Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Protobranching as Repulsion-Induced Attraction: A Prototype for Geminal Stabilization

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Contents

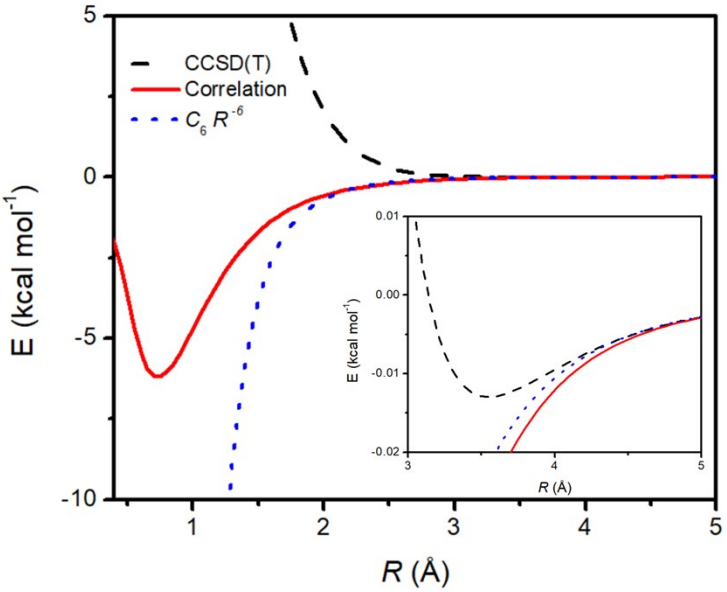


Figure S1. The CCSD(T)/aug-cc-pV5z energy of ^{2}HHe (dashed black line) as a function of distance. The solid red line is the associated correlation energy while the dotted blue line presents the atom-pairwise dipole-dipole term (C_6 = -43.3 kcal mol^{-1} Å^6). The correlation energy displays a minimum of -6.18 kcal mol^{-1} at 0.75 Å. The equilibrium separation is included in the inset (R_{eq} = 3.55 Å, D_o = 0.013 kcal mol^{-1}).

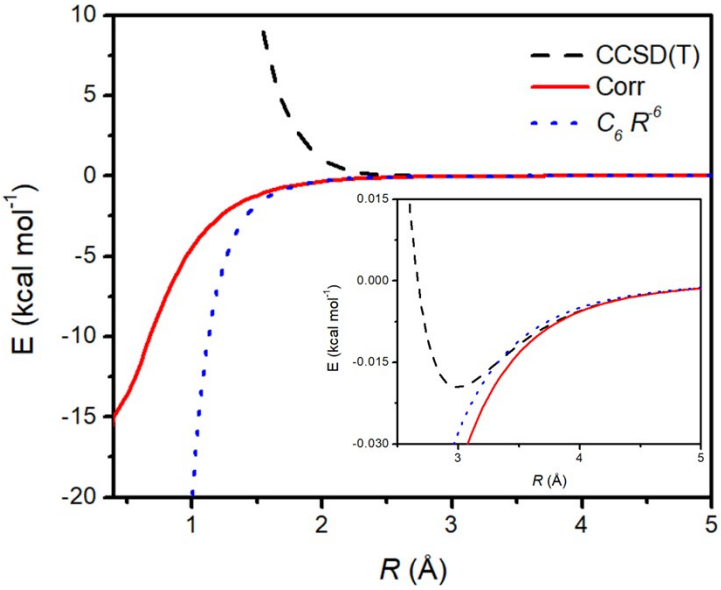


Figure S2. The CCSD(T) energy of ^{2}He$_2$ (dashed black line) as a function of distance (R_{eq} = 3.00 Å, D_o =- 0.020 kcal mol^{-1}). The solid red line is the associated correlation energy while the dotted blue line presents the atom-pairwise dipole-dipole term (C_6 = -20.3 kcal mol^{-1} Å^6). The equilibrium separation is included in the inset.

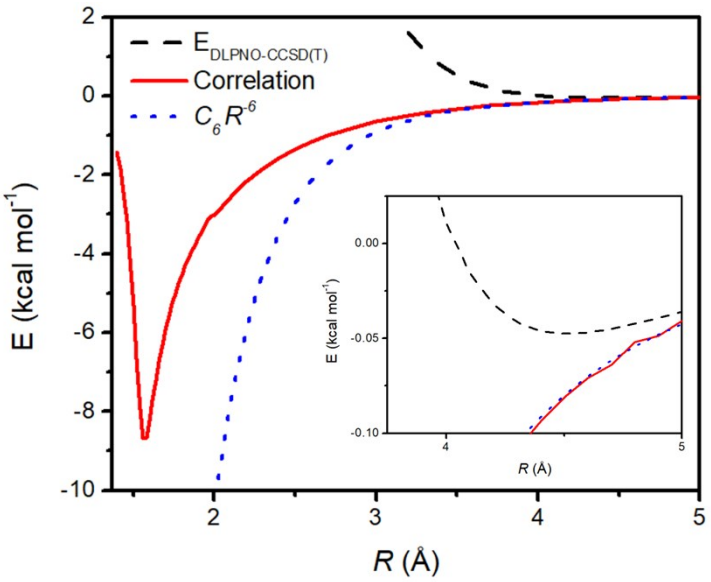


Figure S3. CCSD(T) energy of $^9C_2$ (dashed black line) as a function of distance (R_{eq} = 4.50 Å, D_o = -0.048 kcal mol^{-1}). The equilibrium separation is included in the inset. The solid red line is the associated correlation energy while the dotted blue line presents the atom-pairwise dipole-dipole term (C_6 = -664.0 kcal mol^{-1} Å^6). The correlation energy displays a minimum of -8.68 kcal mol^{-1} at 1.56 Å

I. Exponential Fits of Argon Dimer

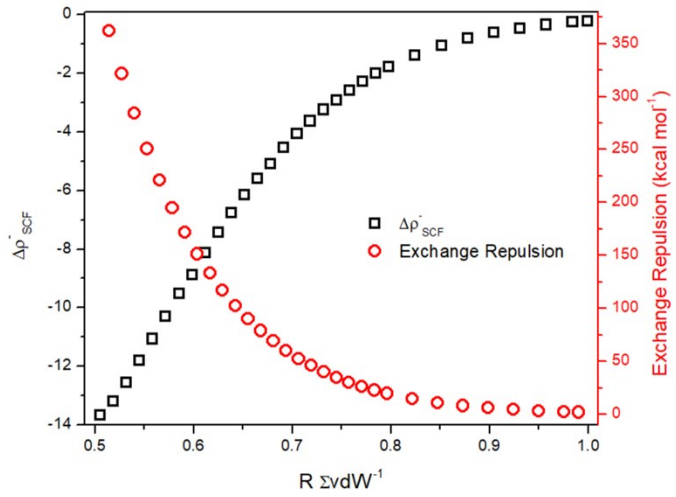


Figure S4. The variation of $\Delta\rho^-_{SCF}$ (black) and exchange repulsion (red) with respect to internuclear separation for Ar_2.

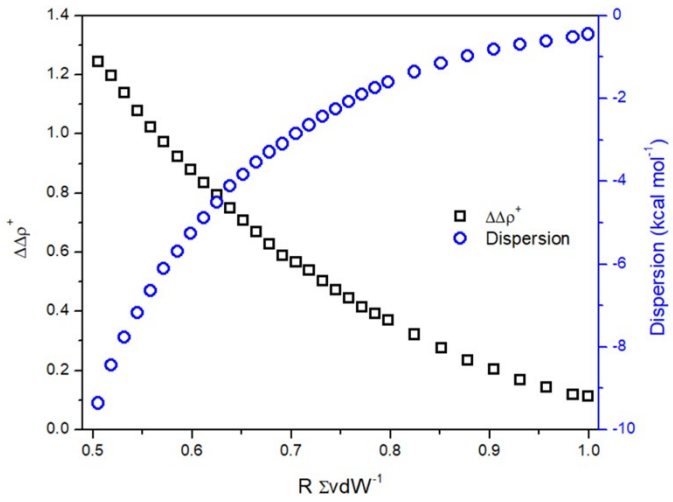


Figure S5. The variation of $\Delta\Delta\rho^{+}$ (black) and exchange repulsion (red) with respect to the internuclear separation for Ar_2.

Figure 4.

$$\text{Exchange Repulsion} = 71.266\, e^{-\left(\frac{\Delta\rho^{-}_{SCF}}{0.876}\right)} - 67.561 \qquad R^2 = 0.998$$

Figure 5.

$$\text{Dispersion} = -3.779\,\Delta\Delta\rho^{+} + 3.782 \qquad R^2 = 0.999$$

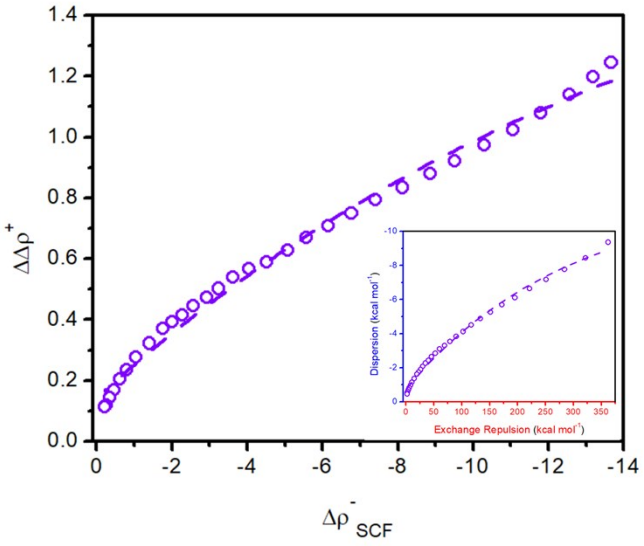
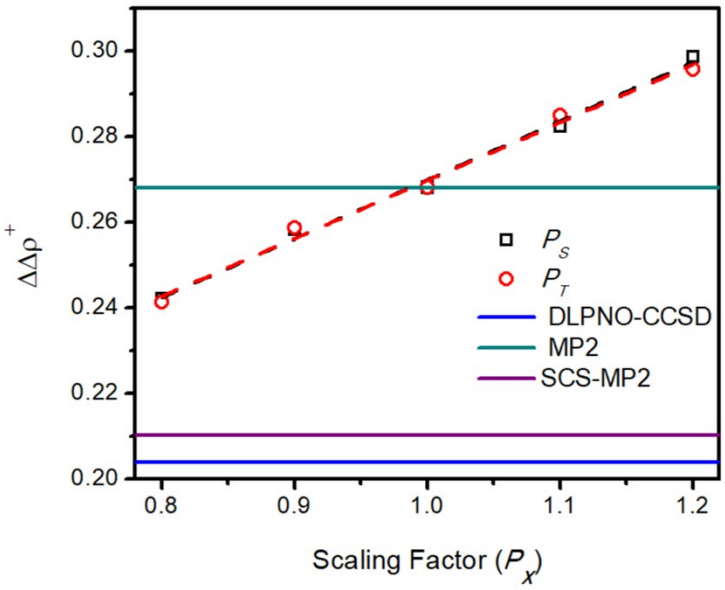


Figure S6. The relationship between $\Delta\Delta\rho^{+}$ and $\Delta\rho^{-}_{SCF}$ where the purple dashed line is an exponential fit. The inset depicts the exponential relationship between Dispersion and Exchange Repulsion as calculated with LED. The exponential fits are provided below:

$$\Delta\Delta\rho^{+} = -0.018e^{\left(\frac{\Delta\rho^{-}_{SCF}}{0.160}\right)} + 0.019 \qquad R^2 = 0.991$$



$$\text{Dispersion} = 11.47e^{\left(\frac{-\text{ Exchange Repulsion}}{290.2}\right)} - 12.20 \quad R^2 = 0.994$$

III. Impact of MP2-derived singlet and triplet correlation on electron density

Figure S7. The relationship of the $\Delta\Delta\rho^{+}$ term, in terms of the specified MP2 electron density, with respect to the singlet (black) and triplet (red) correlation scaling factors at the Ar_2 at a separation of 0.90 ΣvdW^{-1}. The solid blue, purple, and cyan lines present the $\Delta\Delta\rho$ values at its geometry for DLPNO-CCSD, SCS-MP2, and MP2, respectively. The overlapping dashed black and red lines are the respective linear fits for the singlet (P_S) and triplet (P_T) scaling factors.

IV. Functional forms of B3LYP-D3, B3LYP-D3M, and D3(Ar_2) for Ar_2:

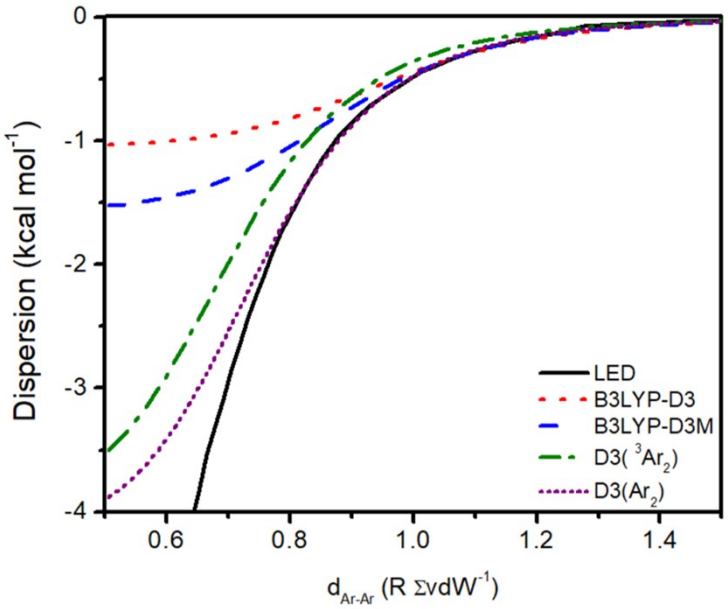


Figure S8. The potential of the specified empirical dispersion correction for Ar_2 (C_6 = -890.8 kcal mol^{-1} Å^6, C_8 = -8890.4 kcal mol^{-1} Å^6)

V.

Gaussian16 and ORCA 4.1 syntax for the D3($^3Ar_2$) correction.

Gaussian:

```
# b3lyp/aug-cc-pVQZ iop(3/174=1000000,3/175=03505000,3/177=00610000,3/178=4634550)
empiricaldispersion=gd3bj
```

ORCA:

```
! d3bj b3lyp aug-cc-pVQZ aug-cc-pVQZ/C RIJK aug-cc-pVQZ/JK TightSCF
%method
D3S6=1.00000
D3S8=0.35050
D3A1=0.06010
D3A2=4.63455
End
```

Gaussian16 and ORCA 4.1 syntax for the D3(Ar_2) correction.

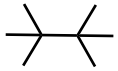
Gaussian:

```
# b3lyp/aug-cc-pVQZ iop(3/174=1000000,3/175=0998380,3/177=0110190,3/178=4645400) empiricaldispersion=gd3bj
```

ORCA:

```
! d3bj b3lyp aug-cc-pVQZ aug-cc-pVQZ/C RIJK aug-cc-pVQZ/JK TightSCF
%method
D3S6=1.00000
D3S8=0.99838
D3A1=0.11019
D3A2=4.64540
End
```

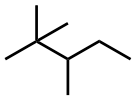
VI. Cartesian coordinates of the eighteen isomers of octane and assoicated low-lying *gauche*-conformations. The gauche conformations are denoted by the aasociated C-C bonds. 1, 2, 3, 4, and 5 refer to a *gauche*-conformation (g) relative to the alkyl substituents along the C_2-C_3, C_3-C_4, C_5-C_6, C_6-C_7, and C_7-C_8 bond, respectively for the longest chain within the configuration.

