	-0.395280	0.531770
Xb	-0.674830	0.395280	-0.674830	0.531770
Xb	0.674830	0.674830	0.395280	0.531770
Xb	0.395280	0.674830	0.674830	0.531770
Xb	-0.674830	-0.395280	0.674830	0.531770
Xb	-0.558730	0.000000	0.000000	0.425830
Xb	0.000000	-0.558730	0.000000	0.425830
Xb	0.558730	0.000000	0.000000	0.425830
Xb	0.000000	0.000000	0.558730	0.425830
Xb	0.000000	0.558730	0.000000	0.425830
Xb	0.000000	0.000000	-0.558730	0.425830
Xb	-0.842870	0.842870	-0.652610	0.221870
Xb	0.842870	-0.842870	-0.652610	0.221870
Xb	-0.842870	-0.842870	0.652610	0.221870
Xb	0.842870	0.842870	0.652610	0.221870
Xb	-0.652610	0.842870	-0.842870	0.221870
Xb	0.842870	-0.652610	-0.842870	0.221870
Xb	-0.842870	-0.652610	0.842870	0.221870
Xb	-0.652610	-0.842870	0.842870	0.221870
Xb	-0.842870	0.652610	-0.842870	0.221870
Xb	0.652610	-0.842870	-0.842870	0.221870
Xb	0.842870	0.652610	0.842870	0.221870
Xb	0.652610	0.842870	0.842870	0.221870

LOL Topologies

Xb	0.154770	0.154770	0.154770	0.161420
Xb	-0.154770	0.154770	-0.154770	0.161420
Xb	0.154770	-0.154770	-0.154770	0.161420
Xb	-0.154770	-0.154770	0.154770	0.161420
Xc	0.489960	-0.771450	-0.489960	0.530900
Xc	0.489960	0.489960	0.771450	0.530900
Xc	-0.771450	-0.489960	0.489960	0.530900
Xc	0.489960	-0.489960	-0.771450	0.530900
Xc	0.489960	0.771450	0.489960	0.530900
Xc	0.771450	-0.489960	-0.489960	0.530900
Xc	0.771450	0.489960	0.489960	0.530900
Xc	-0.771450	0.489960	-0.489960	0.530900
Xc	-0.489960	0.489960	-0.771450	0.530900
Xc	-0.489960	0.771450	-0.489970	0.530900
Xc	-0.489960	-0.489970	0.771450	0.530900
Xc	-0.489960	-0.771450	0.489960	0.530900
Xc	-0.984770	-0.984770	0.984770	0.525870
Xc	0.984770	-0.984770	-0.984770	0.525870
Xc	-0.984770	0.984770	-0.984770	0.525870
Xc	0.984770	0.984770	0.984770	0.525870
Xc	-0.321720	-0.321720	-0.321720	0.357140
Xc	-0.321720	0.321720	0.321720	0.357140
Xc	0.321720	-0.321720	0.321720	0.357140
Xc	0.321720	0.321720	-0.321720	0.357140
Xc	-0.906370	-0.716070	0.716060	0.221760
Xc	-0.906370	0.716060	-0.716060	0.221760
Xc	0.716060	-0.716060	-0.906370	0.221760
Xc	-0.716060	0.906370	-0.716060	0.221760
Xc	0.906370	-0.716060	-0.716060	0.221760
Xc	-0.716070	0.716060	-0.906370	0.221760
Xc	0.716060	-0.906370	-0.716060	0.221760
Xc	0.906370	0.716060	0.716060	0.221760
Xc	0.716060	0.716060	0.906370	0.221760
Xc	0.716060	0.906370	0.716060	0.221760
Xc	-0.716060	-0.716060	0.906370	0.221760
Xc	-0.716070	-0.906370	0.716060	0.221760
Xc	0.277920	0.000000	0.000000	0.149870
Xc	-0.277920	0.000000	0.000000	0.149870
Xc	0.000000	0.277920	0.000000	0.149870
Xc	0.000000	0.000000	0.277920	0.149870
Xc	0.000000	-0.277920	0.000000	0.149870
Xc	0.000000	0.000000	-0.277920	0.149870
Xd	0.867070	0.867070	0.867070	0.192380
Xd	-0.867070	-0.867070	0.867070	0.192380
Xd	-0.867070	0.867070	-0.867070	0.192380
Xd	0.867070	-0.867070	-0.867070	0.192380
Xd	0.676910	-0.676910	-0.676910	0.182580
Xd	-0.676910	0.676910	-0.676910	0.182580
Xd	-0.676910	-0.676910	0.676910	0.182580
Xd	0.676910	0.676910	0.676910	0.182580
Xd	-0.164530	-0.164530	-0.164530	0.141300
Xd	0.164530	-0.164530	0.164530	0.141300
Xd	-0.164530	0.164530	0.164530	0.141300
Xd	0.164530	0.164530	-0.164530	0.141300

**PF5 15**

Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	0.000000	0.000000	0.000700	0.805920
Xa	0.000010	-0.000010	-1.611360	0.801150
Xa	0.000000	0.000000	1.613150	0.798680
Xa	0.784880	-1.359450	0.002240	0.781950
Xa	0.784880	1.359450	0.002240	0.781950
Xa	-1.576000	0.000000	-0.007970	0.772670
Xa	-1.647730	0.000000	-0.350500	0.578010
Xa	0.823870	1.426980	-0.350500	0.578010
Xa	0.823870	-1.426980	-0.350500	0.578010
Xa	-1.647760	0.000000	0.351540	0.578010
Xa	0.823880	-1.427000	0.351540	0.578010
Xa	0.823880	1.427000	0.351540	0.578010
Xa	0.355930	0.000000	-1.673410	0.571420
Xa	-0.177960	-0.308240	-1.673410	0.571420
Xa	-0.177960	0.308240	-1.673410	0.571420
Xa	-0.177960	-0.308240	1.674520	0.571420
Xa	0.355930	0.000000	1.674520	0.571420
Xa	-0.177960	0.308240	1.674520	0.571420
Xa	-0.093670	-0.162240	0.000580	0.571190
Xa	-0.093670	0.162240	0.000580	0.571190
Xa	0.187340	0.000000	0.000580	0.571190
Xa	0.000000	0.000000	-0.186450	0.570710
Xa	0.000000	0.000000	0.187590	0.570710
Xa	0.000000	0.000000	-0.852200	0.569550
Xa	0.000000	0.000000	0.853330	0.569540
Xa	0.424360	0.735010	0.000550	0.566170
Xa	0.424360	-0.735010	0.000550	0.566170
Xa	-0.848710	0.000000	0.000550	0.566170
Xa	0.000000	0.000000	1.154140	0.545680
Xa	0.000000	0.000000	-1.153050	0.545670
Xb	0.039220	0.000000	-0.182300	0.570710
Xb	-0.019610	0.033970	-0.182300	0.570710
Xb	-0.019610	-0.033970	-0.182300	0.570710
Xb	-0.019580	0.033910	0.183450	0.570710
Xb	0.039160	0.000000	0.183450	0.570710
Xb	-0.019580	-0.033910	0.183450	0.570710
Xb	0.176900	0.306410	-1.680960	0.569230
Xb	0.176900	-0.306410	-1.680960	0.569230
Xb	-0.353810	0.000000	-1.680960	0.569230
Xb	-0.353810	0.000000	1.682070	0.569230
Xb	0.176900	0.306410	1.682070	0.569230
Xb	0.176900	-0.306410	1.682070	0.569230
Xb	1.130750	-1.248110	0.000530	0.561970
Xb	0.515520	1.603320	0.000530	0.561970
Xb	1.130750	1.248110	0.000530	0.561970
Xb	0.515520	-1.603320	0.000530	0.561970
Xb	-1.646270	-0.355210	0.000530	0.561970
Xb	-1.646270	0.355210	0.000530	0.561970
Xb	0.000000	0.000000	1.084710	0.544770
Xb	0.000000	0.000000	-1.083580	0.544760
Xb	0.428070	-1.183860	0.000190	0.540330
Xb	0.428070	1.183860	0.000190	0.540330
Xb	0.811220	-0.962650	0.000190	0.540330
Xb	0.811220	0.962650	0.000190	0.540330
Xb	-1.239290	-0.221210	0.000190	0.540330
Xb	-1.239290	0.221210	0.000190	0.540330
Xb	-0.097210	0.168370	1.258110	0.539760
Xb	0.194410	0.000000	1.258110	0.539760
Xb	-0.097210	-0.168370	1.258110	0.539760
Xb	0.194400	0.000000	-1.256990	0.539750
Xb	-0.097200	0.168350	-1.256990	0.539750
Xb	-0.097200	-0.168350	-1.256990	0.539750
Xb	-0.588420	0.000000	-0.584550	0.365900