2,2,3,3-Tetramethylbutane 

C	0.779000	0.000000	-0.000000
C	-0.779000	-0.000000	-0.000000
C	1.326000	1.413000	-0.161000
H	0.907000	2.100000	0.577000
H	2.410000	1.404000	-0.024000
H	1.122000	1.813000	-1.155000
C	1.327000	-0.567000	1.304000
H	0.908000	-1.549000	1.530000
H	2.411000	-0.680000	1.227000
H	1.123000	0.094000	2.148000
C	1.327000	-0.846000	-1.143000
H	2.411000	-0.723000	-1.203000
H	1.123000	-1.907000	-0.993000
H	0.908000	-0.550000	-2.107000
C	-1.326000	-1.413000	-0.161000
H	-2.410000	-1.404000	-0.024000
H	-1.122000	-1.813000	-1.155000
H	-0.907000	-2.100000	0.577000
C	-1.327000	0.846000	-1.143000
H	-2.411000	0.723000	-1.203000
H	-1.123000	1.907000	-0.993000
H	-0.908000	0.550000	-2.107000
C	-1.327000	0.567000	1.304000

H	-2.411000	0.680000	1.227000
H	-1.123000	-0.094000	2.148000
H	-0.908000	1.549000	1.530000

Total Energy: -315.607899340



2,2,3-Trimethylpentane

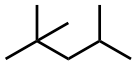
C	2.004000	0.819000	-0.622000
H	1.790000	1.009000	-1.677000
H	1.993000	1.774000	-0.094000
H	3.016000	0.413000	-0.552000
C	1.004000	-0.164000	-0.031000
C	-0.437000	0.313000	-0.310000
H	-0.588000	0.194000	-1.391000
C	-1.490000	-0.536000	0.394000
H	-1.550000	-0.228000	1.443000
H	-1.184000	-1.585000	0.402000
C	-2.862000	-0.438000	-0.246000
H	-2.829000	-0.787000	-1.282000
H	-3.594000	-1.046000	0.288000
H	-3.233000	0.588000	-0.256000
C	1.233000	-1.513000	-0.700000
H	0.561000	-2.282000	-0.318000
H	1.084000	-1.438000	-1.780000
H	2.256000	-1.853000	-0.523000
C	1.266000	-0.298000	1.462000
H	2.308000	-0.580000	1.634000
H	1.086000	0.642000	1.987000
H	0.634000	-1.066000	1.911000
C	-0.651000	1.779000	0.027000
H	-1.698000	2.056000	-0.105000
H	-0.389000	1.982000	1.069000
H	-0.058000	2.439000	-0.605000

Total Energy: -315.606690155

1g

C	0.578000	-1.659000	-0.766000
H	-0.393000	-2.114000	-0.594000
H	0.682000	-1.481000	-1.840000
H	1.343000	-2.383000	-0.473000
C	0.769000	-0.360000	0.008000
C	-0.272000	0.698000	-0.429000
H	-0.363000	0.608000	-1.520000
C	-1.671000	0.537000	0.165000
H	-2.265000	1.374000	-0.214000
H	-1.611000	0.691000	1.247000
C	-2.433000	-0.744000	-0.122000
H	-2.039000	-1.596000	0.431000
H	-3.481000	-0.630000	0.166000
H	-2.405000	-0.993000	-1.185000
C	0.678000	-0.639000	1.501000
H	0.774000	0.281000	2.083000
H	-0.269000	-1.112000	1.767000
H	1.483000	-1.310000	1.806000
C	2.180000	0.126000	-0.305000
H	2.895000	-0.679000	-0.123000
H	2.269000	0.424000	-1.353000
H	2.469000	0.974000	0.317000
C	0.181000	2.119000	-0.121000
H	-0.603000	2.831000	-0.388000
H	0.381000	2.242000	0.947000
H	1.081000	2.398000	-0.666000

Total Energy: -315.602673697

2,2,4-Trimethylpentane 

C	-2.261000	-0.196000	1.067000
H	-2.225000	-1.197000	1.505000
H	-2.132000	0.530000	1.873000
H	-3.254000	-0.051000	0.635000
C	-1.180000	-0.030000	0.010000
C	0.174000	-0.297000	0.669000
H	0.248000	0.313000	1.577000
H	0.166000	-1.339000	1.005000
C	1.417000	-0.053000	-0.189000
H	1.127000	-0.107000	-1.243000
C	2.018000	1.319000	0.066000
H	2.371000	1.386000	1.099000
H	2.873000	1.503000	-0.590000
H	1.293000	2.118000	-0.090000
C	-1.425000	-1.038000	-1.102000
H	-0.671000	-0.963000	-1.889000
H	-1.405000	-2.058000	-0.711000
H	-2.402000	-0.871000	-1.562000
C	-1.259000	1.377000	-0.560000
H	-2.249000	1.558000	-0.984000
H	-1.083000	2.126000	0.216000
H	-0.524000	1.529000	-1.353000
C	2.461000	-1.127000	0.059000
H	2.755000	-1.134000	1.113000
H	2.075000	-2.119000	-0.186000
H	3.361000	-0.953000	-0.536000

Total Energy: -315.606211537

1g

C	-2.224000	-1.097000	-0.354000
H	-2.148000	-1.393000	-1.403000
H	-2.110000	-1.994000	0.260000
H	-3.226000	-0.695000	-0.187000
C	-1.161000	-0.061000	-0.008000
C	0.204000	-0.676000	-0.343000
H	0.164000	-1.732000	-0.054000
H	0.326000	-0.670000	-1.434000
C	1.463000	-0.098000	0.289000
H	1.356000	-0.161000	1.377000
C	2.650000	-0.960000	-0.110000
H	2.804000	-0.918000	-1.192000
H	3.568000	-0.616000	0.371000
H	2.492000	-2.006000	0.163000
C	-1.447000	1.185000	-0.835000
H	-0.748000	1.993000	-0.627000
H	-1.390000	0.957000	-1.903000
H	-2.455000	1.552000	-0.625000
C	-1.262000	0.268000	1.473000
H	-2.271000	0.608000	1.718000
H	-1.046000	-0.612000	2.084000
H	-0.565000	1.057000	1.758000
C	1.741000	1.350000	-0.076000
H	1.723000	1.485000	-1.161000
H	1.013000	2.034000	0.360000
H	2.729000	1.650000	0.282000

Total Energy: -315.605796754

2g

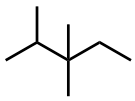
C	-2.308000	-0.620000	-0.662000
H	-2.494000	-0.137000	-1.625000
H	-2.177000	-1.690000	-0.840000
H	-3.194000	-0.485000	-0.038000
C	-1.077000	-0.026000	0.014000
C	0.086000	-0.188000	-0.975000
H	0.014000	-1.195000	-1.400000
H	-0.120000	0.498000	-1.805000
C	1.548000	0.005000	-0.562000
H	2.091000	0.047000	-1.515000
C	1.848000	1.305000	0.164000
H	1.438000	1.299000	1.176000
H	2.927000	1.446000	0.253000
H	1.436000	2.168000	-0.363000
C	-1.375000	1.440000	0.303000
H	-0.568000	1.928000	0.846000
H	-1.542000	1.991000	-0.626000
H	-2.282000	1.523000	0.909000
C	-0.852000	-0.760000	1.326000
H	-1.760000	-0.723000	1.933000
H	-0.602000	-1.809000	1.155000
H	-0.048000	-0.308000	1.908000
C	2.131000	-1.175000	0.200000
H	1.737000	-1.244000	1.213000
H	1.916000	-2.118000	-0.308000
H	3.217000	-1.076000	0.276000

Total Energy: -315.588944735

3g

C	2.261000	0.196000	1.067000
H	2.225000	1.197000	1.505000
H	2.131000	-0.530000	1.873000
H	3.254000	0.051000	0.635000
C	1.180000	0.030000	0.010000
C	-0.174000	0.297000	0.669000
H	-0.248000	-0.312000	1.577000
H	-0.166000	1.339000	1.005000
C	-1.417000	0.053000	-0.189000
H	-1.127000	0.107000	-1.244000
C	-2.018000	-1.319000	0.066000
H	-2.371000	-1.386000	1.099000
H	-2.873000	-1.503000	-0.590000
H	-1.293000	-2.118000	-0.090000
C	1.425000	1.038000	-1.102000
H	0.672000	0.963000	-1.889000
H	1.405000	2.058000	-0.711000
H	2.402000	0.871000	-1.562000
C	1.259000	-1.377000	-0.560000
H	2.249000	-1.557000	-0.985000
H	1.083000	-2.126000	0.217000
H	0.524000	-1.529000	-1.353000
C	-2.461000	1.127000	0.059000
H	-2.755000	1.134000	1.113000
H	-2.075000	2.119000	-0.186000
H	-3.361000	0.953000	-0.536000

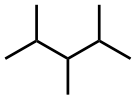
Total Energy: -315.603237992



2,3,3-Trimethylpentane

C	2.299000	-0.722000	-0.111000
H	2.500000	-0.693000	0.963000
H	2.096000	-1.756000	-0.388000
H	3.216000	-0.418000	-0.620000
C	1.163000	0.220000	-0.475000
H	1.084000	0.245000	-1.569000
C	-0.216000	-0.258000	0.030000
C	-1.251000	0.834000	-0.260000
H	-1.096000	1.189000	-1.285000
H	-1.048000	1.686000	0.394000
C	-2.704000	0.429000	-0.093000
H	-2.899000	0.018000	0.900000
H	-3.357000	1.295000	-0.220000
H	-3.005000	-0.318000	-0.828000
C	1.530000	1.622000	-0.012000
H	0.845000	2.380000	-0.389000
H	1.542000	1.686000	1.079000
H	2.533000	1.878000	-0.362000
C	-0.181000	-0.552000	1.522000
H	0.156000	0.315000	2.093000
H	-1.174000	-0.822000	1.885000
H	0.484000	-1.387000	1.745000
C	-0.602000	-1.528000	-0.715000
H	-0.711000	-1.332000	-1.786000
H	0.148000	-2.309000	-0.588000
H	-1.548000	-1.926000	-0.346000

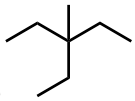
Total Energy: -315.605865048



2,3,4-Trimethylpentane

C	-1.520000	-1.588000	-0.380000
H	-1.524000	-1.534000	-1.473000
H	-0.750000	-2.299000	-0.082000
H	-2.485000	-1.992000	-0.065000
C	-1.302000	-0.209000	0.219000
H	-1.197000	-0.318000	1.305000
C	-0.029000	0.462000	-0.306000
H	-0.198000	0.661000	-1.374000
C	1.201000	-0.450000	-0.230000
H	0.963000	-1.347000	-0.808000
C	2.418000	0.181000	-0.886000
H	2.811000	1.008000	-0.290000
H	3.219000	-0.553000	-0.991000
H	2.178000	0.566000	-1.880000
C	-2.529000	0.650000	-0.044000
H	-2.480000	1.612000	0.464000
H	-2.637000	0.839000	-1.117000
H	-3.434000	0.142000	0.295000
C	0.207000	1.796000	0.384000
H	-0.598000	2.500000	0.175000
H	0.263000	1.671000	1.468000
H	1.135000	2.261000	0.051000
C	1.532000	-0.883000	1.187000
H	1.780000	-0.021000	1.811000
H	0.701000	-1.411000	1.658000
H	2.397000	-1.550000	1.191000

Total Energy: -315.605131312



3-Ethyl-3-methylpentane

C	0.209000	0.231000	2.571000
H	-0.649000	-0.435000	2.675000
H	1.112000	-0.365000	2.717000
H	0.161000	0.956000	3.386000
C	0.209000	0.936000	1.229000
H	-0.713000	1.517000	1.131000
H	1.026000	1.666000	1.201000
C	0.352000	0.035000	-0.000000
C	0.209000	0.936000	-1.229000
H	1.026000	1.666000	-1.201000
H	-0.713000	1.517000	-1.131000
C	0.209000	0.231000	-2.571000
H	-0.649000	-0.435000	-2.675000
H	0.161000	0.956000	-3.386000
H	1.112000	-0.365000	-2.717000
C	-0.699000	-1.073000	-0.000000
H	-0.526000	-1.712000	0.871000
H	-0.526000	-1.712000	-0.871000
C	1.728000	-0.614000	-0.000000
H	1.865000	-1.247000	-0.878000
H	2.515000	0.144000	-0.000000
H	1.865000	-1.247000	0.878000
C	-2.138000	-0.596000	0.000000
H	-2.828000	-1.441000	0.000000
H	-2.359000	0.010000	0.881000
H	-2.359000	0.010000	-0.881000

Total Energy: -315.605552923

1g

C	-1.598000	1.741000	-0.469000
H	-2.458000	1.082000	-0.335000
H	-1.483000	2.326000	0.446000
H	-1.841000	2.438000	-1.274000
C	-0.338000	0.963000	-0.795000
H	-0.492000	0.395000	-1.718000
H	0.468000	1.670000	-1.008000
C	0.139000	0.005000	0.297000
C	1.312000	-0.825000	-0.230000
H	0.972000	-1.398000	-1.097000
H	1.576000	-1.560000	0.539000
C	2.555000	-0.047000	-0.619000
H	2.967000	0.507000	0.226000
H	3.332000	-0.724000	-0.977000
H	2.351000	0.667000	-1.420000
C	-0.983000	-0.943000	0.728000
H	-1.756000	-0.357000	1.232000
H	-0.575000	-1.617000	1.489000
C	0.577000	0.788000	1.526000
H	1.015000	0.117000	2.270000
H	1.319000	1.548000	1.277000
H	-0.271000	1.290000	1.995000
C	-1.621000	-1.759000	-0.379000
H	-2.411000	-2.398000	0.021000
H	-2.072000	-1.118000	-1.140000
H	-0.899000	-2.407000	-0.877000

Total Energy: -315.603487286

1g2g

C	-0.226000	2.139000	0.387000
H	0.609000	2.365000	-0.278000
H	-1.133000	2.149000	-0.215000
H	-0.298000	2.957000	1.108000
C	-0.017000	0.821000	1.113000
H	0.916000	0.896000	1.681000
H	-0.804000	0.684000	1.862000
C	0.045000	-0.454000	0.259000
C	0.814000	-0.227000	-1.040000
H	0.302000	0.538000	-1.628000
H	0.760000	-1.148000	-1.631000
C	2.268000	0.170000	-0.866000
H	2.856000	-0.638000	-0.429000
H	2.720000	0.419000	-1.829000
H	2.373000	1.041000	-0.217000
C	-1.352000	-0.997000	-0.061000
H	-1.817000	-1.298000	0.884000
H	-1.214000	-1.920000	-0.635000
C	0.737000	-1.530000	1.086000
H	0.797000	-2.470000	0.532000
H	1.748000	-1.233000	1.367000
H	0.179000	-1.717000	2.007000
C	-2.314000	-0.094000	-0.808000
H	-3.209000	-0.651000	-1.093000
H	-2.640000	0.745000	-0.192000
H	-1.874000	0.308000	-1.723000

Total Energy: -315.582553168

1g2g3g

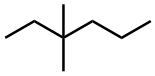
C	-1.598000	1.741000	-0.469000
H	-2.458000	1.082000	-0.336000
H	-1.483000	2.325000	0.447000
H	-1.841000	2.438000	-1.273000
C	-0.338000	0.963000	-0.795000
H	-0.492000	0.395000	-1.718000
H	0.468000	1.670000	-1.008000
C	0.139000	0.005000	0.297000
C	1.312000	-0.825000	-0.230000
H	0.972000	-1.397000	-1.098000
H	1.576000	-1.560000	0.539000
C	2.555000	-0.047000	-0.619000
H	2.967000	0.507000	0.226000
H	3.332000	-0.724000	-0.977000
H	2.351000	0.667000	-1.420000
C	-0.983000	-0.943000	0.728000
H	-1.756000	-0.356000	1.232000
H	-0.575000	-1.617000	1.489000
C	0.577000	0.788000	1.526000
H	1.016000	0.117000	2.270000
H	1.319000	1.548000	1.277000
H	-0.271000	1.290000	1.995000
C	-1.621000	-1.759000	-0.379000
H	-2.411000	-2.398000	0.022000
H	-2.072000	-1.119000	-1.140000
H	-0.898000	-2.407000	-0.877000

Total Energy: -315.602975543

1g3g

C	-1.598000	1.741000	-0.469000
H	-2.458000	1.082000	-0.336000
H	-1.483000	2.325000	0.447000
H	-1.841000	2.438000	-1.273000
C	-0.338000	0.963000	-0.795000
H	-0.492000	0.395000	-1.718000
H	0.468000	1.670000	-1.008000
C	0.139000	0.005000	0.297000
C	1.312000	-0.825000	-0.230000
H	0.972000	-1.397000	-1.098000
H	1.576000	-1.560000	0.539000
C	2.555000	-0.047000	-0.619000
H	2.967000	0.507000	0.226000
H	3.332000	-0.724000	-0.977000
H	2.351000	0.667000	-1.420000
C	-0.983000	-0.943000	0.728000
H	-1.756000	-0.356000	1.232000
H	-0.575000	-1.617000	1.489000
C	0.577000	0.788000	1.526000
H	1.016000	0.117000	2.270000
H	1.319000	1.548000	1.277000
H	-0.271000	1.290000	1.995000
C	-1.621000	-1.759000	-0.379000
H	-2.411000	-2.398000	0.022000
H	-2.072000	-1.119000	-1.140000
H	-0.898000	-2.407000	-0.877000

Total Energy: -315.601938904



3,3-Dimethylhexane

C	1.099000	2.094000	-0.017000
H	0.069000	2.318000	0.269000
H	1.701000	2.085000	0.893000
H	1.454000	2.918000	-0.638000
C	1.194000	0.779000	-0.765000
H	0.592000	0.838000	-1.677000
H	2.226000	0.621000	-1.096000
C	0.763000	-0.458000	0.024000
C	-0.650000	-0.303000	0.586000
H	-0.638000	0.470000	1.361000
H	-0.914000	-1.235000	1.099000
C	-1.736000	0.031000	-0.417000
H	-1.764000	-0.729000	-1.204000
H	-1.503000	0.977000	-0.913000
C	-3.099000	0.128000	0.241000
H	-3.102000	0.900000	1.015000
H	-3.880000	0.375000	-0.481000
H	-3.369000	-0.817000	0.719000
C	1.713000	-0.695000	1.188000
H	1.684000	0.129000	1.904000
H	1.440000	-1.608000	1.723000
H	2.742000	-0.805000	0.835000
C	0.832000	-1.662000	-0.904000
H	0.521000	-2.572000	-0.385000
H	0.191000	-1.532000	-1.778000
H	1.854000	-1.810000	-1.261000

Total Energy: -315.607683161

1g

C	-2.151000	-1.613000	0.007000
H	-1.352000	-2.334000	-0.174000
H	-2.311000	-1.553000	1.085000
H	-3.063000	-2.018000	-0.436000
C	-1.830000	-0.255000	-0.586000
H	-1.692000	-0.357000	-1.668000
H	-2.690000	0.409000	-0.449000
C	-0.597000	0.454000	-0.018000
C	0.638000	-0.414000	-0.250000
H	0.671000	-0.692000	-1.311000
H	0.521000	-1.349000	0.307000
C	1.972000	0.200000	0.132000
H	1.948000	0.516000	1.179000
H	2.151000	1.101000	-0.459000
C	3.116000	-0.774000	-0.075000
H	3.172000	-1.092000	-1.119000
H	4.078000	-0.331000	0.192000
H	2.980000	-1.671000	0.534000
C	-0.791000	0.724000	1.467000
H	-0.821000	-0.203000	2.043000
H	0.019000	1.337000	1.864000
H	-1.727000	1.261000	1.639000
C	-0.457000	1.781000	-0.748000
H	0.359000	2.380000	-0.341000
H	-0.266000	1.621000	-1.813000
H	-1.376000	2.364000	-0.655000

Total Energy: -315.606584608

1g2g

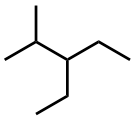
C	1.097000	2.094000	-0.017000
H	0.067000	2.318000	0.269000
H	1.699000	2.085000	0.894000
H	1.453000	2.919000	-0.637000
C	1.193000	0.779000	-0.765000
H	0.593000	0.838000	-1.677000
H	2.226000	0.622000	-1.096000
C	0.763000	-0.458000	0.024000
C	-0.649000	-0.303000	0.586000
H	-0.638000	0.469000	1.362000
H	-0.914000	-1.235000	1.099000
C	-1.735000	0.031000	-0.417000
H	-1.763000	-0.727000	-1.205000
H	-1.503000	0.979000	-0.911000
C	-3.099000	0.127000	0.241000
H	-3.103000	0.897000	1.016000
H	-3.880000	0.374000	-0.481000
H	-3.369000	-0.819000	0.717000
C	1.714000	-0.695000	1.188000
H	1.685000	0.128000	1.904000
H	1.441000	-1.608000	1.723000
H	2.742000	-0.805000	0.834000
C	0.832000	-1.662000	-0.904000
H	0.522000	-2.572000	-0.385000
H	0.191000	-1.532000	-1.778000
H	1.854000	-1.809000	-1.262000

Total Energy: -315.607683207

2g

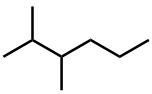
C	2.574000	-1.175000	-0.096000
H	3.165000	-0.517000	-0.736000
H	2.848000	-0.969000	0.940000
H	2.873000	-2.201000	-0.316000
C	1.085000	-0.994000	-0.326000
H	0.852000	-1.212000	-1.374000
H	0.545000	-1.734000	0.270000
C	0.531000	0.393000	0.005000
C	-0.942000	0.463000	-0.402000
H	-1.004000	0.326000	-1.489000
H	-1.300000	1.480000	-0.204000
C	-1.885000	-0.519000	0.265000
H	-1.827000	-0.410000	1.352000
H	-1.580000	-1.544000	0.040000
C	-3.318000	-0.311000	-0.187000
H	-3.408000	-0.437000	-1.269000
H	-3.999000	-1.020000	0.290000
H	-3.661000	0.698000	0.056000
C	1.274000	1.460000	-0.785000
H	1.229000	1.253000	-1.858000
H	0.825000	2.441000	-0.613000
H	2.323000	1.520000	-0.493000
C	0.677000	0.687000	1.491000
H	0.192000	1.634000	1.741000
H	0.227000	-0.097000	2.102000
H	1.728000	0.770000	1.774000

Total Energy: -315.606515716

3-Ethyl-2-methylpentane 

C	-2.212000	0.838000	0.384000
H	-2.311000	0.624000	1.453000
H	-1.876000	1.870000	0.279000
H	-3.206000	0.766000	-0.062000
C	-1.261000	-0.150000	-0.270000
H	-1.112000	0.158000	-1.311000
C	0.111000	-0.166000	0.411000
H	-0.042000	-0.572000	1.422000
C	1.073000	-1.100000	-0.316000
H	1.115000	-0.819000	-1.373000
H	0.667000	-2.113000	-0.291000
C	2.475000	-1.128000	0.261000
H	2.452000	-1.326000	1.336000
H	3.075000	-1.910000	-0.209000
H	2.997000	-0.180000	0.112000
C	-1.900000	-1.529000	-0.278000
H	-1.322000	-2.253000	-0.852000
H	-1.997000	-1.909000	0.744000
H	-2.901000	-1.486000	-0.712000
C	0.700000	1.231000	0.582000
H	1.632000	1.151000	1.146000
H	0.032000	1.829000	1.205000
C	0.963000	1.957000	-0.724000
H	0.043000	2.104000	-1.293000
H	1.400000	2.941000	-0.542000
H	1.657000	1.401000	-1.358000

Total Energy: -315.604241762



2,3-dimethylhexane

C	1.931000	-1.433000	-0.787000
H	1.263000	-2.169000	-0.334000
H	1.740000	-1.423000	-1.863000
H	2.954000	-1.781000	-0.628000
C	1.729000	-0.057000	-0.179000
H	2.457000	0.618000	-0.645000
C	0.345000	0.515000	-0.506000
H	0.198000	0.370000	-1.585000
C	-0.780000	-0.218000	0.209000
H	-0.759000	0.038000	1.274000
H	-0.614000	-1.298000	0.151000
C	-2.161000	0.080000	-0.343000
H	-2.174000	-0.148000	-1.414000
H	-2.375000	1.149000	-0.255000
C	-3.245000	-0.710000	0.363000
H	-3.262000	-0.478000	1.431000
H	-4.235000	-0.492000	-0.042000
H	-3.072000	-1.785000	0.263000
C	2.018000	-0.094000	1.312000
H	1.881000	0.883000	1.780000
H	1.362000	-0.806000	1.817000
H	3.048000	-0.409000	1.494000
C	0.290000	2.007000	-0.230000
H	-0.646000	2.446000	-0.579000
H	0.369000	2.210000	0.841000
H	1.109000	2.529000	-0.732000

Total Energy: -315.605268377

1g

C	1.931000	-1.434000	-0.787000
H	1.263000	-2.170000	-0.333000
H	1.739000	-1.424000	-1.862000
H	2.954000	-1.782000	-0.628000
C	1.729000	-0.057000	-0.179000
H	2.457000	0.618000	-0.645000
C	0.345000	0.515000	-0.507000
H	0.198000	0.369000	-1.585000
C	-0.780000	-0.218000	0.209000
H	-0.759000	0.038000	1.274000
H	-0.614000	-1.298000	0.151000
C	-2.161000	0.080000	-0.343000
H	-2.175000	-0.148000	-1.414000
H	-2.375000	1.149000	-0.255000
C	-3.245000	-0.710000	0.364000
H	-3.262000	-0.478000	1.432000
H	-4.235000	-0.492000	-0.041000
H	-3.072000	-1.785000	0.264000
C	2.018000	-0.093000	1.311000
H	1.882000	0.884000	1.779000
H	1.362000	-0.805000	1.817000
H	3.048000	-0.408000	1.494000
C	0.290000	2.007000	-0.231000
H	-0.646000	2.446000	-0.580000
H	0.368000	2.210000	0.840000
H	1.109000	2.528000	-0.732000

Total Energy: -315.605268378

1g3g

C	1.839000	-1.581000	-0.398000
H	1.530000	-2.038000	0.545000
H	1.291000	-2.072000	-1.205000
H	2.902000	-1.797000	-0.530000
C	1.591000	-0.083000	-0.392000
H	2.015000	0.324000	-1.318000
C	0.095000	0.250000	-0.436000
H	-0.302000	-0.283000	-1.308000
C	-0.657000	-0.243000	0.791000
H	-0.242000	0.240000	1.681000
H	-0.486000	-1.317000	0.911000
C	-2.157000	0.003000	0.757000
H	-2.357000	1.078000	0.769000
H	-2.595000	-0.394000	1.678000
C	-2.846000	-0.630000	-0.438000
H	-2.622000	-1.699000	-0.494000
H	-3.930000	-0.517000	-0.377000
H	-2.520000	-0.176000	-1.376000
C	2.322000	0.567000	0.769000
H	2.183000	1.649000	0.786000
H	1.976000	0.166000	1.725000
H	3.394000	0.370000	0.702000
C	-0.132000	1.735000	-0.660000
H	-1.171000	1.946000	-0.918000
H	0.105000	2.310000	0.238000
H	0.494000	2.107000	-1.474000

Total Energy: -315.604830670

2g

C	-2.722000	-0.025000	-0.376000
H	-3.154000	0.035000	0.627000
H	-2.869000	0.938000	-0.865000
H	-3.289000	-0.772000	-0.937000
C	-1.255000	-0.412000	-0.297000
H	-0.847000	-0.395000	-1.314000
C	-0.458000	0.589000	0.540000
H	-0.928000	0.613000	1.532000
C	0.994000	0.170000	0.749000
H	1.033000	-0.749000	1.341000
H	1.489000	0.937000	1.355000
C	1.795000	-0.035000	-0.523000
H	1.761000	0.872000	-1.133000
H	1.337000	-0.825000	-1.125000
C	3.238000	-0.397000	-0.230000
H	3.297000	-1.316000	0.360000
H	3.812000	-0.552000	-1.146000
H	3.729000	0.393000	0.344000
C	-1.131000	-1.826000	0.243000
H	-0.107000	-2.198000	0.197000
H	-1.454000	-1.864000	1.288000
H	-1.761000	-2.513000	-0.325000
C	-0.531000	1.992000	-0.043000
H	0.127000	2.672000	0.503000
H	-0.222000	1.998000	-1.091000
H	-1.540000	2.400000	0.006000

Total Energy: -315.605275756

2g3g

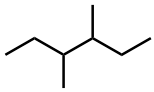
C	-2.455000	-0.291000	-0.584000
H	-3.047000	-0.068000	0.310000
H	-2.591000	0.528000	-1.290000
H	-2.868000	-1.194000	-1.038000
C	-0.995000	-0.497000	-0.213000
H	-0.428000	-0.613000	-1.144000
C	-0.427000	0.711000	0.530000
H	-0.987000	0.787000	1.472000
C	1.047000	0.573000	0.914000
H	1.176000	-0.266000	1.603000
H	1.305000	1.469000	1.486000
C	2.036000	0.426000	-0.241000
H	2.979000	0.901000	0.044000
H	1.677000	0.984000	-1.110000
C	2.335000	-1.008000	-0.643000
H	1.452000	-1.525000	-1.019000
H	3.098000	-1.045000	-1.424000
H	2.709000	-1.577000	0.212000
C	-0.863000	-1.770000	0.603000
H	0.173000	-2.009000	0.838000
H	-1.407000	-1.669000	1.547000
H	-1.288000	-2.621000	0.066000
C	-0.651000	2.005000	-0.239000
H	-0.133000	2.836000	0.245000
H	-0.274000	1.929000	-1.262000
H	-1.708000	2.262000	-0.297000

Total Energy: -315.601510649

3g

C	-2.586000	0.700000	0.476000
H	-2.403000	0.663000	1.555000
H	-2.560000	1.744000	0.166000
H	-3.597000	0.328000	0.299000
C	-1.566000	-0.153000	-0.261000
H	-1.726000	-0.024000	-1.340000
C	-0.130000	0.285000	0.039000
H	0.015000	0.171000	1.121000
C	0.879000	-0.609000	-0.674000
H	0.640000	-0.615000	-1.744000
H	0.756000	-1.636000	-0.323000
C	2.338000	-0.223000	-0.488000
H	2.536000	0.744000	-0.959000
H	2.957000	-0.949000	-1.023000
C	2.761000	-0.179000	0.968000
H	2.545000	-1.129000	1.464000
H	3.831000	0.015000	1.067000
H	2.231000	0.604000	1.515000
C	-1.803000	-1.615000	0.082000
H	-1.212000	-2.291000	-0.537000
H	-1.548000	-1.806000	1.129000
H	-2.854000	-1.875000	-0.055000
C	0.094000	1.743000	-0.321000
H	1.111000	2.059000	-0.087000
H	-0.064000	1.899000	-1.393000
H	-0.582000	2.404000	0.219000

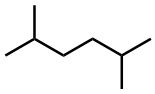
Total Energy: -315.604597064



2,4-dimethylhexane

C	-2.942000	-0.845000	0.314000
H	-3.019000	-1.479000	-0.574000
H	-2.829000	-1.499000	1.182000
H	-3.884000	-0.301000	0.418000
C	-1.767000	0.106000	0.183000
H	-1.739000	0.732000	1.082000
C	-0.469000	-0.683000	0.107000
H	-0.380000	-1.302000	1.009000
H	-0.543000	-1.382000	-0.735000
C	0.809000	0.128000	-0.045000
H	0.763000	0.671000	-0.997000
C	2.003000	-0.814000	-0.118000
H	1.790000	-1.585000	-0.866000
H	2.094000	-1.337000	0.841000
C	3.314000	-0.135000	-0.461000
H	3.620000	0.571000	0.313000
H	4.119000	-0.864000	-0.574000
H	3.230000	0.418000	-1.400000
C	-1.947000	1.011000	-1.021000
H	-1.163000	1.767000	-1.086000
H	-1.922000	0.424000	-1.944000
H	-2.909000	1.528000	-0.981000
C	0.962000	1.139000	1.075000
H	0.980000	0.631000	2.044000
H	1.886000	1.710000	0.978000
H	0.137000	1.853000	1.088000

Total Energy: -315.607015734



2,5-dimethylhexane

C	3.047000	-0.836000	-0.414000
H	3.084000	-1.434000	0.502000
H	2.882000	-1.518000	-1.251000
H	4.025000	-0.368000	-0.544000
C	1.944000	0.202000	-0.321000
H	1.940000	0.785000	-1.250000
C	0.589000	-0.477000	-0.195000
H	0.471000	-1.186000	-1.023000
H	0.588000	-1.076000	0.723000
C	-0.589000	0.477000	-0.195000
H	-0.471000	1.186000	-1.023000
H	-0.588000	1.076000	0.723000
C	-1.944000	-0.202000	-0.321000
H	-1.940000	-0.785000	-1.250000
C	-3.047000	0.836000	-0.414000
H	-3.084000	1.434000	0.502000
H	-2.882000	1.518000	-1.251000
H	-4.025000	0.368000	-0.544000
C	2.207000	1.151000	0.834000
H	1.474000	1.957000	0.876000
H	2.166000	0.610000	1.785000
H	3.198000	1.603000	0.751000
C	-2.207000	-1.151000	0.834000
H	-1.473000	-1.957000	0.876000
H	-2.166000	-0.610000	1.785000
H	-3.198000	-1.603000	0.751000

Total Energy: -315.607518606

1g

C	-2.503000	1.147000	-0.501000
H	-2.006000	1.824000	0.198000
H	-2.292000	1.495000	-1.515000
H	-3.578000	1.235000	-0.330000
C	-2.040000	-0.286000	-0.302000
H	-2.621000	-0.917000	-0.984000
C	-0.573000	-0.476000	-0.674000
H	-0.346000	-1.546000	-0.643000
H	-0.431000	-0.160000	-1.714000
C	0.414000	0.272000	0.202000
H	0.379000	-0.120000	1.224000
H	0.123000	1.325000	0.266000
C	1.853000	0.203000	-0.288000
H	1.877000	0.598000	-1.311000
C	2.745000	1.072000	0.579000
H	2.747000	0.704000	1.610000
H	3.777000	1.066000	0.221000
H	2.396000	2.107000	0.596000
C	-2.329000	-0.750000	1.115000
H	-1.982000	-1.774000	1.276000
H	-1.831000	-0.108000	1.845000
H	-3.400000	-0.718000	1.325000
C	2.375000	-1.222000	-0.317000
H	2.314000	-1.667000	0.681000
H	1.807000	-1.854000	-1.001000
H	3.421000	-1.248000	-0.629000

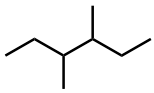
Total Energy: -315.606190531

1g3g

C	2.329000	-0.750000	1.115000
H	1.831000	-0.108000	1.845000
H	1.983000	-1.773000	1.277000
H	3.401000	-0.716000	1.326000
C	2.040000	-0.286000	-0.302000
H	2.620000	-0.918000	-0.984000
C	0.573000	-0.476000	-0.674000
H	0.430000	-0.162000	-1.714000
H	0.346000	-1.546000	-0.641000
C	-0.414000	0.272000	0.202000
H	-0.123000	1.325000	0.266000
H	-0.379000	-0.120000	1.224000
C	-1.853000	0.203000	-0.288000
H	-1.876000	0.598000	-1.311000
C	-2.375000	-1.222000	-0.317000
H	-2.314000	-1.667000	0.681000
H	-3.421000	-1.248000	-0.629000
H	-1.807000	-1.853000	-1.001000
C	2.503000	1.147000	-0.502000
H	2.291000	1.494000	-1.516000
H	2.005000	1.824000	0.196000
H	3.578000	1.235000	-0.331000
C	-2.745000	1.072000	0.579000
H	-2.748000	0.704000	1.609000
H	-2.395000	2.107000	0.596000
H	-3.776000	1.067000	0.221000

Total Energy: -315.606190518

‘



3,4-dimethylhexane

C	-2.785000	-1.145000	0.135000
H	-3.480000	-0.318000	-0.026000
H	-2.720000	-1.709000	-0.799000
H	-3.224000	-1.800000	0.890000
C	-1.415000	-0.653000	0.563000
H	-1.509000	-0.072000	1.486000
H	-0.789000	-1.516000	0.804000
C	-0.720000	0.198000	-0.491000
H	-0.748000	-0.364000	-1.434000
C	0.761000	0.441000	-0.177000
H	1.121000	1.159000	-0.925000
C	1.585000	-0.827000	-0.350000
H	1.337000	-1.273000	-1.318000
H	1.294000	-1.559000	0.410000
C	3.083000	-0.596000	-0.274000
H	3.389000	-0.257000	0.717000
H	3.635000	-1.512000	-0.492000
H	3.396000	0.163000	-0.996000
C	-1.458000	1.507000	-0.714000
H	-1.532000	2.080000	0.213000
H	-0.940000	2.125000	-1.451000
H	-2.472000	1.338000	-1.077000
C	0.973000	1.055000	1.196000
H	0.332000	1.924000	1.353000
H	0.756000	0.330000	1.984000
H	2.005000	1.385000	1.326000

Total Energy: -315.604413408

1g

C	-2.405000	-0.694000	0.922000
H	-1.663000	-1.332000	1.406000
H	-2.534000	0.194000	1.544000
H	-3.353000	-1.235000	0.920000
C	-1.987000	-0.327000	-0.490000
H	-1.884000	-1.236000	-1.086000
H	-2.786000	0.252000	-0.963000
C	-0.700000	0.492000	-0.573000
H	-0.472000	0.615000	-1.640000
C	0.502000	-0.216000	0.057000
H	0.325000	-0.274000	1.139000
C	1.782000	0.587000	-0.149000
H	1.636000	1.596000	0.241000
H	1.957000	0.696000	-1.226000
C	3.009000	-0.010000	0.513000
H	3.306000	-0.954000	0.055000
H	3.861000	0.669000	0.442000
H	2.824000	-0.200000	1.574000
C	-0.921000	1.876000	0.019000
H	-0.972000	1.833000	1.110000
H	-0.124000	2.570000	-0.247000
H	-1.861000	2.302000	-0.341000
C	0.659000	-1.628000	-0.477000
H	-0.212000	-2.245000	-0.258000
H	0.795000	-1.612000	-1.563000
H	1.526000	-2.125000	-0.040000