LOL Topologies

Xb	0.294210	0.509590	-0.584550	0.365900
Xb	0.294210	-0.509590	-0.584550	0.365900
Xb	0.294220	-0.509600	0.585670	0.365900
Xb	-0.588440	0.000000	0.585670	0.365900
Xb	0.294220	0.509600	0.585670	0.365900
Xb	0.855870	0.000000	0.000550	0.318010
Xb	-0.427940	0.741210	0.000550	0.318010
Xb	-0.427940	-0.741210	0.000550	0.318010
Xb	0.000000	0.000000	-0.082450	0.272210
Xb	0.000000	0.000000	0.083590	0.272210
Xb	0.792860	1.373280	-0.154670	0.222460
Xb	0.792860	-1.373280	-0.154670	0.222460
Xb	-1.585720	0.000000	-0.154670	0.222460
Xb	-1.585740	0.000000	0.155720	0.222460
Xb	0.792870	-1.373290	0.155720	0.222460
Xb	0.792870	1.373290	0.155720	0.222460
Xb	0.156110	0.000000	-1.621050	0.218900
Xb	-0.078050	0.135190	-1.621050	0.218900
Xb	-0.078050	-0.135190	-1.621050	0.218900
Xb	-0.078050	0.135190	1.622160	0.218900
Xb	0.156110	0.000000	1.622160	0.218900
Xb	-0.078050	-0.135190	1.622160	0.218900
Xb	0.246090	0.426250	0.000560	0.178240
Xb	0.246090	-0.426250	0.000560	0.178240
Xb	-0.492190	0.000000	0.000560	0.178240
Xb	0.000000	0.000000	0.495350	0.177150
Xb	0.000000	0.000000	-0.494220	0.177150
Xc	0.093530	0.161990	0.000560	0.569740
Xc	0.093530	-0.161990	0.000560	0.569740
Xc	-0.187050	0.000000	0.000560	0.569740
Xc	0.969540	1.679300	0.000510	0.540010
Xc	0.969540	-1.679300	0.000510	0.540010
Xc	-1.939090	0.000000	0.000510	0.540010
Xc	0.612930	1.061630	-0.196660	0.539790
Xc	0.612930	-1.061630	-0.196660	0.539790
Xc	-1.225870	0.000000	-0.196660	0.539790
Xc	0.612940	-1.061650	0.197740	0.539790
Xc	0.612940	1.061650	0.197740	0.539790
Xc	-1.225880	0.000000	0.197740	0.539790
Xc	0.101260	-0.175400	1.266380	0.539050
Xc	0.101260	0.175400	1.266380	0.539050
Xc	-0.202530	0.000000	1.266380	0.539050
Xc	0.101260	0.175380	-1.265260	0.539050
Xc	-0.202520	0.000000	-1.265260	0.539050
Xc	0.101260	-0.175380	-1.265260	0.539050
Xc	0.000000	0.000000	1.976170	0.538350
Xc	0.000000	0.000000	-1.975060	0.538350
Xc	-0.378220	-0.655090	-0.384810	0.302760
Xc	-0.378220	0.655090	-0.384810	0.302760
Xc	0.756440	0.000000	-0.384810	0.302760
Xc	-0.378220	0.655100	0.385940	0.302750
Xc	-0.378220	-0.655100	0.385940	0.302750
Xc	0.756440	0.000000	0.385940	0.302750
Xc	-0.041530	-0.071930	0.000570	0.271860
Xc	-0.041530	0.071930	0.000570	0.271860
Xc	0.083050	0.000000	0.000570	0.271860
Xc	0.078080	0.135240	-1.621240	0.218730
Xc	-0.156160	0.000000	-1.621240	0.218730
Xc	0.078080	-0.135240	-1.621240	0.218730
Xc	-0.156160	0.000000	1.622340	0.218730
Xc	0.078080	-0.135240	1.622340	0.218730
Xc	0.078080	0.135240	1.622340	0.218730
Xc	0.930450	-1.297790	0.000530	0.214630
Xc	0.658690	1.454690	0.000530	0.214630
Xc	0.658690	-1.454690	0.000530	0.214630
Xc	0.930450	1.297790	0.000530	0.214630
Xc	-1.589140	-0.156900	0.000530	0.214630
Xc	-1.589140	0.156900	0.000530	0.214630
Xc	0.180510	-0.312660	-0.366770	0.159850
Xc	-0.361030	0.000000	-0.366770	0.159850
Xc	0.180510	0.312660	-0.366770	0.159850