Total Energy: -315.603761748

1g3g

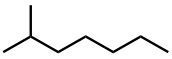
C	-2.409000	1.095000	-0.633000
H	-2.168000	1.630000	0.288000
H	-2.032000	1.688000	-1.468000
H	-3.497000	1.061000	-0.718000
C	-1.823000	-0.304000	-0.634000
H	-2.222000	-0.864000	0.215000
H	-2.162000	-0.835000	-1.529000
C	-0.297000	-0.357000	-0.607000
H	-0.026000	-1.416000	-0.526000
C	0.297000	0.357000	0.607000
H	0.026000	1.416000	0.526000
C	1.823000	0.304000	0.634000
H	2.162000	0.835000	1.529000
H	2.222000	0.864000	-0.215000
C	2.409000	-1.095000	0.633000
H	2.168000	-1.630000	-0.288000
H	3.497000	-1.061000	0.718000
H	2.032000	-1.688000	1.468000
C	0.283000	0.174000	-1.907000
H	0.173000	1.259000	-1.974000
H	1.346000	-0.053000	-1.998000
H	-0.225000	-0.267000	-2.767000
C	-0.283000	-0.174000	1.907000
H	-1.346000	0.053000	1.998000
H	-0.173000	-1.259000	1.974000
H	0.225000	0.267000	2.767000

Total Energy: -315.604096481

2g

C	-2.785000	-1.145000	0.135000
H	-3.480000	-0.319000	-0.026000
H	-2.719000	-1.710000	-0.799000
H	-3.224000	-1.800000	0.890000
C	-1.415000	-0.653000	0.563000
H	-1.509000	-0.072000	1.486000
H	-0.789000	-1.516000	0.804000
C	-0.720000	0.198000	-0.491000
H	-0.748000	-0.364000	-1.434000
C	0.761000	0.441000	-0.177000
H	1.121000	1.159000	-0.925000
C	1.585000	-0.827000	-0.350000
H	1.337000	-1.274000	-1.318000
H	1.294000	-1.559000	0.410000
C	3.083000	-0.596000	-0.274000
H	3.389000	-0.257000	0.717000
H	3.635000	-1.513000	-0.492000
H	3.396000	0.162000	-0.997000
C	-1.457000	1.507000	-0.714000
H	-1.532000	2.080000	0.213000
H	-0.940000	2.126000	-1.451000
H	-2.472000	1.338000	-1.077000
C	0.974000	1.056000	1.196000
H	0.332000	1.924000	1.352000
H	0.756000	0.330000	1.984000
H	2.005000	1.384000	1.326000

Total Energy: -315.604413414

2-methylheptane 

C	3.350000	-0.962000	0.002000
H	3.428000	-1.092000	1.086000
H	3.172000	-1.945000	-0.440000
H	4.313000	-0.595000	-0.359000
C	2.228000	0.004000	-0.332000
H	2.181000	0.113000	-1.423000
C	0.894000	-0.555000	0.136000
H	0.773000	-1.565000	-0.272000
H	0.924000	-0.670000	1.227000
C	-0.314000	0.276000	-0.249000
H	-0.303000	0.453000	-1.331000
H	-0.257000	1.262000	0.222000
C	-1.625000	-0.378000	0.139000
H	-1.631000	-0.568000	1.218000
H	-1.698000	-1.361000	-0.341000
C	-2.840000	0.450000	-0.230000
H	-2.830000	0.641000	-1.309000
H	-2.766000	1.431000	0.252000
C	-4.144000	-0.217000	0.161000
H	-4.184000	-0.391000	1.239000
H	-5.008000	0.392000	-0.111000
H	-4.249000	-1.186000	-0.333000
C	2.512000	1.369000	0.270000
H	1.765000	2.109000	-0.022000
H	2.517000	1.307000	1.362000
H	3.490000	1.739000	-0.047000

Total Energy: -315.605634110

1g

C	-2.658000	-1.249000	-0.419000
H	-2.083000	-1.271000	-1.347000
H	-2.422000	-2.155000	0.145000
H	-3.716000	-1.284000	-0.689000
C	-2.346000	-0.000000	0.387000
H	-3.000000	-0.000000	1.266000
C	-0.913000	-0.000000	0.908000
H	-0.773000	0.876000	1.551000
H	-0.772000	-0.877000	1.551000
C	0.169000	0.000000	-0.155000
H	0.059000	0.876000	-0.801000
H	0.059000	-0.875000	-0.802000
C	1.563000	-0.000000	0.440000
H	1.682000	-0.876000	1.089000
H	1.682000	0.875000	1.089000
C	2.661000	0.000000	-0.606000
H	2.540000	0.876000	-1.253000
H	2.540000	-0.875000	-1.253000
C	4.049000	-0.000000	0.003000
H	4.198000	-0.882000	0.632000
H	4.828000	0.000000	-0.762000
H	4.199000	0.881000	0.633000
C	-2.659000	1.249000	-0.419000
H	-2.423000	2.155000	0.145000
H	-2.083000	1.271000	-1.347000
H	-3.716000	1.284000	-0.688000

Total Energy: -315.604509563

1g2g

C	2.139000	-0.031000	1.386000
H	1.165000	0.250000	1.795000
H	2.359000	-1.049000	1.718000
H	2.884000	0.636000	1.823000
C	2.144000	0.073000	-0.128000
H	3.161000	-0.155000	-0.469000
C	1.238000	-0.975000	-0.780000
H	1.123000	-0.724000	-1.841000
H	1.764000	-1.935000	-0.751000
C	-0.137000	-1.195000	-0.169000
H	-0.030000	-1.528000	0.868000
H	-0.606000	-2.031000	-0.700000
C	-1.089000	-0.015000	-0.213000
H	-1.095000	0.418000	-1.220000
H	-0.740000	0.777000	0.456000
C	-2.503000	-0.395000	0.181000
H	-2.487000	-0.850000	1.178000
H	-2.869000	-1.171000	-0.500000
C	-3.451000	0.788000	0.171000
H	-3.496000	1.242000	-0.822000
H	-4.465000	0.496000	0.452000
H	-3.119000	1.559000	0.871000
C	1.847000	1.495000	-0.577000
H	1.855000	1.572000	-1.667000
H	0.874000	1.838000	-0.226000
H	2.600000	2.184000	-0.186000

Total Energy: -315.601271504

1g2g3g

C	-2.432000	-0.021000	-0.980000
H	-1.658000	-0.137000	-1.743000
H	-2.973000	-0.968000	-0.908000
H	-3.130000	0.742000	-1.332000
C	-1.827000	0.376000	0.354000
H	-2.657000	0.545000	1.051000
C	-0.989000	-0.749000	0.967000
H	-0.430000	-0.348000	1.817000
H	-1.681000	-1.487000	1.386000
C	-0.047000	-1.507000	0.041000
H	-0.632000	-1.985000	-0.749000
H	0.397000	-2.325000	0.619000
C	1.081000	-0.710000	-0.594000
H	0.676000	0.039000	-1.280000
H	1.678000	-1.386000	-1.216000
C	2.000000	-0.033000	0.404000
H	2.403000	-0.787000	1.088000
H	1.426000	0.663000	1.021000
C	3.134000	0.711000	-0.273000
H	2.745000	1.489000	-0.936000
H	3.794000	1.191000	0.452000
H	3.738000	0.033000	-0.882000
C	-1.086000	1.698000	0.243000
H	-0.670000	1.998000	1.207000
H	-0.266000	1.648000	-0.474000
H	-1.763000	2.489000	-0.090000

Total Energy: -315.601152141

1g2g3g4g

C	2.562000	-0.594000	0.501000
H	2.002000	-0.706000	1.432000
H	2.786000	-1.595000	0.124000
H	3.508000	-0.104000	0.743000
C	1.779000	0.219000	-0.513000
H	2.424000	0.361000	-1.387000
C	0.543000	-0.529000	-1.021000
H	-0.076000	0.166000	-1.598000
H	0.886000	-1.285000	-1.735000
C	-0.315000	-1.251000	0.008000
H	0.301000	-1.979000	0.542000
H	-1.058000	-1.842000	-0.537000
C	-1.039000	-0.382000	1.026000
H	-0.315000	0.081000	1.701000
H	-1.659000	-1.034000	1.652000
C	-1.925000	0.693000	0.419000
H	-1.310000	1.410000	-0.131000
H	-2.397000	1.258000	1.228000
C	-2.996000	0.136000	-0.500000
H	-3.604000	-0.612000	0.018000
H	-3.664000	0.923000	-0.855000
H	-2.559000	-0.347000	-1.376000
C	1.477000	1.608000	0.027000
H	0.931000	2.206000	-0.706000
H	0.880000	1.570000	0.939000
H	2.405000	2.135000	0.264000

Total Energy: -315.600667495

1g2g4g

C	-1.833000	1.482000	0.374000
H	-0.898000	1.531000	0.937000
H	-1.772000	2.208000	-0.440000
H	-2.638000	1.793000	1.045000
C	-2.080000	0.079000	-0.150000
H	-3.060000	0.081000	-0.642000
C	-1.070000	-0.318000	-1.229000
H	-1.171000	-1.391000	-1.424000
H	-1.357000	0.189000	-2.156000
C	0.394000	0.005000	-0.972000
H	0.509000	1.085000	-0.848000
H	0.956000	-0.250000	-1.877000
C	1.037000	-0.715000	0.200000
H	0.749000	-1.771000	0.172000
H	0.651000	-0.316000	1.142000
C	2.552000	-0.603000	0.209000
H	2.949000	-1.032000	-0.717000
H	2.952000	-1.211000	1.026000
C	3.044000	0.825000	0.359000
H	2.634000	1.282000	1.264000
H	4.133000	0.867000	0.427000
H	2.742000	1.443000	-0.489000
C	-2.173000	-0.919000	0.993000
H	-2.349000	-1.930000	0.619000
H	-1.261000	-0.939000	1.590000
H	-2.998000	-0.659000	1.661000

Total Energy: -315.600666298

1g3g

C	-2.457000	1.338000	0.408000
H	-2.172000	1.110000	1.438000
H	-1.932000	2.249000	0.109000
H	-3.529000	1.547000	0.403000
C	-2.125000	0.180000	-0.517000
H	-2.497000	0.435000	-1.516000
C	-0.620000	-0.027000	-0.652000
H	-0.439000	-0.840000	-1.365000
H	-0.187000	0.874000	-1.097000
C	0.107000	-0.347000	0.642000
H	-0.381000	-1.193000	1.135000
H	0.026000	0.500000	1.330000
C	1.575000	-0.678000	0.438000
H	1.663000	-1.539000	-0.235000
H	2.011000	-0.992000	1.392000
C	2.399000	0.470000	-0.115000
H	2.261000	1.349000	0.525000
H	2.028000	0.750000	-1.104000
C	3.873000	0.128000	-0.208000
H	4.031000	-0.737000	-0.858000
H	4.458000	0.958000	-0.610000
H	4.278000	-0.123000	0.776000
C	-2.841000	-1.083000	-0.072000
H	-2.601000	-1.927000	-0.724000
H	-2.562000	-1.357000	0.948000
H	-3.924000	-0.942000	-0.087000

Total Energy: -315.603661452

1g3g4g

C	1.984000	1.512000	-0.277000
H	1.657000	1.369000	-1.309000
H	1.343000	2.272000	0.177000
H	3.003000	1.902000	-0.306000
C	1.925000	0.206000	0.498000
H	2.327000	0.396000	1.500000
C	0.490000	-0.276000	0.688000
H	0.499000	-1.175000	1.315000
H	-0.055000	0.486000	1.254000
C	-0.263000	-0.581000	-0.593000
H	0.300000	-1.304000	-1.187000
H	-0.336000	0.323000	-1.203000
C	-1.656000	-1.137000	-0.346000
H	-1.570000	-2.102000	0.166000
H	-2.132000	-1.341000	-1.311000
C	-2.565000	-0.226000	0.465000
H	-2.177000	-0.128000	1.483000
H	-3.544000	-0.703000	0.561000
C	-2.732000	1.151000	-0.149000
H	-3.085000	1.078000	-1.181000
H	-3.452000	1.751000	0.410000
H	-1.787000	1.699000	-0.164000
C	2.802000	-0.846000	-0.157000
H	2.753000	-1.795000	0.382000
H	2.495000	-1.029000	-1.189000
H	3.846000	-0.523000	-0.180000

Total Energy: -315.603617882

1g4g

C	2.545000	-0.587000	1.132000
H	1.847000	-0.164000	1.859000
H	2.480000	-1.676000	1.200000
H	3.551000	-0.289000	1.433000
C	2.231000	-0.101000	-0.272000
H	3.000000	-0.501000	-0.942000
C	0.894000	-0.633000	-0.775000
H	0.757000	-0.314000	-1.815000
H	0.935000	-1.728000	-0.795000
C	-0.321000	-0.207000	0.026000
H	-0.372000	0.884000	0.065000
H	-0.227000	-0.549000	1.062000
C	-1.610000	-0.756000	-0.556000
H	-1.518000	-1.843000	-0.653000
H	-1.738000	-0.368000	-1.573000
C	-2.846000	-0.429000	0.265000
H	-2.726000	-0.841000	1.272000
H	-3.710000	-0.937000	-0.173000
C	-3.134000	1.059000	0.355000
H	-3.226000	1.497000	-0.643000
H	-4.065000	1.252000	0.892000
H	-2.336000	1.591000	0.877000
C	2.304000	1.415000	-0.342000
H	2.064000	1.778000	-1.344000
H	1.603000	1.875000	0.359000
H	3.304000	1.769000	-0.084000

Total Energy: -315.603819653

2g

C	3.166000	-0.047000	-0.853000
H	3.797000	-0.496000	-0.080000
H	3.113000	-0.749000	-1.688000
H	3.662000	0.861000	-1.202000
C	1.786000	0.254000	-0.298000
H	1.194000	0.716000	-1.096000
C	1.098000	-1.039000	0.117000
H	1.045000	-1.699000	-0.756000
H	1.739000	-1.548000	0.847000
C	-0.294000	-0.876000	0.701000
H	-0.241000	-0.329000	1.647000
H	-0.691000	-1.866000	0.949000
C	-1.269000	-0.175000	-0.224000
H	-1.279000	-0.683000	-1.196000
H	-0.928000	0.847000	-0.421000
C	-2.679000	-0.125000	0.331000
H	-2.661000	0.372000	1.307000
H	-3.028000	-1.146000	0.516000
C	-3.646000	0.590000	-0.591000
H	-3.696000	0.094000	-1.564000
H	-4.657000	0.616000	-0.178000
H	-3.329000	1.622000	-0.764000
C	1.878000	1.237000	0.854000
H	0.893000	1.541000	1.212000
H	2.416000	0.789000	1.694000
H	2.418000	2.139000	0.555000

Total Energy: -315.605487439

2g3g

C	2.513000	1.350000	-0.326000
H	3.316000	0.820000	-0.846000
H	2.070000	2.057000	-1.030000
H	2.962000	1.919000	0.491000
C	1.479000	0.365000	0.189000
H	0.701000	0.935000	0.712000
C	0.830000	-0.367000	-0.976000
H	0.411000	0.374000	-1.663000
H	1.616000	-0.887000	-1.536000
C	-0.246000	-1.369000	-0.587000
H	0.211000	-2.211000	-0.061000
H	-0.683000	-1.784000	-1.502000
C	-1.358000	-0.789000	0.271000
H	-0.954000	-0.470000	1.238000
H	-2.084000	-1.578000	0.496000
C	-2.083000	0.378000	-0.369000
H	-2.451000	0.075000	-1.356000
H	-1.380000	1.197000	-0.545000
C	-3.235000	0.876000	0.481000
H	-2.881000	1.202000	1.463000
H	-3.749000	1.720000	0.015000
H	-3.971000	0.085000	0.645000
C	2.107000	-0.597000	1.180000
H	1.367000	-1.265000	1.625000
H	2.860000	-1.216000	0.682000
H	2.602000	-0.057000	1.990000

Total Energy: -315.605352812

2g3g4g

C	-2.457000	1.396000	-0.116000
H	-3.031000	1.321000	0.812000
H	-1.904000	2.337000	-0.091000
H	-3.168000	1.441000	-0.945000
C	-1.520000	0.210000	-0.255000
H	-0.975000	0.318000	-1.199000
C	-0.509000	0.210000	0.882000
H	0.011000	1.173000	0.885000
H	-1.057000	0.159000	1.830000
C	0.511000	-0.916000	0.837000
H	0.008000	-1.874000	0.999000
H	1.201000	-0.799000	1.677000
C	1.300000	-0.987000	-0.461000
H	0.630000	-1.268000	-1.280000
H	2.038000	-1.792000	-0.382000
C	2.015000	0.304000	-0.826000
H	1.279000	1.094000	-1.006000
H	2.540000	0.160000	-1.775000
C	3.000000	0.762000	0.232000
H	3.731000	-0.022000	0.449000
H	3.548000	1.649000	-0.092000
H	2.495000	1.009000	1.168000
C	-2.306000	-1.087000	-0.308000
H	-1.661000	-1.948000	-0.490000
H	-2.829000	-1.253000	0.639000
H	-3.056000	-1.057000	-1.102000

Total Energy: -315.605086932

2g4g

C	3.232000	-0.312000	-0.340000
H	3.681000	-0.179000	0.648000
H	3.355000	-1.360000	-0.623000
H	3.795000	0.300000	-1.048000
C	1.767000	0.082000	-0.312000
H	1.361000	-0.051000	-1.321000
C	1.000000	-0.833000	0.633000
H	1.130000	-1.868000	0.296000
H	1.467000	-0.772000	1.623000
C	-0.483000	-0.535000	0.759000
H	-0.621000	0.449000	1.215000
H	-0.933000	-1.254000	1.452000
C	-1.227000	-0.598000	-0.561000
H	-0.989000	-1.547000	-1.055000
H	-0.865000	0.192000	-1.227000
C	-2.734000	-0.467000	-0.417000
H	-3.104000	-1.268000	0.231000
H	-3.202000	-0.621000	-1.394000
C	-3.167000	0.878000	0.138000
H	-2.781000	1.694000	-0.479000
H	-4.255000	0.966000	0.165000
H	-2.799000	1.030000	1.154000
C	1.615000	1.542000	0.073000
H	0.578000	1.874000	0.011000
H	1.958000	1.702000	1.099000
H	2.211000	2.182000	-0.582000

Total Energy: -315.604868728

3g

C	-2.961000	1.253000	-0.045000
H	-2.765000	1.668000	0.949000
H	-2.724000	2.025000	-0.781000
H	-4.030000	1.038000	-0.109000
C	-2.130000	0.003000	-0.267000
H	-2.355000	-0.387000	-1.268000
C	-0.648000	0.340000	-0.225000
H	-0.450000	1.151000	-0.935000
H	-0.413000	0.740000	0.768000
C	0.269000	-0.825000	-0.546000
H	-0.084000	-1.307000	-1.464000
H	0.201000	-1.580000	0.244000
C	1.723000	-0.421000	-0.718000
H	1.803000	0.311000	-1.530000
H	2.306000	-1.293000	-1.034000
C	2.353000	0.157000	0.535000
H	2.221000	-0.551000	1.360000
H	1.823000	1.068000	0.828000
C	3.826000	0.466000	0.351000
H	3.974000	1.187000	-0.457000
H	4.269000	0.884000	1.257000
H	4.384000	-0.438000	0.091000
C	-2.495000	-1.062000	0.751000
H	-1.972000	-2.001000	0.566000
H	-2.234000	-0.725000	1.760000
H	-3.568000	-1.266000	0.735000

Total Energy: -315.605013100

3g4g

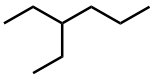
C	-2.891000	-0.509000	-0.928000
H	-2.631000	0.062000	-1.824000
H	-2.832000	-1.571000	-1.180000
H	-3.927000	-0.276000	-0.673000
C	-1.949000	-0.159000	0.210000
H	-2.240000	-0.745000	1.091000
C	-0.522000	-0.539000	-0.150000
H	-0.501000	-1.591000	-0.458000
H	-0.223000	0.041000	-1.031000
C	0.482000	-0.335000	0.968000
H	0.102000	-0.811000	1.878000
H	0.570000	0.729000	1.198000
C	1.857000	-0.900000	0.651000
H	1.780000	-1.987000	0.544000
H	2.522000	-0.718000	1.502000
C	2.495000	-0.322000	-0.603000
H	1.907000	-0.608000	-1.480000
H	3.480000	-0.779000	-0.738000
C	2.640000	1.187000	-0.559000
H	3.196000	1.500000	0.329000
H	3.171000	1.562000	-1.436000
H	1.666000	1.681000	-0.528000
C	-2.068000	1.314000	0.558000
H	-1.463000	1.579000	1.426000
H	-1.736000	1.928000	-0.284000
H	-3.104000	1.582000	0.777000

Total Energy: -315.604918714

4g

C	3.285000	-0.746000	-0.427000
H	3.551000	-1.098000	0.577000
H	3.121000	-1.629000	-1.053000
H	4.150000	-0.207000	-0.827000
C	2.045000	0.144000	-0.374000
H	1.815000	0.472000	-1.399000
C	0.842000	-0.653000	0.141000
H	0.749000	-1.571000	-0.456000
H	1.051000	-0.984000	1.169000
C	-0.489000	0.091000	0.107000
H	-0.660000	0.486000	-0.904000
H	-0.452000	0.963000	0.771000
C	-1.669000	-0.787000	0.512000
H	-1.491000	-1.197000	1.516000
H	-1.726000	-1.656000	-0.159000
C	-3.005000	-0.051000	0.498000
H	-2.974000	0.766000	1.231000
H	-3.796000	-0.731000	0.838000
C	-3.360000	0.505000	-0.877000
H	-3.427000	-0.296000	-1.621000
H	-4.320000	1.030000	-0.868000
H	-2.600000	1.213000	-1.225000
C	2.320000	1.385000	0.473000
H	1.484000	2.090000	0.460000
H	2.503000	1.105000	1.518000
H	3.206000	1.919000	0.114000

Total Energy: -315.604094973

3-ethylhexane 

C	0.962000	-2.550000	0.231000
H	1.362000	-2.567000	1.249000
H	-0.116000	-2.707000	0.298000
H	1.385000	-3.401000	-0.307000
C	1.296000	-1.243000	-0.460000
H	2.375000	-1.188000	-0.636000
H	0.831000	-1.221000	-1.451000
C	0.879000	0.001000	0.314000
H	1.439000	0.002000	1.259000
C	-0.600000	-0.001000	0.680000
H	-0.814000	0.870000	1.307000
H	-0.812000	-0.872000	1.307000
C	-1.552000	-0.002000	-0.500000
H	-1.361000	-0.876000	-1.129000
H	-1.363000	0.873000	-1.129000
C	-3.002000	-0.003000	-0.057000
H	-3.224000	0.878000	0.552000
H	-3.687000	-0.004000	-0.907000
H	-3.222000	-0.885000	0.551000
C	1.293000	1.246000	-0.460000
H	2.372000	1.193000	-0.635000
H	0.828000	1.223000	-1.451000
C	0.956000	2.552000	0.231000
H	1.356000	2.570000	1.249000
H	1.377000	3.404000	-0.307000
H	-0.123000	2.706000	0.298000

Total Energy: -315.604198881

1g

C	2.149000	-1.921000	-0.120000
H	2.104000	-2.294000	0.907000
H	1.400000	-2.461000	-0.701000
H	3.128000	-2.182000	-0.527000
C	1.921000	-0.422000	-0.159000
H	2.760000	0.082000	0.332000
H	1.924000	-0.081000	-1.199000
C	0.630000	0.026000	0.514000
H	0.633000	-0.389000	1.531000
C	-0.592000	-0.531000	-0.200000
H	-0.537000	-1.623000	-0.203000
H	-0.567000	-0.227000	-1.253000
C	-1.919000	-0.120000	0.408000
H	-2.045000	0.963000	0.332000
H	-1.910000	-0.351000	1.479000
C	-3.093000	-0.812000	-0.258000
H	-3.012000	-1.898000	-0.160000
H	-4.045000	-0.506000	0.179000
H	-3.125000	-0.580000	-1.325000
C	0.583000	1.545000	0.656000
H	-0.247000	1.820000	1.312000
H	1.494000	1.869000	1.170000
C	0.453000	2.297000	-0.656000
H	-0.478000	2.046000	-1.169000
H	0.455000	3.375000	-0.488000
H	1.276000	2.068000	-1.335000

Total Energy: -315.603626610

1g2g

C	0.768000	-2.493000	-0.213000
H	1.195000	-2.868000	0.721000
H	-0.318000	-2.564000	-0.127000
H	1.081000	-3.162000	-1.016000
C	1.215000	-1.067000	-0.471000
H	2.303000	-1.044000	-0.589000
H	0.799000	-0.715000	-1.419000
C	0.831000	-0.113000	0.650000
H	1.227000	-0.551000	1.575000
C	-0.684000	-0.001000	0.843000
H	-0.890000	0.877000	1.466000
H	-1.033000	-0.861000	1.424000
C	-1.535000	0.076000	-0.413000
H	-1.417000	-0.843000	-0.994000
H	-1.197000	0.886000	-1.060000
C	-3.002000	0.269000	-0.076000
H	-3.157000	1.203000	0.470000
H	-3.623000	0.298000	-0.974000
H	-3.366000	-0.545000	0.556000
C	1.527000	1.239000	0.514000
H	1.362000	1.806000	1.436000
H	2.605000	1.055000	0.459000
C	1.113000	2.097000	-0.668000
H	0.085000	2.448000	-0.568000
H	1.752000	2.980000	-0.742000
H	1.192000	1.553000	-1.611000

Total Energy: -315.600173497

1g2g4g

C	-0.177000	2.491000	0.047000
H	-0.468000	2.723000	1.075000
H	0.911000	2.402000	0.025000
H	-0.451000	3.343000	-0.578000
C	-0.852000	1.220000	-0.432000
H	-1.926000	1.400000	-0.519000
H	-0.505000	0.972000	-1.441000
C	-0.627000	0.022000	0.480000
H	-1.092000	0.257000	1.447000
C	0.851000	-0.238000	0.751000
H	0.935000	-1.111000	1.409000
H	1.271000	0.601000	1.314000
C	1.703000	-0.471000	-0.482000
H	1.651000	0.403000	-1.137000
H	1.303000	-1.310000	-1.058000
C	3.151000	-0.747000	-0.123000
H	3.233000	-1.636000	0.508000
H	3.765000	-0.909000	-1.011000
H	3.579000	0.091000	0.433000
C	-1.316000	-1.226000	-0.059000
H	-0.929000	-1.449000	-1.058000
H	-1.038000	-2.075000	0.574000
C	-2.828000	-1.120000	-0.116000
H	-3.155000	-0.362000	-0.829000
H	-3.278000	-2.068000	-0.418000
H	-3.236000	-0.854000	0.863000

Total Energy: -315.603579245

1g3g

C	-2.328000	-1.632000	0.038000
H	-2.037000	-2.213000	-0.842000
H	-1.885000	-2.112000	0.912000
H	-3.412000	-1.703000	0.140000
C	-1.883000	-0.188000	-0.099000
H	-2.442000	0.284000	-0.914000
H	-2.145000	0.360000	0.811000
C	-0.395000	-0.024000	-0.377000
H	-0.164000	-0.646000	-1.250000
C	0.442000	-0.528000	0.791000
H	0.229000	-1.590000	0.945000
H	0.118000	-0.018000	1.704000
C	1.943000	-0.359000	0.623000
H	2.440000	-0.744000	1.519000
H	2.195000	0.704000	0.573000
C	2.491000	-1.069000	-0.600000
H	2.089000	-0.646000	-1.522000
H	3.579000	-0.995000	-0.649000
H	2.228000	-2.130000	-0.583000
C	-0.059000	1.415000	-0.755000
H	0.973000	1.463000	-1.112000
H	-0.686000	1.700000	-1.606000
C	-0.246000	2.422000	0.365000
H	0.402000	2.199000	1.215000
H	-0.006000	3.431000	0.024000
H	-1.275000	2.434000	0.727000

Total Energy: -315.603388630

1g3g4g

C	1.790000	-2.074000	0.373000
H	1.455000	-2.138000	1.412000
H	1.176000	-2.757000	-0.215000
H	2.818000	-2.439000	0.332000
C	1.699000	-0.646000	-0.133000
H	2.450000	-0.045000	0.384000
H	1.960000	-0.612000	-1.198000
C	0.334000	0.001000	0.052000
H	0.116000	0.002000	1.129000
C	-0.748000	-0.805000	-0.654000
H	-0.760000	-1.817000	-0.241000
H	-0.469000	-0.906000	-1.710000
C	-2.156000	-0.240000	-0.559000
H	-2.839000	-0.924000	-1.072000
H	-2.221000	0.708000	-1.101000
C	-2.624000	-0.043000	0.871000
H	-2.029000	0.714000	1.386000
H	-3.668000	0.276000	0.908000
H	-2.536000	-0.972000	1.440000
C	0.338000	1.448000	-0.419000
H	0.519000	1.464000	-1.501000
H	-0.659000	1.871000	-0.273000
C	1.347000	2.336000	0.286000
H	2.374000	2.060000	0.047000
H	1.214000	3.382000	0.002000
H	1.229000	2.268000	1.371000

Total Energy: -315.603112713

1g4g

C	1.230000	2.447000	-0.195000
H	1.133000	2.468000	-1.284000
H	0.313000	2.861000	0.227000
H	2.047000	3.118000	0.079000
C	1.498000	1.036000	0.294000
H	2.499000	0.742000	-0.027000
H	1.511000	1.019000	1.391000
C	0.497000	-0.002000	-0.194000
H	0.524000	0.001000	-1.294000
C	-0.918000	0.353000	0.236000
H	-1.155000	1.362000	-0.114000
H	-0.954000	0.396000	1.332000
C	-2.001000	-0.583000	-0.267000
H	-1.880000	-1.574000	0.175000
H	-1.887000	-0.713000	-1.349000
C	-3.391000	-0.063000	0.044000
H	-3.558000	0.910000	-0.426000
H	-4.167000	-0.744000	-0.311000
H	-3.526000	0.065000	1.121000
C	0.881000	-1.400000	0.273000
H	0.817000	-1.431000	1.368000
H	0.139000	-2.112000	-0.095000
C	2.256000	-1.859000	-0.175000
H	3.055000	-1.285000	0.295000
H	2.418000	-2.910000	0.075000
H	2.365000	-1.755000	-1.258000

Total Energy: -315.603176865

2g

C	-2.216000	1.711000	-0.034000
H	-3.008000	0.965000	-0.123000
H	-2.209000	2.061000	1.002000
H	-2.486000	2.556000	-0.670000
C	-0.864000	1.143000	-0.421000
H	-0.906000	0.745000	-1.440000
H	-0.132000	1.954000	-0.446000
C	-0.359000	0.056000	0.518000
H	-0.221000	0.515000	1.506000
C	0.995000	-0.478000	0.074000
H	0.919000	-0.867000	-0.947000
H	1.260000	-1.333000	0.706000
C	2.125000	0.533000	0.132000
H	2.163000	0.970000	1.136000
H	1.924000	1.359000	-0.554000
C	3.466000	-0.087000	-0.209000
H	3.452000	-0.512000	-1.216000
H	4.274000	0.646000	-0.167000
H	3.710000	-0.896000	0.485000
C	-1.366000	-1.077000	0.694000
H	-0.936000	-1.813000	1.381000
H	-2.261000	-0.691000	1.188000
C	-1.767000	-1.768000	-0.596000
H	-0.903000	-2.194000	-1.110000
H	-2.467000	-2.583000	-0.399000
H	-2.255000	-1.076000	-1.285000

Total Energy: -315.603521872

2g3g

C	-1.498000	2.072000	0.020000
H	-2.481000	1.608000	0.126000
H	-1.194000	2.427000	1.009000
H	-1.613000	2.945000	-0.626000
C	-0.476000	1.103000	-0.541000
H	-0.818000	0.718000	-1.508000
H	0.451000	1.645000	-0.746000
C	-0.166000	-0.065000	0.382000
H	0.273000	0.351000	1.297000
C	0.855000	-1.011000	-0.235000
H	0.418000	-1.481000	-1.121000
H	1.048000	-1.820000	0.479000
C	2.180000	-0.375000	-0.623000
H	2.028000	0.333000	-1.442000
H	2.835000	-1.155000	-1.021000
C	2.875000	0.324000	0.531000
H	3.001000	-0.356000	1.378000
H	3.863000	0.684000	0.240000
H	2.301000	1.184000	0.883000
C	-1.420000	-0.824000	0.810000
H	-1.112000	-1.659000	1.449000
H	-2.035000	-0.175000	1.439000
C	-2.265000	-1.352000	-0.334000
H	-1.698000	-2.027000	-0.979000
H	-3.127000	-1.906000	0.043000
H	-2.644000	-0.540000	-0.958000

Total Energy: -315.603210846

2g3g4g

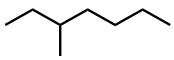
C	-1.346000	2.336000	0.286000
H	-2.374000	2.060000	0.047000
H	-1.228000	2.268000	1.371000
H	-1.214000	3.382000	0.002000
C	-0.338000	1.448000	-0.420000
H	-0.520000	1.464000	-1.501000
H	0.659000	1.871000	-0.274000
C	-0.334000	0.001000	0.052000
H	-0.116000	0.002000	1.128000
C	0.748000	-0.805000	-0.654000
H	0.469000	-0.906000	-1.710000
H	0.760000	-1.817000	-0.241000
C	2.156000	-0.240000	-0.559000
H	2.221000	0.707000	-1.101000
H	2.839000	-0.924000	-1.072000
C	2.624000	-0.043000	0.871000
H	2.536000	-0.972000	1.440000
H	3.668000	0.275000	0.908000
H	2.029000	0.714000	1.385000
C	-1.699000	-0.646000	-0.133000
H	-2.450000	-0.045000	0.384000
H	-1.960000	-0.613000	-1.198000
C	-1.790000	-2.073000	0.373000
H	-1.454000	-2.138000	1.412000
H	-2.818000	-2.439000	0.333000
H	-1.176000	-2.757000	-0.215000

Total Energy: -315.603112699

2g4g

C	2.256000	-1.860000	0.176000
H	3.055000	-1.285000	-0.294000
H	2.364000	-1.756000	1.259000
H	2.417000	-2.910000	-0.075000
C	0.881000	-1.400000	-0.274000
H	0.818000	-1.431000	-1.368000
H	0.139000	-2.111000	0.095000
C	0.497000	-0.002000	0.194000
H	0.524000	0.001000	1.293000
C	-0.918000	0.353000	-0.236000
H	-0.954000	0.395000	-1.333000
H	-1.155000	1.362000	0.113000
C	-2.001000	-0.582000	0.267000
H	-1.887000	-0.712000	1.350000
H	-1.880000	-1.574000	-0.175000
C	-3.391000	-0.063000	-0.044000
H	-3.526000	0.065000	-1.121000
H	-4.167000	-0.743000	0.312000
H	-3.558000	0.911000	0.425000
C	1.498000	1.036000	-0.295000
H	2.499000	0.741000	0.026000
H	1.510000	1.020000	-1.391000
C	1.230000	2.447000	0.195000
H	1.134000	2.468000	1.284000
H	2.047000	3.118000	-0.079000
H	0.313000	2.861000	-0.226000