LOL Topologies

Xc	0.180520	0.312670	0.367890	0.159850
Xc	-0.361040	0.000000	0.367890	0.159850
Xc	0.180520	-0.312670	0.367890	0.159850
Xc	-0.266650	-0.461860	0.000550	0.147030
Xc	-0.266650	0.461860	0.000550	0.147030
Xc	0.533310	0.000000	0.000550	0.147030
Xd	0.041540	-0.071940	0.000570	0.271770
Xd	0.041540	0.071940	0.000570	0.271770
Xd	-0.083070	0.000000	0.000570	0.271770
Xd	0.867740	-1.502960	0.000520	0.198520
Xd	0.867740	1.502960	0.000520	0.198520
Xd	-1.735470	0.000000	0.000520	0.198520
Xd	0.000000	0.000000	1.771720	0.198390
Xd	0.000000	0.000000	-1.770610	0.198390
Xd	0.000000	0.000000	1.444960	0.190530
Xd	0.000000	0.000000	-1.444960	0.190520
Xd	-1.409800	0.000000	0.000530	0.189980
Xd	0.704900	1.220920	0.000530	0.189980
Xd	0.704900	-1.220920	0.000530	0.189980
Xd	0.490130	0.000000	-0.212020	0.145850
Xd	-0.245060	0.424460	-0.212020	0.145850
Xd	-0.245060	-0.424460	-0.212020	0.145850
Xd	-0.245070	-0.424470	0.213150	0.145850
Xd	-0.245070	0.424470	0.213150	0.145850
Xd	0.490130	0.000000	0.213150	0.145850

**SF4 16**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Xa	0.000000	-1.697280	0.306740	0.803410
Xa	0.000000	1.698520	0.306490	0.799340
Xa	0.000000	0.000000	0.377660	0.799290
Xa	-1.236600	-0.000960	-0.644730	0.799190
Xa	1.236600	0.000960	-0.644730	0.799190
Xa	0.000000	0.000000	1.120070	0.679840
Xa	0.591980	0.000000	-0.148270	0.588550
Xa	-0.591980	0.000000	-0.148270	0.588550
Xa	-1.278790	0.353640	-0.674480	0.580900
Xa	-1.278790	-0.353640	-0.674480	0.580900
Xa	1.278790	0.353640	-0.674480	0.580900
Xa	1.278790	-0.353640	-0.674480	0.580900
Xa	0.000000	0.000000	0.549070	0.575830
Xa	0.000000	-1.765310	-0.047290	0.573240
Xa	0.000000	1.765310	-0.047290	0.573240
Xa	0.000000	1.723850	0.667480	0.572610
Xa	0.000000	-1.723850	0.667480	0.572610
Xa	0.000000	0.000000	0.206060	0.570910
Xa	0.000000	0.798440	0.301550	0.565280
Xa	0.000000	-0.798440	0.301550	0.565280
Xa	0.860930	0.000000	-0.378940	0.531990
Xa	-0.860930	0.000000	-0.378940	0.531990
Xb	0.000000	-0.076590	0.223950	0.570870
Xb	0.000000	0.076590	0.223950	0.570870
Xb	1.500330	0.000000	-0.399000	0.570090
Xb	-1.500330	0.000000	-0.399000	0.570090
Xb	1.048290	0.000000	-0.951780	0.568760
Xb	-1.048290	0.000000	-0.951780	0.568760
Xb	-0.351060	1.749180	0.234940	0.566380
Xb	-0.351060	-1.749180	0.234940	0.566380
Xb	0.351060	-1.749180	0.234940	0.566380
Xb	0.351060	1.749180	0.234940	0.566380
Xb	-0.827070	0.000000	-0.339370	0.531570
Xb	0.827070	0.000000	-0.339370	0.531570
Xb	0.837430	0.000000	-0.521030	0.530310
Xb	-0.837430	0.000000	-0.521030	0.530310
Xb	0.000000	1.081300	0.286550	0.508550
Xb	0.000000	-1.081300	0.286550	0.508550
Xb	0.000000	-0.657710	0.723310	0.498130
Xb	0.000000	0.657710	0.723310	0.498130
Xb	-0.749610	0.000000	0.460220	0.462590
Xb	0.749610	0.000000	0.460220	0.462590
Xb	0.409730	-0.540380	0.031870	0.422580
Xb	-0.409730	-0.540380	0.031870	0.422580
Xb	0.409730	0.540380	0.031870	0.422580
Xb	-0.409730	0.540380	0.031870	0.422580
Xb	0.000000	0.000000	-0.388080	0.411410
Xb	0.000000	0.000000	0.455180	0.278940
Xb	0.000000	0.000000	0.301820	0.277590
Xb	-1.241560	0.155070	-0.648680	0.223270
Xb	1.241560	0.155070	-0.648680	0.223270
Xb	1.241560	-0.155070	-0.648680	0.223270
Xb	-1.241560	-0.155070	-0.648680	0.223270
Xb	0.000000	1.713850	0.151590	0.219560
Xb	0.000000	-1.713850	0.151590	0.219560
Xb	0.000000	1.695810	0.463340	0.219410
Xb	0.000000	-1.695810	0.463340	0.219410
Xb	0.000000	0.000000	0.801960	0.195210
Xb	-0.362690	0.000000	0.117190	0.180350
Xb	0.362690	0.000000	0.117190	0.180350
Xc	-0.133750	0.000000	0.269450	0.570120
Xc	0.133750	0.000000	0.269450	0.570120
Xc	0.000000	-2.061490	0.339570	0.534190

LOL Topologies

Xc	0.000000	2.061490	0.339570	0.534190
Xc	0.000000	-1.305200	0.394580	0.532620
Xc	0.000000	1.305200	0.394580	0.532620
Xc	-1.519750	0.000000	-0.874150	0.526870
Xc	1.519750	0.000000	-0.874150	0.526870
Xc	1.044150	0.000000	-0.280150	0.526500
Xc	-1.044150	0.000000	-0.280150	0.526500
Xc	-0.558200	-0.500990	0.302900	0.416340
Xc	0.558200	-0.500990	0.302900	0.416340
Xc	0.558200	0.500990	0.302900	0.416340
Xc	-0.558200	0.500990	0.302900	0.416340
Xc	0.000000	-0.406850	-0.266690	0.388830
Xc	0.000000	0.406850	-0.266690	0.388830
Xc	0.000000	-0.075360	0.363300	0.276320
Xc	0.000000	0.075360	0.363300	0.276320
Xc	-1.341620	0.000000	-0.528580	0.217700
Xc	1.341620	0.000000	-0.528580	0.217700
Xc	-1.143330	0.000000	-0.770580	0.217620
Xc	1.143330	0.000000	-0.770580	0.217620
Xc	-0.156780	-1.706050	0.303090	0.216440
Xc	0.156780	1.706050	0.303090	0.216440
Xc	-0.156780	1.706050	0.303090	0.216440
Xc	0.156780	-1.706050	0.303090	0.216440
Xc	0.447440	0.000000	0.438430	0.173660
Xc	-0.447440	0.000000	0.438430	0.173660
Xc	-0.262330	-0.346560	0.231780	0.167530
Xc	0.262330	-0.346560	0.231780	0.167530
Xc	-0.262330	0.346560	0.231780	0.167530
Xc	0.262330	0.346560	0.231780	0.167530
Xc	0.000000	0.000000	-0.083750	0.166300
Xd	-0.076020	0.000000	0.366550	0.275660
Xd	0.076020	0.000000	0.366550	0.275660
Xd	0.000000	-1.857630	0.317300	0.197360
Xd	0.000000	1.857630	0.317300	0.197360
Xd	-1.360830	0.000000	-0.746260	0.192310
Xd	1.360830	0.000000	-0.746260	0.192310
Xd	0.000000	-1.532590	0.298500	0.191410
Xd	0.000000	1.532590	0.298500	0.191410
Xd	1.106680	0.000000	-0.537660	0.183790
Xd	-1.106680	0.000000	-0.537660	0.183790
Xd	0.317010	-0.327870	0.338080	0.167330
Xd	-0.317010	0.327870	0.338080	0.167330
Xd	-0.317010	-0.327870	0.338080	0.167330
Xd	0.317010	0.327870	0.338080	0.167330
Xd	0.000000	-0.271790	0.001600	0.163280
Xd	0.000000	0.271790	0.001600	0.163280



**ClF3 14**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

Cl	0.000000	0.000000	0.098858	0.000000
F	0.000000	0.000000	-1.577642	0.000000
F	1.756627	0.000000	0.085300	0.000000
F	-1.756627	0.000000	0.085300	0.000000
Xa	-1.756780	-0.000900	0.085320	0.800890
Xa	1.756780	0.000900	0.085320	0.800890
Xa	0.000000	0.001010	-1.575890	0.797490
Xa	0.000000	0.661360	0.238530	0.688350
Xa	0.000000	-0.661360	0.238530	0.688350
Xa	0.000000	0.021070	0.099270	0.625940
Xa	0.000000	-0.354510	-1.610630	0.588630
Xa	0.000000	0.354510	-1.610630	0.588630
Xa	-1.791040	0.356960	0.068080	0.581780
Xa	1.791040	0.356960	0.068080	0.581780
Xa	-1.791040	-0.356960	0.068080	0.581780
Xa	1.791040	-0.356960	0.068080	0.581780
Xa	0.000000	0.000000	-0.693580	0.577880
Xa	0.000000	-0.156270	0.119220	0.575380
Xa	0.000000	0.156270	0.119220	0.575380
Xa	-0.773600	0.000000	0.057190	0.533970
Xa	0.773600	0.000000	0.057190	0.533970
Xa	0.000000	0.000000	-1.121370	0.494520
Xb	0.355260	0.000000	-1.610000	0.584710
Xb	-0.355260	0.000000	-1.610000	0.584710
Xb	0.000000	0.000000	0.258400	0.572330
Xb	1.746740	0.000000	0.448350	0.568090
Xb	-1.746740	0.000000	0.448350	0.568090
Xb	-1.830970	0.000000	-0.268050	0.567440
Xb	1.830970	0.000000	-0.268050	0.567440
Xb	0.000000	0.000000	0.783080	0.528470
Xb	0.000000	0.352080	-0.515720	0.526670
Xb	0.000000	-0.352080	-0.515720	0.526670
Xb	-0.659650	-0.259780	0.112530	0.514770
Xb	-0.659650	0.259780	0.112530	0.514770
Xb	0.659650	-0.259780	0.112530	0.514770
Xb	0.659650	0.259780	0.112530	0.514770
Xb	-0.052110	0.000000	-1.133870	0.494420
Xb	0.052110	0.000000	-1.133870	0.494420
Xb	0.000000	0.000000	-1.059100	0.493650
Xb	-1.117730	0.000000	0.051100	0.478840
Xb	1.117730	0.000000	0.051100	0.478840
Xb	0.000000	-0.070910	0.100440	0.287870
Xb	0.000000	0.070910	0.100440	0.287870
Xb	0.000000	0.154360	-1.582040	0.226350
Xb	0.000000	-0.154360	-1.582040	0.226350
Xb	1.761630	0.155190	0.083190	0.223450
Xb	1.761630	-0.155190	0.083190	0.223450
Xb	-1.761630	0.155190	0.083190	0.223450
Xb	-1.761630	-0.155190	0.083190	0.223450
Xb	0.000000	-0.375210	0.178900	0.200410
Xb	0.000000	0.375210	0.178900	0.200410
Xc	0.000000	0.000000	-0.062060	0.568600
Xc	-2.120840	0.000000	0.138430	0.520990
Xc	2.120840	0.000000	0.138430	0.520990
Xc	1.354810	0.000000	0.038000	0.513650
Xc	-1.354810	0.000000	0.038000	0.513650
Xc	0.000000	0.000000	-1.948300	0.496790
Xc	0.000000	-0.054950	-1.135440	0.494400
Xc	0.000000	0.054950	-1.135440	0.494400
Xc	0.543780	0.000000	0.518680	0.473320
Xc	-0.543780	0.000000	0.518680	0.473320
Xc	-0.510440	0.000000	-0.392840	0.439650
Xc	0.510440	0.000000	-0.392840	0.439650

LOL Topologies

Xc	0.000000	0.000000	0.170320	0.280770
Xc	0.154850	0.000000	-1.582260	0.224320
Xc	-0.154850	0.000000	-1.582260	0.224320
Xc	-1.779460	0.000000	-0.069910	0.216680
Xc	1.779460	0.000000	-0.069910	0.216680
Xc	-1.745900	0.000000	0.242070	0.216460
Xc	1.745900	0.000000	0.242070	0.216460
Xc	0.000000	0.000000	0.501480	0.182430
Xc	0.000000	0.000000	-0.315120	0.175740
Xd	0.000000	0.000000	0.026930	0.279900
Xd	-1.917770	0.000000	0.104080	0.191480
Xd	1.917770	0.000000	0.104080	0.191480
Xd	1.590860	0.000000	0.068820	0.185300
Xd	-1.590860	0.000000	0.068820	0.185300
Xd	0.000000	0.000000	-1.742590	0.179090
Xd	0.000000	0.000000	-1.406290	0.169640
Xd	-0.317300	0.000000	-0.175070	0.169000
Xd	0.317300	0.000000	-0.175070	0.169000