Total Energy: -315.603176869



3-methylheptane

C	3.631000	-0.309000	0.355000
H	3.929000	0.671000	-0.019000
H	3.585000	-0.249000	1.446000
H	4.424000	-1.013000	0.094000
C	2.298000	-0.750000	-0.217000
H	2.097000	-1.782000	0.090000
H	2.349000	-0.762000	-1.312000
C	1.117000	0.114000	0.203000
H	1.087000	0.128000	1.301000
C	-0.181000	-0.507000	-0.290000
H	-0.171000	-0.521000	-1.387000
H	-0.208000	-1.556000	0.025000
C	-1.443000	0.178000	0.192000
H	-1.416000	0.263000	1.285000
H	-1.488000	1.202000	-0.191000
C	-2.704000	-0.554000	-0.222000
H	-2.673000	-1.575000	0.172000
H	-2.721000	-0.650000	-1.313000
C	-3.966000	0.140000	0.252000
H	-4.865000	-0.400000	-0.052000
H	-3.978000	0.224000	1.342000
H	-4.030000	1.152000	-0.156000
C	1.272000	1.543000	-0.285000
H	1.297000	1.566000	-1.380000
H	0.444000	2.172000	0.043000
H	2.193000	1.997000	0.081000

Total Energy: -315.604811241

1g

C	2.935000	-0.989000	-0.611000
H	2.205000	-1.696000	-1.010000
H	3.139000	-0.247000	-1.385000
H	3.861000	-1.539000	-0.432000
C	2.439000	-0.338000	0.668000
H	3.219000	0.322000	1.060000
H	2.280000	-1.112000	1.426000
C	1.152000	0.467000	0.518000
H	0.917000	0.874000	1.510000
C	-0.016000	-0.417000	0.107000
H	0.145000	-0.782000	-0.913000
H	-0.033000	-1.304000	0.751000
C	-1.368000	0.265000	0.177000
H	-1.513000	0.682000	1.181000
H	-1.396000	1.115000	-0.512000
C	-2.518000	-0.669000	-0.149000
H	-2.499000	-1.516000	0.545000
H	-2.364000	-1.091000	-1.148000
C	-3.867000	0.020000	-0.084000
H	-4.683000	-0.666000	-0.320000
H	-4.049000	0.426000	0.914000
H	-3.914000	0.852000	-0.791000
C	1.333000	1.639000	-0.431000
H	1.453000	1.293000	-1.461000
H	0.474000	2.310000	-0.408000
H	2.219000	2.222000	-0.168000

Total Energy: -315.603941424

1g2g3g

C	1.929000	1.687000	0.357000
H	1.303000	1.727000	1.251000
H	2.892000	1.262000	0.646000
H	2.107000	2.715000	0.035000
C	1.271000	0.881000	-0.747000
H	1.897000	0.917000	-1.644000
H	0.324000	1.354000	-1.020000
C	1.016000	-0.582000	-0.398000
H	0.480000	-1.021000	-1.247000
C	0.146000	-0.747000	0.841000
H	-0.057000	-1.815000	0.977000
H	0.719000	-0.436000	1.719000
C	-1.172000	0.006000	0.806000
H	-1.711000	-0.176000	1.742000
H	-0.985000	1.085000	0.774000
C	-2.069000	-0.374000	-0.356000
H	-2.218000	-1.460000	-0.353000
H	-1.569000	-0.139000	-1.300000
C	-3.409000	0.332000	-0.304000
H	-4.046000	0.056000	-1.147000
H	-3.944000	0.085000	0.617000
H	-3.277000	1.417000	-0.326000
C	2.312000	-1.354000	-0.229000
H	2.880000	-0.987000	0.629000
H	2.113000	-2.414000	-0.059000
H	2.946000	-1.265000	-1.115000

Total Energy: -315.604417988

1g2g

C	-1.809000	1.697000	-0.602000
H	-0.855000	1.737000	-1.132000
H	-2.547000	1.267000	-1.282000
H	-2.113000	2.725000	-0.396000
C	-1.697000	0.898000	0.683000
H	-2.647000	0.947000	1.225000
H	-0.953000	1.367000	1.333000
C	-1.335000	-0.572000	0.485000
H	-1.182000	-0.998000	1.484000
C	-0.041000	-0.761000	-0.292000
H	0.171000	-1.834000	-0.358000
H	-0.185000	-0.423000	-1.324000
C	1.161000	-0.057000	0.304000
H	1.002000	1.027000	0.295000
H	1.263000	-0.339000	1.359000
C	2.451000	-0.370000	-0.427000
H	2.339000	-0.100000	-1.483000
H	2.622000	-1.452000	-0.408000
C	3.648000	0.350000	0.162000
H	4.569000	0.112000	-0.374000
H	3.508000	1.433000	0.124000
H	3.790000	0.074000	1.210000
C	-2.464000	-1.340000	-0.180000
H	-2.639000	-0.979000	-1.196000
H	-2.224000	-2.403000	-0.247000
H	-3.397000	-1.237000	0.379000

Total Energy: -315.604620490

1g2g3g4g

C	-2.407000	-1.224000	0.125000
H	-1.865000	-1.644000	0.974000
H	-3.149000	-0.526000	0.517000
H	-2.947000	-2.042000	-0.357000
C	-1.466000	-0.548000	-0.855000
H	-2.035000	-0.202000	-1.724000
H	-0.754000	-1.286000	-1.235000
C	-0.698000	0.639000	-0.281000
H	-0.015000	0.983000	-1.066000
C	0.137000	0.266000	0.935000
H	0.689000	1.154000	1.258000
H	-0.533000	0.019000	1.764000
C	1.104000	-0.885000	0.716000
H	1.678000	-1.041000	1.636000
H	0.542000	-1.808000	0.549000
C	2.074000	-0.677000	-0.437000
H	1.520000	-0.626000	-1.379000
H	2.722000	-1.554000	-0.515000
C	2.926000	0.568000	-0.284000
H	3.660000	0.650000	-1.088000
H	2.317000	1.474000	-0.301000
H	3.470000	0.555000	0.665000
C	-1.622000	1.795000	0.057000
H	-2.306000	1.529000	0.866000
H	-1.051000	2.666000	0.386000
H	-2.223000	2.090000	-0.807000

Total Energy: -315.604167200

2g

C	-3.001000	-1.362000	-0.096000
H	-3.798000	-0.674000	0.190000
H	-3.026000	-1.465000	-1.184000
H	-3.238000	-2.337000	0.335000
C	-1.641000	-0.876000	0.367000
H	-0.902000	-1.658000	0.177000
H	-1.652000	-0.720000	1.453000
C	-1.182000	0.414000	-0.299000
H	-1.134000	0.231000	-1.381000
C	0.208000	0.821000	0.165000
H	0.459000	1.784000	-0.293000
H	0.181000	0.999000	1.247000
C	1.311000	-0.168000	-0.156000
H	1.150000	-1.106000	0.384000
H	1.275000	-0.420000	-1.223000
C	2.691000	0.361000	0.186000
H	2.718000	0.628000	1.248000
H	2.866000	1.290000	-0.365000
C	3.792000	-0.635000	-0.122000
H	4.778000	-0.238000	0.127000
H	3.651000	-1.559000	0.444000
H	3.794000	-0.897000	-1.183000
C	-2.161000	1.548000	-0.051000
H	-2.276000	1.721000	1.023000
H	-1.802000	2.476000	-0.501000
H	-3.147000	1.337000	-0.464000

Total Energy: -315.604635606

2g3g

C	2.367000	1.713000	-0.064000
H	3.341000	1.224000	-0.112000
H	2.084000	1.989000	-1.084000
H	2.490000	2.635000	0.508000
C	1.315000	0.817000	0.561000
H	0.399000	1.395000	0.707000
H	1.640000	0.501000	1.559000
C	0.993000	-0.423000	-0.259000
H	0.627000	-0.089000	-1.238000
C	-0.095000	-1.262000	0.398000
H	-0.301000	-2.123000	-0.247000
H	0.305000	-1.671000	1.333000
C	-1.400000	-0.540000	0.685000
H	-2.108000	-1.253000	1.121000
H	-1.248000	0.230000	1.448000
C	-2.035000	0.092000	-0.539000
H	-2.134000	-0.666000	-1.324000
H	-1.370000	0.862000	-0.942000
C	-3.389000	0.702000	-0.236000
H	-3.835000	1.161000	-1.121000
H	-4.084000	-0.056000	0.136000
H	-3.304000	1.474000	0.534000
C	2.224000	-1.281000	-0.488000
H	2.664000	-1.579000	0.469000
H	1.966000	-2.192000	-1.033000
H	2.990000	-0.756000	-1.060000

Total Energy: -315.604560445

2g3g4g

C	-2.619000	-1.224000	-0.482000
H	-3.406000	-0.477000	-0.593000
H	-2.231000	-1.448000	-1.480000
H	-3.080000	-2.134000	-0.093000
C	-1.507000	-0.740000	0.430000
H	-0.813000	-1.565000	0.610000
H	-1.919000	-0.467000	1.409000
C	-0.732000	0.449000	-0.117000
H	-0.303000	0.151000	-1.081000
C	0.406000	0.848000	0.811000
H	0.918000	1.713000	0.377000
H	-0.024000	1.198000	1.756000
C	1.424000	-0.243000	1.104000
H	2.228000	0.186000	1.712000
H	0.965000	-1.022000	1.718000
C	2.031000	-0.878000	-0.137000
H	1.253000	-1.403000	-0.699000
H	2.748000	-1.644000	0.174000
C	2.723000	0.123000	-1.043000
H	3.207000	-0.372000	-1.887000
H	2.016000	0.850000	-1.447000
H	3.489000	0.678000	-0.496000
C	-1.635000	1.646000	-0.357000
H	-2.134000	1.938000	0.572000
H	-1.056000	2.503000	-0.708000
H	-2.405000	1.437000	-1.101000

Total Energy: -315.604390441

2g4g

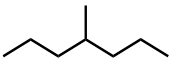
C	-3.110000	-1.062000	0.128000
H	-3.734000	-0.267000	0.540000
H	-3.318000	-1.125000	-0.943000
H	-3.431000	-2.000000	0.585000
C	-1.635000	-0.808000	0.376000
H	-1.068000	-1.690000	0.068000
H	-1.455000	-0.686000	1.451000
C	-1.085000	0.413000	-0.345000
H	-1.229000	0.256000	-1.423000
C	0.407000	0.582000	-0.097000
H	0.742000	1.500000	-0.593000
H	0.563000	0.743000	0.976000
C	1.267000	-0.570000	-0.581000
H	1.079000	-1.460000	0.028000
H	0.969000	-0.827000	-1.604000
C	2.755000	-0.264000	-0.552000
H	2.955000	0.603000	-1.191000
H	3.302000	-1.103000	-0.993000
C	3.285000	0.002000	0.844000
H	4.366000	0.153000	0.838000
H	2.830000	0.892000	1.282000
H	3.068000	-0.841000	1.507000
C	-1.821000	1.678000	0.056000
H	-1.747000	1.834000	1.136000
H	-1.389000	2.552000	-0.437000
H	-2.879000	1.638000	-0.206000

Total Energy: -315.603987075

4g

C	-3.417000	-0.751000	-0.240000
H	-3.899000	0.189000	0.034000
H	-3.394000	-0.807000	-1.332000
H	-4.052000	-1.561000	0.122000
C	-2.017000	-0.854000	0.333000
H	-1.621000	-1.857000	0.139000
H	-2.054000	-0.747000	1.424000
C	-1.032000	0.166000	-0.221000
H	-1.008000	0.047000	-1.313000
C	0.365000	-0.124000	0.308000
H	0.370000	0.030000	1.395000
H	0.576000	-1.186000	0.150000
C	1.467000	0.706000	-0.320000
H	1.445000	0.567000	-1.407000
H	1.275000	1.767000	-0.140000
C	2.855000	0.367000	0.199000
H	2.874000	0.500000	1.286000
H	3.572000	1.086000	-0.209000
C	3.309000	-1.039000	-0.149000
H	4.335000	-1.217000	0.180000
H	2.679000	-1.796000	0.321000
H	3.272000	-1.201000	-1.230000
C	-1.468000	1.585000	0.095000
H	-1.507000	1.734000	1.178000
H	-0.779000	2.321000	-0.321000
H	-2.458000	1.801000	-0.309000

Total Energy: -315.603865456

4-methylheptane 

C	0.449000	-0.580000	3.740000
H	-0.289000	-1.382000	3.822000
H	1.431000	-1.048000	3.633000
H	0.443000	-0.024000	4.680000
C	0.144000	0.315000	2.554000
H	0.883000	1.121000	2.498000
H	-0.825000	0.797000	2.706000
C	0.144000	-0.450000	1.245000
H	1.090000	-0.996000	1.159000
H	-0.645000	-1.213000	1.270000
C	-0.040000	0.404000	-0.000000
H	0.748000	1.170000	-0.000000
C	0.144000	-0.450000	-1.245000
H	-0.645000	-1.213000	-1.270000
H	1.090000	-0.996000	-1.159000
C	0.144000	0.315000	-2.554000
H	0.883000	1.121000	-2.498000
H	-0.825000	0.797000	-2.706000
C	0.449000	-0.580000	-3.740000
H	-0.289000	-1.382000	-3.822000
H	0.443000	-0.024000	-4.680000
H	1.431000	-1.048000	-3.633000
C	-1.385000	1.107000	0.000000
H	-1.509000	1.740000	-0.879000
H	-2.195000	0.369000	0.000000
H	-1.509000	1.740000	0.879000

Total Energy: -315.604716351

1g

C	-3.029000	-0.346000	1.013000
H	-2.824000	-1.354000	1.386000
H	-2.459000	0.353000	1.628000
H	-4.089000	-0.139000	1.174000
C	-2.658000	-0.227000	-0.453000
H	-2.836000	0.796000	-0.795000
H	-3.322000	-0.862000	-1.048000
C	-1.221000	-0.626000	-0.742000
H	-1.098000	-1.692000	-0.520000
H	-1.023000	-0.512000	-1.815000
C	-0.158000	0.149000	0.025000
H	-0.302000	-0.037000	1.096000
C	1.221000	-0.374000	-0.346000
H	1.409000	-0.158000	-1.406000
H	1.218000	-1.466000	-0.256000
C	2.361000	0.178000	0.488000
H	2.140000	0.013000	1.548000
H	2.433000	1.260000	0.354000
C	3.690000	-0.461000	0.136000
H	3.936000	-0.292000	-0.916000
H	4.506000	-0.057000	0.739000
H	3.659000	-1.542000	0.295000
C	-0.277000	1.642000	-0.220000
H	0.484000	2.201000	0.326000
H	-0.158000	1.861000	-1.285000
H	-1.250000	2.024000	0.093000

Total Energy: -315.604517069

1g2g

C	-2.482000	-0.749000	-1.057000
H	-3.105000	0.145000	-1.136000
H	-1.630000	-0.617000	-1.725000
H	-3.061000	-1.596000	-1.431000
C	-2.043000	-0.985000	0.377000
H	-1.330000	-1.814000	0.407000
H	-2.908000	-1.318000	0.958000
C	-1.450000	0.221000	1.092000
H	-2.203000	1.016000	1.130000
H	-1.268000	-0.075000	2.131000
C	-0.148000	0.806000	0.542000
H	0.266000	1.426000	1.348000
C	0.874000	-0.280000	0.250000
H	0.532000	-0.882000	-0.600000
H	0.922000	-0.963000	1.106000
C	2.269000	0.237000	-0.042000
H	2.591000	0.884000	0.781000
H	2.252000	0.865000	-0.937000
C	3.270000	-0.887000	-0.233000
H	2.975000	-1.532000	-1.065000
H	4.271000	-0.506000	-0.445000
H	3.331000	-1.511000	0.662000
C	-0.357000	1.730000	-0.649000
H	0.546000	2.304000	-0.863000
H	-0.617000	1.178000	-1.552000
H	-1.161000	2.442000	-0.450000

Total Energy: -315.600357817

1g2g3g

C	-2.251000	-1.179000	-0.846000
H	-3.152000	-0.633000	-0.555000
H	-1.780000	-0.628000	-1.660000
H	-2.560000	-2.148000	-1.244000
C	-1.314000	-1.354000	0.335000
H	-0.377000	-1.801000	-0.012000
H	-1.750000	-2.084000	1.023000
C	-1.015000	-0.096000	1.137000
H	-1.955000	0.302000	1.534000
H	-0.425000	-0.395000	2.008000
C	-0.274000	1.040000	0.426000
H	0.129000	1.681000	1.220000
C	0.911000	0.548000	-0.389000
H	1.370000	1.405000	-0.895000
H	0.556000	-0.114000	-1.187000
C	1.972000	-0.166000	0.425000
H	1.536000	-1.037000	0.921000
H	2.314000	0.499000	1.225000
C	3.151000	-0.602000	-0.422000
H	3.623000	0.257000	-0.907000
H	3.913000	-1.110000	0.173000
H	2.830000	-1.288000	-1.210000
C	-1.184000	1.916000	-0.419000
H	-0.644000	2.798000	-0.772000
H	-1.559000	1.389000	-1.297000
H	-2.047000	2.259000	0.157000

Total Energy: -315.601112983

1g2g3g4g

C	-2.695000	-0.634000	-0.484000
H	-3.287000	-0.037000	0.214000
H	-2.403000	0.017000	-1.309000
H	-3.344000	-1.409000	-0.896000
C	-1.491000	-1.249000	0.206000
H	-0.853000	-1.730000	-0.541000
H	-1.838000	-2.056000	0.859000
C	-0.659000	-0.302000	1.059000
H	-1.301000	0.131000	1.834000
H	0.083000	-0.906000	1.591000
C	0.078000	0.836000	0.354000
H	0.812000	1.211000	1.076000
C	0.844000	0.364000	-0.872000
H	1.360000	1.227000	-1.311000
H	0.129000	0.024000	-1.628000
C	1.863000	-0.732000	-0.607000
H	2.330000	-1.014000	-1.555000
H	1.355000	-1.630000	-0.242000
C	2.939000	-0.327000	0.382000
H	2.524000	-0.144000	1.375000
H	3.699000	-1.105000	0.482000
H	3.440000	0.591000	0.060000
C	-0.812000	2.018000	0.003000
H	-0.206000	2.865000	-0.327000
H	-1.508000	1.781000	-0.801000
H	-1.398000	2.340000	0.867000