**SF2 13**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

S	0.000000	0.000000	-0.104527	0.000000
F	0.000000	-1.256057	-1.155051	0.000000
F	0.000000	1.256057	-1.155051	0.000000
Xa	-0.000010	0.000000	-0.103960	0.803220
Xa	-0.000230	-1.257080	-1.155900	0.798910
Xa	0.000230	1.257080	-1.155900	0.798910
Xa	0.720380	0.000000	0.121660	0.713460
Xa	-0.352660	1.293400	-1.198960	0.584200
Xa	0.352660	-1.293400	-1.198960	0.584200
Xa	-0.352660	-1.293400	-1.198960	0.584200
Xa	0.352660	1.293400	-1.198960	0.584200
Xa	-0.168620	0.000000	-0.083130	0.575680
Xa	0.168620	0.000000	-0.083130	0.575680
Xa	0.000000	-0.614470	-0.656460	0.563390
Xa	0.000000	0.614470	-0.656460	0.563390
Xa	0.000000	-0.893490	-0.902170	0.524900
Xa	0.000000	0.893490	-0.902170	0.524900
Xb	0.000000	0.000000	0.067170	0.573030
Xb	0.000000	0.000000	-0.278220	0.568570
Xb	0.000000	1.519490	-0.906800	0.567210
Xb	0.000000	-1.519490	-0.906800	0.567210
Xb	0.000000	-1.074070	-1.467000	0.566010
Xb	0.000000	1.074070	-1.467000	0.566010
Xb	0.000000	0.863700	-1.002470	0.524340
Xb	0.000000	-0.863700	-1.002470	0.524340
Xb	0.000000	1.035760	-0.801600	0.522460
Xb	0.000000	-1.035760	-0.801600	0.522460
Xb	0.000000	-0.823220	-0.821950	0.521540
Xb	0.000000	0.823220	-0.821950	0.521540
Xb	0.411320	0.520980	-0.492900	0.486840
Xb	-0.411320	0.520980	-0.492900	0.486840
Xb	-0.411320	-0.520980	-0.492900	0.486840
Xb	0.411320	-0.520980	-0.492900	0.486840
Xb	-0.076180	0.000000	-0.102260	0.282620
Xb	0.076180	0.000000	-0.102260	0.282620
Xb	0.154650	-1.260960	-1.160290	0.225320
Xb	-0.154650	-1.260960	-1.160290	0.225320
Xb	0.154650	1.260960	-1.160290	0.225320
Xb	-0.154650	1.260960	-1.160290	0.225320
Xb	-0.399920	0.000000	0.034950	0.194510
Xb	0.399920	0.000000	0.034950	0.194510
Xc	0.000000	0.120220	-0.229740	0.568140
Xc	0.000000	-0.120230	-0.229740	0.568140
Xc	0.000000	-1.543710	-1.381670	0.525280
Xc	0.000000	1.543710	-1.381670	0.525280
Xc	-0.049470	1.029900	-0.809360	0.522460
Xc	0.049470	1.029900	-0.809360	0.522460
Xc	-0.049470	-1.029900	-0.809360	0.522460
Xc	0.049470	-1.029900	-0.809360	0.522460
Xc	0.000000	-0.740940	0.093670	0.374620
Xc	0.000000	0.740940	0.093670	0.374620
Xc	0.000000	0.000000	-0.891950	0.366290
Xc	0.000000	0.000000	-0.027850	0.276130
Xc	0.000000	0.000000	-0.181840	0.275010
Xc	0.000000	-1.361330	-1.038490	0.216360
Xc	0.000000	1.361330	-1.038490	0.216360
Xc	0.000000	1.165030	-1.283010	0.216350
Xc	0.000000	-1.165030	-1.283010	0.216350
Xc	0.000000	0.000000	0.339080	0.176840
Xc	0.000000	-0.362700	-0.383470	0.170390
Xc	0.000000	0.362700	-0.383470	0.170390
Xd	0.000000	0.074970	-0.123040	0.274070
Xd	0.000000	-0.074970	-0.123040	0.274070

LOL Topologies

Xd	0.000000	-1.382270	-1.255910	0.191660
Xd	0.000000	1.382270	-1.255910	0.191660
Xd	0.000000	1.125530	-1.049580	0.182830
Xd	0.000000	-1.125530	-1.049580	0.182830
Xd	0.000000	-0.448100	0.031540	0.157230
Xd	0.000000	0.448100	0.031540	0.157230
Xd	0.000000	0.000000	-0.578960	0.156260

**PF3 12**

Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

P	0.000000	0.000000	-0.194008	0.000000
F	1.399964	0.000000	0.605282	0.000000
F	-0.699982	-1.212405	0.605282	0.000000
F	-0.699982	1.212405	0.605282	0.000000
Xa	0.000000	0.000000	-0.193640	0.804880
Xa	1.398670	0.000000	0.604580	0.799320
Xa	-0.700610	-1.213490	0.602200	0.792250
Xa	-0.700610	1.213490	0.602200	0.792250
Xa	0.000000	0.000000	-0.378710	0.575350
Xa	0.000000	0.000000	-0.006410	0.570880
Xa	-0.819330	1.419120	0.334280	0.568430
Xa	-0.819330	-1.419120	0.334280	0.568430
Xa	1.638660	0.000000	0.334280	0.568430
Xa	-0.648740	-1.123650	0.951480	0.567810
Xa	-0.648740	1.123650	0.951480	0.567810
Xa	1.297480	0.000000	0.951480	0.567810
Xa	1.010580	0.000000	0.447480	0.546740
Xa	-0.505290	-0.875190	0.447480	0.546740
Xa	-0.505290	0.875190	0.447480	0.546740
Xb	0.069610	0.120570	-0.068220	0.570180
Xb	-0.139220	0.000000	-0.068220	0.570180
Xb	0.069610	-0.120570	-0.068220	0.570180
Xb	-1.003190	1.062650	0.733060	0.564650
Xb	-1.003190	-1.062650	0.733060	0.564650
Xb	1.421880	-0.337460	0.733060	0.564650
Xb	1.421880	0.337460	0.733060	0.564650
Xb	-0.418690	-1.400110	0.733060	0.564650
Xb	-0.418690	1.400110	0.733060	0.564650
Xb	-0.501080	0.867900	0.600570	0.545410
Xb	1.002160	0.000000	0.600570	0.545410
Xb	-0.501080	-0.867900	0.600570	0.545410
Xb	0.852980	0.000000	0.328960	0.531380
Xb	-0.426490	0.738700	0.328960	0.531380
Xb	-0.426490	-0.738700	0.328960	0.531380
Xb	0.000000	0.000000	-0.276420	0.273570
Xb	0.000000	0.000000	-0.110770	0.272210
Xb	-0.743140	1.287160	0.474430	0.217580
Xb	-0.743140	-1.287160	0.474430	0.217580
Xb	1.486280	0.000000	0.474430	0.217580
Xb	1.334830	0.000000	0.747900	0.217540
Xb	-0.667410	-1.156000	0.747900	0.217540
Xb	-0.667410	1.156000	0.747900	0.217540
Xb	0.000000	0.000000	-0.667490	0.188130
Xb	-0.223220	-0.386630	0.026450	0.174120
Xb	-0.223220	0.386630	0.026450	0.174120
Xb	0.446450	0.000000	0.026450	0.174120
Xc	0.159030	0.000000	-0.094680	0.569630
Xc	-0.079510	0.137720	-0.094680	0.569630
Xc	-0.079510	-0.137720	-0.094680	0.569630
Xc	1.720090	0.000000	0.776560	0.544810
Xc	-0.860040	-1.489640	0.776560	0.544810
Xc	-0.860040	1.489640	0.776560	0.544810
Xc	-0.595530	-1.031490	0.271580	0.540870
Xc	-0.595530	1.031490	0.271580	0.540870
Xc	1.191060	0.000000	0.271580	0.540870
Xc	0.041030	-0.071060	-0.180350	0.270320
Xc	0.041030	0.071060	-0.180350	0.270320
Xc	-0.082060	0.000000	-0.180350	0.270320
Xc	-0.568220	1.296960	0.619030	0.215960
Xc	-0.839090	-1.140570	0.619030	0.215960
Xc	-0.839090	1.140570	0.619030	0.215960
Xc	1.407310	0.156390	0.619030	0.215960
Xc	1.407310	-0.156390	0.619030	0.215960

LOL Topologies

Xc	-0.568220	-1.296960	0.619030	0.215960
Xc	0.487410	0.000000	-0.331460	0.164990
Xc	-0.243710	0.422110	-0.331460	0.164990
Xc	-0.243710	-0.422110	-0.331460	0.164990
Xc	-0.372480	0.000000	0.174520	0.154500
Xc	0.186240	-0.322570	0.174520	0.154500
Xc	0.186240	0.322570	0.174520	0.154500
Xd	-0.041070	0.071140	-0.180800	0.270260
Xd	-0.041070	-0.071140	-0.180800	0.270260
Xd	0.082140	0.000000	-0.180800	0.270260
Xd	-0.769760	-1.333260	0.682060	0.201290
Xd	-0.769760	1.333260	0.682060	0.201290
Xd	1.539520	0.000000	0.682060	0.201290
Xd	-0.628270	-1.088190	0.524910	0.194410
Xd	-0.628270	1.088190	0.524910	0.194410
Xd	1.256530	0.000000	0.524910	0.194410
Xd	0.262920	-0.455400	-0.145970	0.149690
Xd	0.262920	0.455400	-0.145970	0.149690
Xd	-0.525850	0.000000	-0.145970	0.149690
Xd	0.000000	0.000000	0.341130	0.146430

**NH3 18**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

N	0.000000	0.000000	0.117476	0.000000
H	-0.471152	0.816060	-0.281879	0.000000
H	0.942305	0.000000	-0.281879	0.000000
H	-0.471152	-0.816060	-0.281879	0.000000
Xa	-0.379390	-0.657120	-0.208970	0.899810
Xa	0.758770	0.000000	-0.208970	0.899810
Xa	-0.379390	0.657120	-0.208970	0.899810
Xa	0.000000	0.000000	0.117940	0.798790
Xa	0.000000	0.000000	0.594800	0.622070
Xb	-0.213120	-0.369140	0.369290	0.562360
Xb	-0.213120	0.369140	0.369290	0.562360
Xb	0.426240	0.000000	0.369290	0.562360
Xb	0.150910	0.261380	-0.294760	0.514390
Xb	-0.301820	0.000000	-0.294760	0.514390
Xb	0.150910	-0.261380	-0.294760	0.514390
Xb	0.000000	0.000000	0.326730	0.201390
Xb	0.000000	0.000000	-0.105560	0.186080
Xc	0.000000	0.000000	-0.378960	0.501130
Xc	-0.494460	0.000000	0.112500	0.475990
Xc	0.247230	0.428220	0.112500	0.475990
Xc	0.247230	-0.428220	0.112500	0.475990
Xc	-0.110920	0.192120	0.103350	0.172040
Xc	0.221840	0.000000	0.103350	0.172040
Xc	-0.110920	-0.192120	0.103350	0.172040
Xd	-0.226130	0.000000	0.098300	0.165040
Xd	0.113060	0.195830	0.098300	0.165040
Xd	0.113060	-0.195830	0.098300	0.165040

**BH3 17**

XYZ coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

B	0.000000	0.000000	0.000000	0.000000
H	-0.599891	1.039042	0.000000	0.000000
H	-0.599891	-1.039042	0.000000	0.000000
H	1.199782	0.000000	0.000000	0.000000
Xa	-0.392030	-0.679010	0.000000	0.927560
Xa	0.784060	0.000000	0.000000	0.927560
Xa	-0.392030	0.679010	0.000000	0.927560
Xa	0.000400	-0.000690	0.000000	0.794360
Xb	-0.703120	0.000000	0.000000	0.490880
Xb	0.351560	-0.608920	0.000000	0.490880
Xb	0.351560	0.608920	0.000000	0.490880
Xb	0.317300	0.000000	0.000000	0.174510
Xb	-0.158650	-0.274790	0.000000	0.174510
Xb	-0.158650	0.274790	0.000000	0.174510
Xc	-0.337010	0.000000	0.000000	0.153530
Xc	0.168510	-0.291860	0.000000	0.153530
Xc	0.168510	0.291860	0.000000	0.153530
Xc	0.000000	0.000000	-0.764600	0.144640
Xc	0.000000	0.000000	0.764600	0.144640
Xd	0.000000	0.000000	-0.427320	0.056640
Xd	0.000000	0.000000	0.427320	0.056640