Total Energy: -315.600565946

2g

C	3.515000	-0.884000	0.114000
H	4.101000	-0.069000	-0.318000
H	3.626000	-0.828000	1.200000
H	3.955000	-1.826000	-0.218000
C	2.056000	-0.773000	-0.285000
H	1.503000	-1.621000	0.128000
H	1.963000	-0.846000	-1.374000
C	1.434000	0.529000	0.180000
H	1.448000	0.568000	1.277000
H	2.066000	1.358000	-0.158000
C	0.012000	0.778000	-0.302000
H	0.017000	0.725000	-1.399000
C	-0.947000	-0.287000	0.209000
H	-0.928000	-0.280000	1.306000
H	-0.586000	-1.274000	-0.095000
C	-2.378000	-0.136000	-0.271000
H	-2.382000	-0.048000	-1.363000
H	-2.804000	0.794000	0.113000
C	-3.249000	-1.302000	0.154000
H	-3.267000	-1.397000	1.243000
H	-4.279000	-1.183000	-0.187000
H	-2.867000	-2.243000	-0.251000
C	-0.433000	2.171000	0.106000
H	-1.405000	2.431000	-0.315000
H	-0.509000	2.242000	1.195000
H	0.287000	2.922000	-0.227000

Total Energy: -315.604609279

2g3g

C	-3.081000	-1.106000	-0.261000
H	-3.828000	-0.310000	-0.303000
H	-2.866000	-1.408000	-1.289000
H	-3.529000	-1.960000	0.252000
C	-1.820000	-0.629000	0.434000
H	-1.105000	-1.454000	0.496000
H	-2.049000	-0.346000	1.468000
C	-1.183000	0.549000	-0.275000
H	-0.889000	0.248000	-1.287000
H	-1.935000	1.335000	-0.406000
C	0.019000	1.145000	0.443000
H	-0.332000	1.516000	1.413000
C	1.107000	0.116000	0.732000
H	0.734000	-0.615000	1.456000
H	1.944000	0.624000	1.223000
C	1.630000	-0.629000	-0.482000
H	1.993000	0.082000	-1.228000
H	0.813000	-1.181000	-0.956000
C	2.743000	-1.593000	-0.116000
H	2.395000	-2.329000	0.613000
H	3.112000	-2.135000	-0.989000
H	3.587000	-1.062000	0.331000
C	0.562000	2.329000	-0.337000
H	1.414000	2.784000	0.175000
H	0.893000	2.026000	-1.333000
H	-0.205000	3.096000	-0.467000

Total Energy: -315.604600611

2g3g4g

C	3.041000	0.208000	-0.219000
H	3.478000	-0.691000	-0.661000
H	2.832000	0.905000	-1.035000
H	3.794000	0.665000	0.426000
C	1.773000	-0.123000	0.542000
H	1.365000	0.790000	0.984000
H	2.004000	-0.790000	1.380000
C	0.730000	-0.782000	-0.338000
H	0.523000	-0.148000	-1.207000
H	1.150000	-1.709000	-0.744000
C	-0.576000	-1.108000	0.367000
H	-0.329000	-1.710000	1.251000
C	-1.327000	0.123000	0.875000
H	-0.746000	0.607000	1.666000
H	-2.242000	-0.237000	1.354000
C	-1.689000	1.166000	-0.180000
H	-2.648000	1.619000	0.084000
H	-1.851000	0.677000	-1.145000
C	-0.667000	2.279000	-0.339000
H	0.300000	1.905000	-0.675000
H	-1.005000	3.023000	-1.063000
H	-0.507000	2.792000	0.614000
C	-1.461000	-1.957000	-0.530000
H	-2.398000	-2.216000	-0.033000
H	-1.708000	-1.430000	-1.455000
H	-0.956000	-2.884000	-0.809000

Total Energy: -315.601363110

n-octane 

C	-3.361000	2.907000	0.000000
H	-3.016000	3.454000	0.881000
H	-3.016000	3.454000	-0.881000
H	-4.452000	2.927000	0.000000
C	-2.824000	1.489000	0.000000
H	-3.201000	0.949000	-0.875000
H	-3.201000	0.950000	0.876000
C	-1.309000	1.437000	0.000000
H	-0.928000	1.976000	-0.876000
H	-0.928000	1.976000	0.875000
C	-0.757000	0.026000	0.000000
H	-1.138000	-0.513000	-0.875000
H	-1.138000	-0.513000	0.876000
C	0.757000	-0.026000	-0.000000
H	1.138000	0.513000	-0.876000
H	1.138000	0.513000	0.875000
C	1.309000	-1.437000	-0.000000
H	0.928000	-1.976000	-0.875000
H	0.928000	-1.976000	0.876000
C	2.824000	-1.489000	-0.000000
H	3.201000	-0.950000	-0.876000
H	3.201000	-0.949000	0.875000
C	3.361000	-2.907000	-0.000000
H	3.016000	-3.454000	-0.881000
H	4.452000	-2.927000	-0.000000
H	3.016000	-3.454000	0.881000

Total Energy: -315.603915580

1g

C	-3.661000	1.035000	-0.300000
H	-2.951000	1.822000	-0.044000
H	-3.667000	0.935000	-1.389000
H	-4.652000	1.372000	0.010000
C	-3.296000	-0.283000	0.358000
H	-4.083000	-1.016000	0.157000
H	-3.267000	-0.155000	1.445000
C	-1.964000	-0.844000	-0.112000
H	-1.814000	-1.835000	0.329000
H	-1.998000	-0.994000	-1.197000
C	-0.772000	0.028000	0.232000
H	-0.767000	0.224000	1.311000
H	-0.869000	1.004000	-0.254000
C	0.550000	-0.593000	-0.172000
H	0.659000	-1.566000	0.321000
H	0.539000	-0.799000	-1.248000
C	1.746000	0.275000	0.161000
H	1.756000	0.483000	1.237000
H	1.638000	1.248000	-0.334000
C	3.069000	-0.346000	-0.241000
H	3.174000	-1.317000	0.254000
H	3.056000	-0.553000	-1.316000
C	4.256000	0.535000	0.098000
H	4.301000	0.731000	1.172000
H	5.200000	0.074000	-0.198000
H	4.182000	1.500000	-0.409000

Total Energy: -315.603161050

1g2g

C	-2.914000	1.321000	-0.468000
H	-1.946000	1.611000	-0.883000
H	-3.519000	0.928000	-1.289000
H	-3.398000	2.227000	-0.098000
C	-2.758000	0.289000	0.632000
H	-3.732000	0.099000	1.094000
H	-2.122000	0.692000	1.425000
C	-2.187000	-1.032000	0.139000
H	-2.098000	-1.720000	0.986000
H	-2.901000	-1.488000	-0.556000
C	-0.836000	-0.916000	-0.546000
H	-0.934000	-0.333000	-1.467000
H	-0.508000	-1.913000	-0.857000
C	0.240000	-0.293000	0.322000
H	-0.039000	0.734000	0.581000
H	0.302000	-0.838000	1.271000
C	1.601000	-0.281000	-0.342000
H	1.534000	0.254000	-1.297000
H	1.893000	-1.308000	-0.592000
C	2.680000	0.354000	0.512000
H	2.386000	1.380000	0.757000
H	2.743000	-0.180000	1.466000
C	4.037000	0.357000	-0.166000
H	4.000000	0.910000	-1.108000
H	4.802000	0.818000	0.462000
H	4.360000	-0.662000	-0.395000

Total Energy: -315.602986650

1g2g3g

C	3.045000	-0.819000	-0.703000
H	2.608000	-0.295000	-1.555000
H	3.931000	-0.258000	-0.390000
H	3.376000	-1.799000	-1.053000
C	2.055000	-0.945000	0.439000
H	2.493000	-1.556000	1.234000
H	1.169000	-1.487000	0.096000
C	1.640000	0.395000	1.024000
H	0.949000	0.224000	1.855000
H	2.521000	0.882000	1.456000
C	1.001000	1.343000	0.019000
H	1.752000	1.662000	-0.709000
H	0.685000	2.250000	0.545000
C	-0.191000	0.757000	-0.719000
H	-0.579000	1.505000	-1.418000
H	0.132000	-0.089000	-1.334000
C	-1.314000	0.305000	0.193000
H	-1.611000	1.137000	0.844000
H	-0.958000	-0.487000	0.859000
C	-2.526000	-0.198000	-0.566000
H	-2.892000	0.596000	-1.226000
H	-2.220000	-1.020000	-1.222000
C	-3.641000	-0.660000	0.351000
H	-3.977000	0.156000	0.997000
H	-4.506000	-1.019000	-0.211000
H	-3.301000	-1.473000	0.998000

Total Energy: -315.602845355

1g2g3g4g

C	3.300000	-0.012000	-0.404000
H	3.012000	1.030000	-0.555000
H	3.873000	-0.065000	0.526000
H	3.965000	-0.292000	-1.223000
C	2.087000	-0.921000	-0.343000
H	2.414000	-1.963000	-0.290000
H	1.516000	-0.830000	-1.272000
C	1.180000	-0.632000	0.843000
H	0.347000	-1.341000	0.837000
H	1.735000	-0.821000	1.768000
C	0.635000	0.787000	0.881000
H	1.456000	1.491000	1.045000
H	-0.022000	0.890000	1.749000
C	-0.116000	1.195000	-0.377000
H	-0.509000	2.208000	-0.241000
H	0.584000	1.252000	-1.216000
C	-1.260000	0.267000	-0.749000
H	-0.870000	-0.728000	-0.988000
H	-1.732000	0.632000	-1.668000
C	-2.319000	0.136000	0.328000
H	-1.874000	-0.287000	1.233000
H	-2.678000	1.134000	0.603000
C	-3.484000	-0.728000	-0.113000
H	-3.145000	-1.735000	-0.371000
H	-4.240000	-0.821000	0.670000
H	-3.969000	-0.308000	-0.998000

Total Energy: -315.602593435

1g2g3g4g5g

C	-3.241000	-0.433000	-0.282000
H	-2.731000	-1.331000	-0.637000
H	-3.711000	-0.678000	0.675000
H	-4.035000	-0.202000	-0.995000
C	-2.279000	0.729000	-0.130000
H	-2.838000	1.632000	0.132000
H	-1.803000	0.937000	-1.092000
C	-1.213000	0.491000	0.928000
H	-0.577000	1.378000	0.999000
H	-1.698000	0.386000	1.904000
C	-0.347000	-0.734000	0.676000
H	-0.957000	-1.637000	0.761000
H	0.401000	-0.805000	1.471000
C	0.347000	-0.734000	-0.676000
H	0.957000	-1.637000	-0.761000
H	-0.401000	-0.805000	-1.471000
C	1.213000	0.491000	-0.928000
H	0.577000	1.378000	-0.999000
H	1.698000	0.386000	-1.904000
C	2.279000	0.729000	0.130000
H	2.838000	1.632000	-0.132000
H	1.803000	0.937000	1.092000
C	3.241000	-0.433000	0.282000
H	3.711000	-0.678000	-0.675000
H	4.035000	-0.202000	0.995000
H	2.731000	-1.331000	0.637000

Total Energy: -315.602309615

1g2g3g5g

C	-2.685000	1.221000	-0.489000
H	-2.123000	1.075000	-1.414000
H	-3.641000	0.701000	-0.600000
H	-2.894000	2.288000	-0.395000
C	-1.922000	0.698000	0.712000
H	-2.468000	0.945000	1.627000
H	-0.960000	1.214000	0.787000
C	-1.692000	-0.804000	0.670000
H	-1.159000	-1.110000	1.575000
H	-2.661000	-1.313000	0.701000
C	-0.928000	-1.284000	-0.556000
H	-1.548000	-1.148000	-1.447000
H	-0.757000	-2.361000	-0.465000
C	0.405000	-0.586000	-0.767000
H	0.879000	-0.982000	-1.671000
H	0.232000	0.477000	-0.958000
C	1.362000	-0.747000	0.399000
H	1.458000	-1.813000	0.631000
H	0.937000	-0.276000	1.292000
C	2.739000	-0.158000	0.142000
H	3.397000	-0.406000	0.980000
H	3.174000	-0.635000	-0.743000
C	2.720000	1.348000	-0.049000
H	2.260000	1.840000	0.813000
H	3.729000	1.748000	-0.163000
H	2.150000	1.633000	-0.935000

Total Energy: -315.602260214

1g2g4g

C	2.538000	1.549000	-0.043000
H	1.484000	1.830000	-0.099000
H	2.873000	1.731000	0.982000
H	3.093000	2.219000	-0.702000
C	2.746000	0.097000	-0.429000
H	3.818000	-0.121000	-0.464000
H	2.371000	-0.070000	-1.443000
C	2.081000	-0.880000	0.529000
H	2.266000	-1.902000	0.182000
H	2.559000	-0.794000	1.510000
C	0.583000	-0.676000	0.688000
H	0.395000	0.298000	1.147000
H	0.194000	-1.421000	1.390000
C	-0.182000	-0.786000	-0.617000
H	0.119000	0.023000	-1.291000
H	0.101000	-1.719000	-1.115000
C	-1.690000	-0.743000	-0.444000
H	-2.004000	-1.560000	0.218000
H	-2.173000	-0.930000	-1.409000
C	-2.207000	0.571000	0.111000
H	-1.788000	0.743000	1.106000
H	-1.845000	1.391000	-0.519000
C	-3.721000	0.610000	0.187000
H	-4.099000	-0.191000	0.828000
H	-4.083000	1.558000	0.589000
H	-4.165000	0.474000	-0.803000

Total Energy: -315.602407126

1g2g5g

C	2.933000	1.179000	0.396000
H	2.074000	1.436000	1.020000
H	3.651000	0.649000	1.028000
H	3.396000	2.113000	0.073000
C	2.522000	0.326000	-0.789000
H	3.384000	0.175000	-1.445000
H	1.779000	0.862000	-1.386000
C	1.971000	-1.034000	-0.387000
H	1.695000	-1.587000	-1.291000
H	2.767000	-1.610000	0.097000
C	0.769000	-0.974000	0.541000
H	1.061000	-0.539000	1.502000
H	0.441000	-1.995000	0.763000
C	-0.402000	-0.194000	-0.023000
H	-0.117000	0.854000	-0.169000
H	-0.646000	-0.584000	-1.016000
C	-1.623000	-0.249000	0.875000
H	-1.332000	0.066000	1.883000
H	-1.957000	-1.289000	0.964000
C	-2.781000	0.610000	0.396000
H	-3.579000	0.585000	1.144000
H	-2.451000	1.653000	0.335000
C	-3.340000	0.175000	-0.946000
H	-3.649000	-0.874000	-0.915000
H	-4.210000	0.771000	-1.227000
H	-2.600000	0.278000	-1.741000

Total Energy: -315.602280460

1g3g

C	-3.443000	-0.882000	-0.639000
H	-3.159000	-0.361000	-1.555000
H	-2.970000	-1.868000	-0.658000
H	-4.524000	-1.030000	-0.666000
C	-3.021000	-0.108000	0.597000
H	-3.410000	-0.611000	1.488000
H	-3.481000	0.886000	0.581000
C	-1.515000	0.042000	0.728000
H	-1.281000	0.531000	1.679000
H	-1.062000	-0.954000	0.774000
C	-0.884000	0.841000	-0.398000
H	-1.438000	1.780000	-0.514000
H	-0.995000	0.301000	-1.344000
C	0.586000	1.149000	-0.175000
H	0.944000	1.803000	-0.977000
H	0.700000	1.716000	0.756000
C	1.469000	-0.082000	-0.119000
H	1.310000	-0.683000	-1.023000
H	1.175000	-0.716000	0.723000
C	2.943000	0.253000	0.006000
H	3.243000	0.878000	-0.841000
H	3.096000	0.863000	0.903000
C	3.820000	-0.982000	0.070000
H	3.698000	-1.592000	-0.829000
H	4.877000	-0.724000	0.159000
H	3.554000	-1.605000	0.928000

Total Energy: -315.602513169

1g4g

C	-3.341000	-1.099000	0.554000
H	-2.496000	-1.746000	0.795000
H	-3.594000	-0.535000	1.456000
H	-4.191000	-1.741000	0.313000
C	-3.016000	-0.160000	-0.593000
H	-3.915000	0.400000	-0.867000
H	-2.737000	-0.744000	-1.477000
C	-1.900000	0.820000	-0.273000
H	-1.783000	1.519000	-1.108000
H	-2.187000	1.425000	0.595000
C	-0.561000	0.161000	0.001000
H	-0.312000	-0.497000	-0.837000
H	-0.633000	-0.480000	0.885000
C	0.550000	1.172000	0.216000
H	0.674000	1.768000	-0.695000
H	0.240000	1.872000	0.998000
C	1.882000	0.553000	0.597000
H	1.763000	-0.025000	1.522000
H	2.599000	1.348000	0.827000
C	2.477000	-0.343000	-0.474000
H	1.805000	-1.183000	-0.669000
H	2.544000	0.220000	-1.412000
C	3.846000	-0.870000	-0.090000
H	3.794000	-1.450000	0.835000
H	4.264000	-1.514000	-0.865000
H	4.547000	-0.048000	0.077000

Total Energy: -315.602478816

1g5g

C	3.595000	0.546000	0.823000
H	3.000000	1.458000	0.888000
H	3.460000	-0.005000	1.759000
H	4.644000	0.841000	0.758000
C	3.186000	-0.305000	-0.365000
H	3.868000	-1.156000	-0.451000
H	3.300000	0.275000	-1.287000
C	1.759000	-0.820000	-0.276000
H	1.568000	-1.500000	-1.113000
H	1.648000	-1.419000	0.636000
C	0.707000	0.272000	-0.284000
H	0.853000	0.907000	-1.166000
H	0.837000	0.923000	0.585000
C	-0.707000	-0.272000	-0.284000
H	-0.853000	-0.907000	-1.166000
H	-0.837000	-0.923000	0.585000
C	-1.759000	0.820000	-0.276000
H	-1.568000	1.500000	-1.113000
H	-1.648000	1.419000	0.636000
C	-3.186000	0.305000	-0.365000
H	-3.868000	1.156000	-0.451000
H	-3.300000	-0.275000	-1.287000
C	-3.595000	-0.546000	0.823000
H	-3.460000	0.005000	1.759000
H	-4.644000	-0.841000	0.758000
H	-3.000000	-1.458000	0.888000