**H3NBH3 19**

Xyz coordinates, LOL value

(3,-3) CP: Xa

(3,-1) CP: Xb

(3,+1) CP: Xc

(3,+3) CP: Xd

B	0.000000	0.000000	-0.835476	0.000000
N	0.000000	0.000000	0.813283	0.000000
H	-0.476483	0.825293	1.186179	0.000000
H	-0.476483	-0.825293	1.186179	0.000000
H	0.952967	0.000000	1.186179	0.000000
H	0.587855	-1.018194	-1.152852	0.000000
H	0.587855	1.018194	-1.152852	0.000000
H	-1.175709	0.000000	-1.152852	0.000000
Xa	-0.383410	-0.664090	1.118240	0.915540
Xa	-0.383410	0.664090	1.118240	0.915540
Xa	0.766830	0.000000	1.118240	0.915540
Xa	0.394350	0.683030	-1.037100	0.897090
Xa	-0.788690	0.000000	-1.037100	0.897090
Xa	0.394350	-0.683030	-1.037100	0.897090
Xa	0.001380	0.000000	0.814900	0.794960
Xa	0.000130	0.000220	-0.831860	0.788770
Xa	0.000000	0.000000	-0.015230	0.666650
Xa	0.000000	0.000000	0.233770	0.655740
Xb	0.000000	0.000000	0.192200	0.655590
Xb	0.417000	0.000000	0.549530	0.545250
Xb	-0.208500	-0.361130	0.549530	0.545250
Xb	-0.208500	0.361130	0.549530	0.545250
Xb	-0.372370	0.000000	1.151570	0.518970
Xb	0.186180	-0.322480	1.151570	0.518970
Xb	0.186180	0.322480	1.151570	0.518970
Xb	-0.332300	0.575550	-1.135890	0.475210
Xb	-0.332300	-0.575550	-1.135890	0.475210
Xb	0.664590	0.000000	-1.135890	0.475210
Xb	-0.529170	0.000000	-0.307930	0.417890
Xb	0.264590	0.458280	-0.307930	0.417890
Xb	0.264590	-0.458280	-0.307930	0.417890
Xb	0.000000	0.000000	0.600480	0.193840
Xb	-0.076360	0.132260	0.973210	0.180350
Xb	0.152720	0.000000	0.973210	0.180350
Xb	-0.076360	-0.132260	0.973210	0.180350
Xb	0.160020	-0.277160	-0.893350	0.163160
Xb	0.160020	0.277160	-0.893350	0.163160
Xb	-0.320030	0.000000	-0.893350	0.163160
Xc	0.000000	0.000000	1.297850	0.481740
Xc	0.238560	0.413200	0.732620	0.473330
Xc	0.238560	-0.413200	0.732620	0.473330
Xc	-0.477120	0.000000	0.732620	0.473330
Xc	-0.303140	-0.525050	-0.435190	0.340550
Xc	0.606280	0.000000	-0.435190	0.340550
Xc	-0.303140	0.525050	-0.435190	0.340550
Xc	0.000000	0.000000	-1.562560	0.295950
Xc	-0.005760	0.000000	1.036800	0.179810
Xc	0.217900	0.000000	0.779750	0.177320
Xc	-0.108950	-0.188710	0.779750	0.177320
Xc	-0.108950	0.188710	0.779750	0.177320
Xc	0.330390	0.000000	-0.929170	0.144440
Xc	-0.165190	-0.286120	-0.929170	0.144440
Xc	-0.165190	0.286120	-0.929170	0.144440
Xc	0.028820	0.049930	-0.479500	0.118490
Xc	0.028820	-0.049930	-0.479500	0.118490
Xc	-0.057650	0.000000	-0.479500	0.118490
Xd	0.112420	0.194730	0.806740	0.170360
Xd	0.112420	-0.194730	0.806740	0.170360
Xd	-0.224850	0.000000	0.806740	0.170360
Xd	-0.076330	-0.132210	-0.505300	0.118060
Xd	-0.076330	0.132210	-0.505300	0.118060
Xd	0.152670	0.000000	-0.505300	0.118060
Xd	0.000000	0.000000	-1.207280	0.107990

### Kinetic Core Radii

Plots of  $v(\mathbf{r})$  for basic atoms H, C, Si, Ge are shown below. Basic atoms constitute fundamental fragments of a molecule; they are chosen to be spherically symmetric and spin-restricted (i.e. spin- $\alpha$  and spin- $\beta$  orbitals are spatially identical; they are equally occupied, and fractional occupations are applied, if necessary, to distribute the electrons equally over symmetry-degenerate states).<sup>S1</sup> The underlying wavefunctions were relativistically optimized (scalar; ZORA),<sup>S2</sup> and use a basis set of valence quadruple zeta quality augmented by four polarization functions (QZ4P).<sup>S3</sup> The abscissae (in a.u.) of plots of  $v(\mathbf{r})$  are logarithmic.

The development of a kinetic core radius  $r_{\text{KC}}$  is not rooted in physical concepts, but is driven by the search for a geometric criterion that allows one to partition an entire set of CP3s into topologically consistent and chemically meaningful subsets. In this work, positions of extrema  $r_{\text{min}}$  and  $r_{\text{max}}$  in  $v$  as well as positions  $r_{1/2}$ , where  $v$  for the first time drops below 0.666, serve as basis for kinetic core radii  $r_{\text{KC}}$ .  $v = 0.666$  roughly corresponds to a  $\tau/\tau_0$  ratio of one half.

According to this pragmatic approach, kinetic core radii were chosen as follows:

For H:

$$- r_{\text{KC}} = r_{1/2}$$

For C:

$$- r_{\text{KC}} = (r_{\text{min}}(\text{last minimum}) + r_{1/2})/2$$

For Si and Ge:

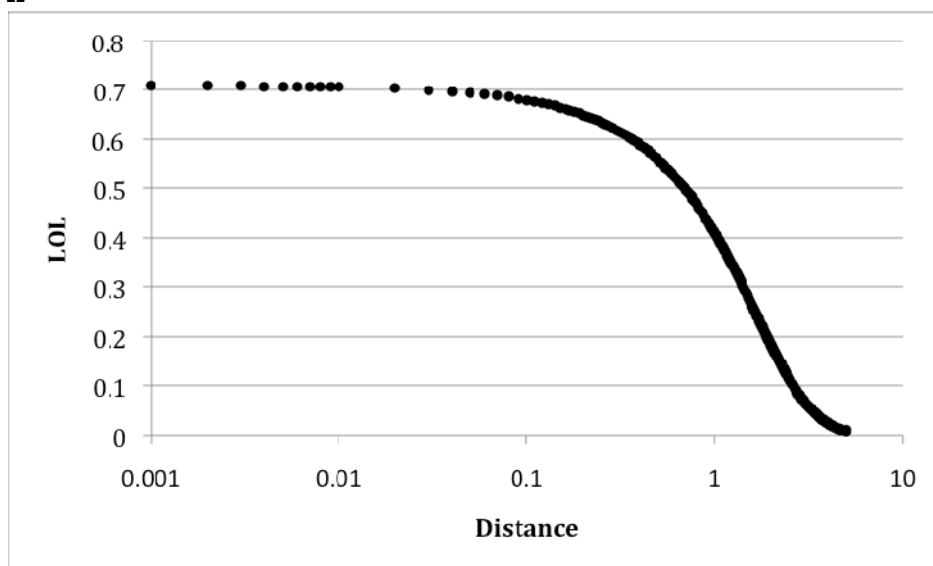
$$- r_{\text{KC}} = (r_{\text{min}}(\text{last minimum}) + r_{\text{min}}(\text{second last minimum}))/2$$

S1: Chemical Physics Letters 265,481 (1997).

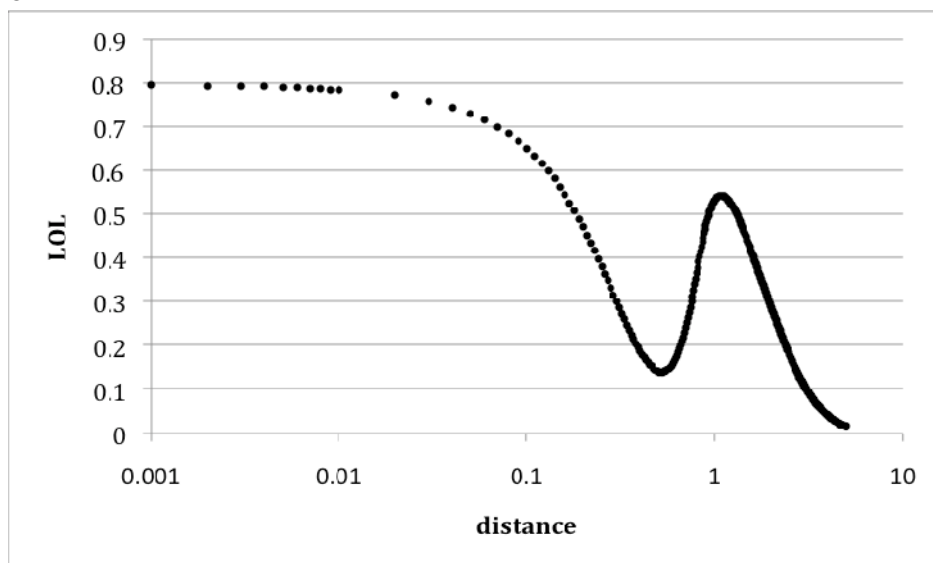
S2: Journal of Chemical Physics 105, 6505 (1994).

S3: Journal of Computational Chemistry 24, 1142 (2003).

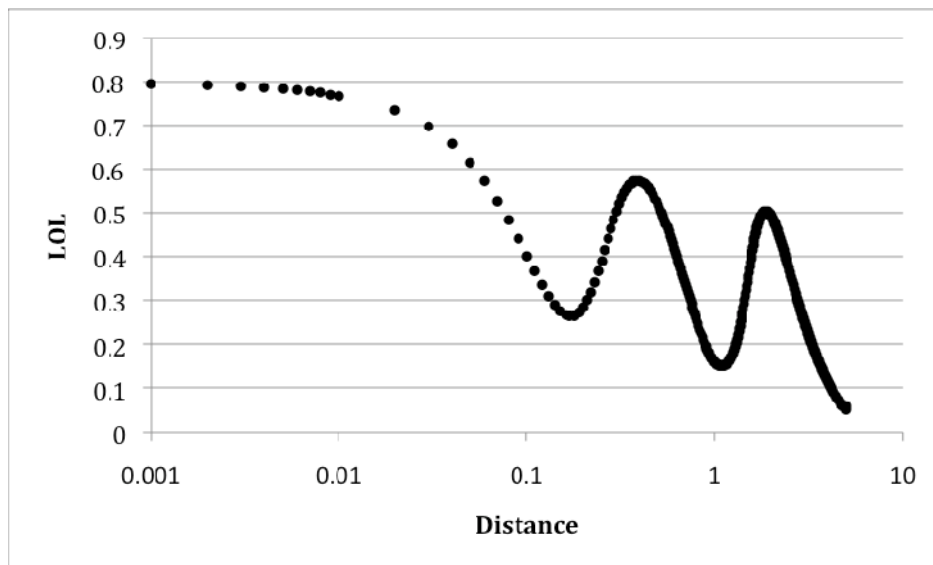
**H**



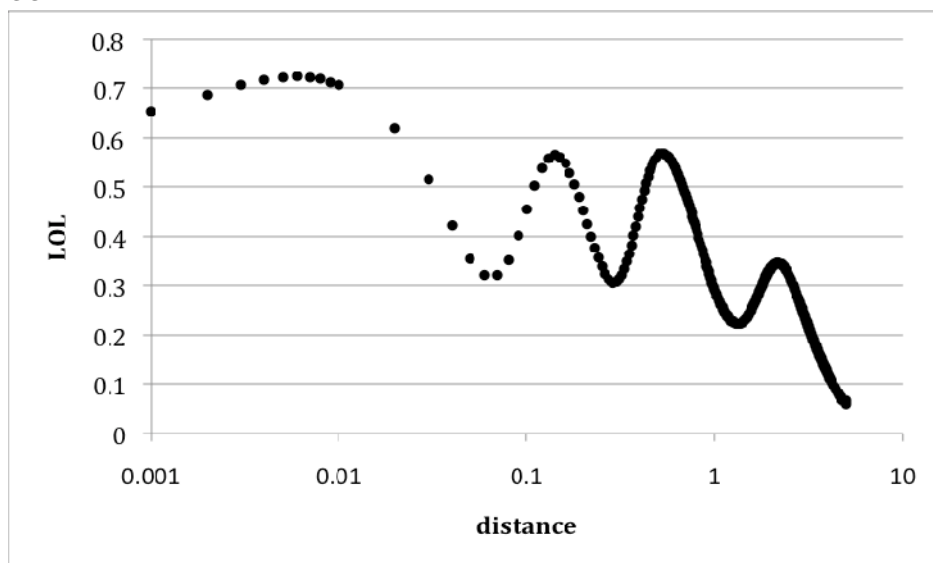
**C**



Si



Ge



### STOs vs. GTOs

The current work utilizes Slater-type functions STOs as basis for molecular orbitals, while the majority of quantum chemical programs exploit Gaussian-type functions GTOs. The difference is explored in  $v(\mathbf{r})$  calculations of  $C_2H_6$ . To achieve consistency, the geometry of ethane has been optimized under  $C_{3v}$ -symmetry constraint using PBE/TZVP(STO) and PBE/TZVP(GTO) calculations. The optimized geometries are virtually identical; a comparison is given in the table below.

QuickTime™ and a decompressor are needed to see this picture.

Both calculations produce consistent  $v(\mathbf{r})$  topologies with  $PoHo\# = 1$ . The details are given in the table below:

	(3, -3)	(3, -1)	(3, 1)	(3, 3)
PBE/TZVP (STO)	9	20	20	8
PBE/TZVP (GTO)	15	26	20	8

Since an STO has a cusp at its origin, while a GTO smoothly proceeds to zero slope, and since the basis functions are centered at atomic positions, the innermost core region is inadequately described by GTOs. The GTO calculations result in six additional (3,-3) CPs, and six additional (3,-1) CPs. These additional CPs are located in close vicinity to the hydrogen atoms, as show in the pictures below:

QuickTime™ and a decompressor are needed to see this picture.

QuickTime™ and a decompressor are needed to see this picture.

PBE/TZVP (STO)

PBE/TZVP (GTO)

A detailed comparison of (3,-3) and (3,-1) CPs is given in the table below:

QuickTime™ and a  
decompressor  
are needed to see this picture.

Notable differences are found for two of the (3,-3) CPs, which are located at approximately the same position close to the carbon atoms, but which show differences in  $v(\mathbf{r})$ . The fact that a GTO approaches zero slope at the position of a nucleus is reflected in the  $v(\mathbf{r})$  values (0.99896) approaching 1.0. Slight differences in the corresponding STO  $v(\mathbf{r})$  values are due to the fact that the (3,-3) CPs are estimated as approximate endpoints of MaxKCLs.

STO and GTO Basis Sets

A detailed comparison of (3,1) and (3,3) CPs is given in the table below:

QuickTime™ and a decompressor are needed to see this picture.

The results of PBE/TZVP(STO) and PBE/TZVP(GTO) calculations are virtually identical.