Total Energy: -315.602415938

2g

C	4.067000	-0.716000	0.039000
H	4.691000	0.135000	-0.246000
H	4.155000	-0.840000	1.121000
H	4.480000	-1.608000	-0.435000
C	2.623000	-0.484000	-0.361000
H	2.026000	-1.362000	-0.096000
H	2.550000	-0.381000	-1.449000
C	2.034000	0.752000	0.293000
H	2.056000	0.627000	1.382000
H	2.683000	1.607000	0.072000
C	0.616000	1.070000	-0.148000
H	0.599000	1.212000	-1.235000
H	0.308000	2.026000	0.289000
C	-0.401000	0.011000	0.232000
H	-0.152000	-0.938000	-0.254000
H	-0.342000	-0.174000	1.311000
C	-1.819000	0.396000	-0.136000
H	-1.874000	0.593000	-1.213000
H	-2.079000	1.341000	0.356000
C	-2.842000	-0.659000	0.232000
H	-2.581000	-1.601000	-0.263000
H	-2.783000	-0.856000	1.308000
C	-4.256000	-0.259000	-0.140000
H	-4.341000	-0.084000	-1.215000
H	-4.981000	-1.029000	0.132000
H	-4.545000	0.666000	0.367000

Total Energy: -315.603193197

2g3g

C	-3.165000	-1.464000	0.047000
H	-4.052000	-1.012000	-0.404000
H	-2.714000	-2.119000	-0.704000
H	-3.494000	-2.089000	0.880000
C	-2.183000	-0.399000	0.493000
H	-1.321000	-0.875000	0.971000
H	-2.643000	0.235000	1.258000
C	-1.712000	0.469000	-0.657000
H	-1.203000	-0.160000	-1.395000
H	-2.587000	0.883000	-1.170000
C	-0.802000	1.610000	-0.235000
H	-1.370000	2.302000	0.396000
H	-0.505000	2.177000	-1.124000
C	0.449000	1.174000	0.511000
H	1.043000	2.061000	0.757000
H	0.172000	0.725000	1.470000
C	1.315000	0.200000	-0.261000
H	1.546000	0.620000	-1.247000
H	0.758000	-0.724000	-0.450000
C	2.605000	-0.142000	0.456000
H	3.171000	0.778000	0.636000
H	2.367000	-0.550000	1.445000
C	3.460000	-1.129000	-0.314000
H	3.728000	-0.729000	-1.295000
H	4.385000	-1.364000	0.216000
H	2.921000	-2.066000	-0.477000

Total Energy: -315.603075549

2g3g4g

C	3.174000	-1.273000	-0.132000
H	3.771000	-1.139000	0.774000
H	2.589000	-2.188000	-0.006000
H	3.861000	-1.428000	-0.966000
C	2.265000	-0.082000	-0.363000
H	1.704000	-0.226000	-1.291000
H	2.866000	0.823000	-0.508000
C	1.302000	0.140000	0.787000
H	0.673000	-0.749000	0.901000
H	1.874000	0.224000	1.717000
C	0.429000	1.373000	0.629000
H	1.067000	2.263000	0.619000
H	-0.214000	1.471000	1.508000
C	-0.429000	1.373000	-0.629000
H	-1.067000	2.263000	-0.619000
H	0.214000	1.471000	-1.508000
C	-1.302000	0.140000	-0.787000
H	-0.673000	-0.749000	-0.901000
H	-1.874000	0.224000	-1.717000
C	-2.265000	-0.082000	0.363000
H	-1.704000	-0.226000	1.291000
H	-2.866000	0.823000	0.508000
C	-3.174000	-1.273000	0.132000
H	-2.589000	-2.188000	0.006000
H	-3.861000	-1.428000	0.966000
H	-3.771000	-1.139000	-0.774000

Total Energy: -315.602912144

2g3g4g5g

C	-3.484000	-0.728000	-0.113000
H	-3.969000	-0.308000	-0.998000
H	-3.145000	-1.735000	-0.371000
H	-4.240000	-0.821000	0.670000
C	-2.319000	0.136000	0.328000
H	-1.874000	-0.287000	1.233000
H	-2.678000	1.134000	0.603000
C	-1.260000	0.267000	-0.749000
H	-0.870000	-0.728000	-0.988000
H	-1.732000	0.632000	-1.668000
C	-0.116000	1.195000	-0.377000
H	-0.509000	2.208000	-0.241000
H	0.584000	1.252000	-1.216000
C	0.635000	0.787000	0.881000
H	1.456000	1.491000	1.045000
H	-0.022000	0.890000	1.749000
C	1.180000	-0.632000	0.843000
H	0.347000	-1.341000	0.837000
H	1.735000	-0.821000	1.768000
C	2.087000	-0.921000	-0.343000
H	2.414000	-1.963000	-0.290000
H	1.516000	-0.830000	-1.272000
C	3.300000	-0.012000	-0.404000
H	3.873000	-0.065000	0.526000
H	3.965000	-0.292000	-1.223000
H	3.012000	1.030000	-0.555000

Total Energy: -315.602593435

2g3g5g

C	-3.107000	1.339000	0.234000
H	-4.033000	0.760000	0.279000
H	-2.843000	1.615000	1.258000
H	-3.314000	2.259000	-0.316000
C	-1.996000	0.534000	-0.411000
H	-1.093000	1.148000	-0.476000
H	-2.268000	0.282000	-1.442000
C	-1.693000	-0.741000	0.350000
H	-1.367000	-0.484000	1.364000
H	-2.620000	-1.312000	0.470000
C	-0.652000	-1.624000	-0.319000
H	-1.051000	-1.982000	-1.273000
H	-0.487000	-2.512000	0.300000
C	0.683000	-0.939000	-0.566000
H	1.368000	-1.652000	-1.038000
H	0.548000	-0.128000	-1.287000
C	1.328000	-0.402000	0.697000
H	1.363000	-1.202000	1.444000
H	0.700000	0.388000	1.124000
C	2.727000	0.149000	0.478000
H	3.159000	0.423000	1.445000
H	3.364000	-0.642000	0.069000
C	2.758000	1.355000	-0.443000
H	2.103000	2.146000	-0.067000
H	3.766000	1.767000	-0.526000
H	2.423000	1.099000	-1.450000

Total Energy: -315.602470708

2g4g

C	-4.021000	-0.484000	-0.187000
H	-4.427000	-0.452000	0.827000
H	-4.348000	0.425000	-0.700000
H	-4.470000	-1.336000	-0.701000
C	-2.508000	-0.575000	-0.163000
H	-2.130000	-0.640000	-1.187000
H	-2.199000	-1.500000	0.337000
C	-1.870000	0.606000	0.545000
H	-2.132000	1.527000	0.011000
H	-2.311000	0.696000	1.544000
C	-0.360000	0.508000	0.668000
H	-0.107000	-0.400000	1.226000
H	0.010000	1.348000	1.266000
C	0.360000	0.508000	-0.668000
H	0.107000	-0.400000	-1.226000
H	-0.010000	1.348000	-1.266000
C	1.870000	0.606000	-0.545000
H	2.132000	1.527000	-0.011000
H	2.311000	0.696000	-1.544000
C	2.508000	-0.575000	0.163000
H	2.130000	-0.640000	1.187000
H	2.199000	-1.500000	-0.337000
C	4.021000	-0.484000	0.187000
H	4.348000	0.425000	0.700000
H	4.470000	-1.336000	0.701000
H	4.427000	-0.452000	-0.827000

Total Energy: -315.602508160

2g5g

C	3.846000	-0.870000	-0.090000
H	4.547000	-0.048000	0.077000
H	3.794000	-1.450000	0.835000
H	4.264000	-1.514000	-0.865000
C	2.477000	-0.343000	-0.474000
H	1.805000	-1.183000	-0.669000
H	2.544000	0.220000	-1.412000
C	1.882000	0.553000	0.597000
H	1.763000	-0.025000	1.522000
H	2.599000	1.348000	0.827000
C	0.550000	1.172000	0.216000
H	0.674000	1.768000	-0.695000
H	0.240000	1.872000	0.998000
C	-0.561000	0.161000	0.001000
H	-0.312000	-0.497000	-0.837000
H	-0.633000	-0.480000	0.885000
C	-1.900000	0.820000	-0.273000
H	-1.783000	1.519000	-1.108000
H	-2.187000	1.425000	0.595000
C	-3.016000	-0.160000	-0.593000
H	-3.915000	0.400000	-0.867000
H	-2.737000	-0.744000	-1.477000
C	-3.341000	-1.099000	0.554000
H	-3.594000	-0.535000	1.456000
H	-4.191000	-1.741000	0.313000
H	-2.496000	-1.746000	0.795000

Total Energy: -315.602478816

3g

C	3.813000	-1.111000	-0.176000
H	3.395000	-2.048000	0.200000
H	3.832000	-1.174000	-1.267000
H	4.846000	-1.041000	0.172000
C	2.984000	0.073000	0.282000
H	3.434000	1.004000	-0.079000
H	2.998000	0.134000	1.376000
C	1.546000	-0.001000	-0.192000
H	1.528000	-0.049000	-1.288000
H	1.103000	-0.938000	0.161000
C	0.710000	1.176000	0.270000
H	1.211000	2.103000	-0.030000
H	0.679000	1.187000	1.366000
C	-0.710000	1.176000	-0.270000
H	-1.211000	2.103000	0.030000
H	-0.679000	1.187000	-1.366000
C	-1.546000	-0.001000	0.192000
H	-1.528000	-0.049000	1.288000
H	-1.103000	-0.938000	-0.161000
C	-2.984000	0.073000	-0.282000
H	-3.434000	1.004000	0.079000
H	-2.998000	0.134000	-1.376000
C	-3.813000	-1.111000	0.176000
H	-3.832000	-1.174000	1.267000
H	-4.846000	-1.041000	-0.172000
H	-3.395000	-2.048000	-0.200000

Total Energy: -315.603245485

3g4g

C	3.460000	-1.129000	-0.314000
H	2.921000	-2.066000	-0.477000
H	3.728000	-0.729000	-1.295000
H	4.385000	-1.364000	0.216000
C	2.605000	-0.142000	0.456000
H	3.171000	0.778000	0.636000
H	2.367000	-0.550000	1.445000
C	1.315000	0.200000	-0.261000
H	1.546000	0.620000	-1.247000
H	0.758000	-0.724000	-0.450000
C	0.449000	1.174000	0.511000
H	1.043000	2.061000	0.757000
H	0.172000	0.725000	1.470000
C	-0.802000	1.610000	-0.235000
H	-1.370000	2.302000	0.396000
H	-0.505000	2.177000	-1.124000
C	-1.712000	0.469000	-0.657000
H	-1.203000	-0.160000	-1.395000
H	-2.587000	0.883000	-1.170000
C	-2.183000	-0.399000	0.493000
H	-1.321000	-0.875000	0.971000
H	-2.643000	0.235000	1.258000
C	-3.165000	-1.464000	0.047000
H	-2.714000	-2.119000	-0.704000
H	-3.494000	-2.089000	0.880000
H	-4.052000	-1.012000	-0.404000

Total Energy: -315.603075549

3g4g5g

C	-3.641000	-0.660000	0.351000
H	-3.301000	-1.473000	0.998000
H	-3.977000	0.156000	0.997000
H	-4.506000	-1.019000	-0.211000
C	-2.526000	-0.198000	-0.566000
H	-2.892000	0.596000	-1.226000
H	-2.220000	-1.020000	-1.222000
C	-1.314000	0.305000	0.193000
H	-1.611000	1.137000	0.844000
H	-0.958000	-0.487000	0.859000
C	-0.191000	0.757000	-0.719000
H	-0.579000	1.505000	-1.418000
H	0.132000	-0.089000	-1.334000
C	1.001000	1.343000	0.019000
H	1.752000	1.662000	-0.709000
H	0.685000	2.250000	0.545000
C	1.640000	0.395000	1.024000
H	0.949000	0.224000	1.855000
H	2.521000	0.882000	1.456000
C	2.055000	-0.945000	0.439000
H	2.493000	-1.556000	1.234000
H	1.169000	-1.487000	0.096000
C	3.045000	-0.819000	-0.703000
H	3.931000	-0.258000	-0.390000
H	3.376000	-1.799000	-1.053000
H	2.608000	-0.295000	-1.555000

Total Energy: -315.602845355

3g5g

C	3.820000	-0.982000	0.070000
H	3.554000	-1.605000	0.928000
H	3.698000	-1.592000	-0.829000
H	4.877000	-0.724000	0.159000
C	2.943000	0.253000	0.006000
H	3.243000	0.878000	-0.841000
H	3.096000	0.863000	0.903000
C	1.469000	-0.082000	-0.119000
H	1.310000	-0.683000	-1.023000
H	1.175000	-0.716000	0.723000
C	0.586000	1.149000	-0.175000
H	0.944000	1.803000	-0.977000
H	0.700000	1.716000	0.756000
C	-0.884000	0.841000	-0.398000
H	-1.438000	1.780000	-0.514000
H	-0.995000	0.301000	-1.344000
C	-1.515000	0.042000	0.728000
H	-1.281000	0.531000	1.679000
H	-1.062000	-0.954000	0.774000
C	-3.021000	-0.108000	0.597000
H	-3.410000	-0.611000	1.488000
H	-3.481000	0.886000	0.581000
C	-3.443000	-0.882000	-0.639000
H	-2.970000	-1.868000	-0.658000
H	-4.524000	-1.030000	-0.666000
H	-3.159000	-0.361000	-1.555000

Total Energy: -315.602513169

VII. Linear fits of the Repulsive and Attractive terms of the eighteen isomers of octane and the sixteen *gauche*-conformations of *n*-octane

$\Delta\Delta_{trv}H°_{gauche}$ is referenced against *trans*-*n*-octane. The variable *n* is the number of *gauche*-conformations with respect to *n*-octane. $\Delta\Delta_{trv}H°_{protobranch}$ is referenced against *trans*-*n*-octane. The variable *n* is the number of geminal-alkyl,alkyl-contacts (protobranches) for the eighteen isomers of octane. Their linear fits (from Figure 7.) are provided below.

$$\Delta\Delta_{trv}H°_{gauche} = -0.0998n - 0.0331 \quad R^2 = 0.991$$

$$\Delta\Delta_{trv}H°_{protobranch} = -0.2840n + 1.6068 \quad R^2 = 0.986$$

$\Delta E^{C\text{-}CCSD}$ is referenced against the singlet and triplet (strong pairs) correlation of *trans*-*n*-octane. The variable *n* is the number of *gauche*-conformations or protobranch interactions, as specified. Their linear fits (from Figure 8.) are provided below:

$$\Delta E^{C\text{-}CCSD}_{gauche} = -0.7598n - 0.1617 \quad R^2 = 0.980$$

$$\Delta E^{C\text{-}CCSD}_{protobranch} = -1.1509n + 6.8763 \quad R^2 = 0.980$$

VIII. Assorted functional performance for the calculation of $\Delta\Delta_f H°$

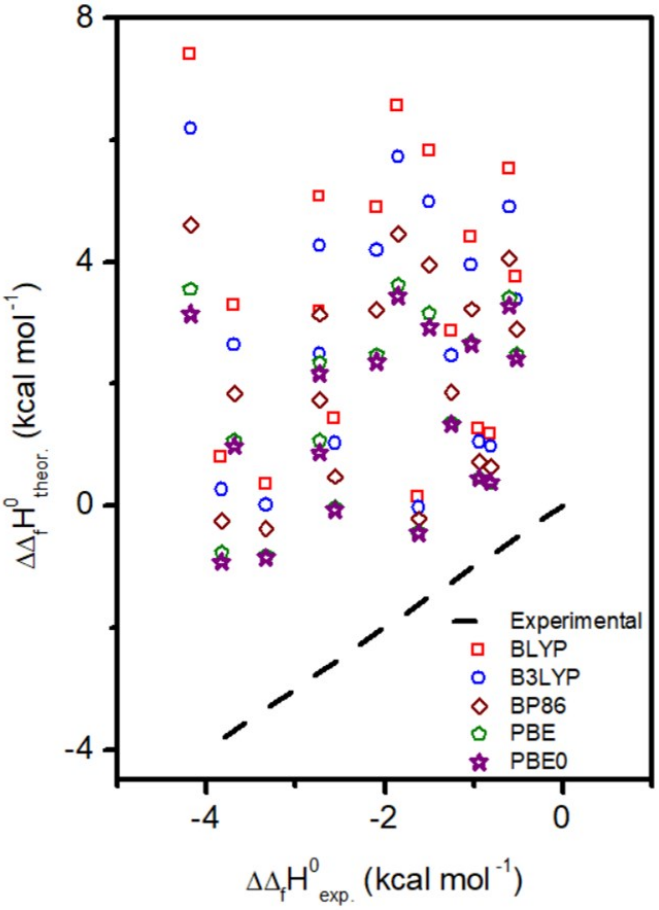


Figure S9. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the following functionals: BLYP (red squares), B3LYP (blue circles), BP86 (brown diamons), PBE (green pentangon), and PBE0 (purple stars).

$$\text{BLYP: } \Delta\Delta_f H°_{theor.} = 0.255\Delta\Delta_f H°_{exp.} + 2.716 \qquad (R^2 = 0.018)$$

$$\text{B3LYP: } \Delta\Delta_f H°_{theor.} = -0.119\Delta\Delta_f H°_{exp.} + 2.460 \qquad (R^2 = 0.005)$$

$$\text{BP86: } \Delta\Delta_f H°_{theor.} = 0.029\Delta\Delta_f H°_{exp.} + 2.055 \qquad (R^2 = 0.018)$$

$$\text{PBE: } \Delta\Delta_f H°_{theor.} = 0.154\Delta\Delta_f H°_{exp.} + 1.742 \qquad (R^2 = 0.016)$$

$$\text{PBE0: } \Delta\Delta_f H°_{theor.} = 0.296\Delta\Delta_f H°_{exp.} + 1.872 \qquad (R^2 = 0.052)$$

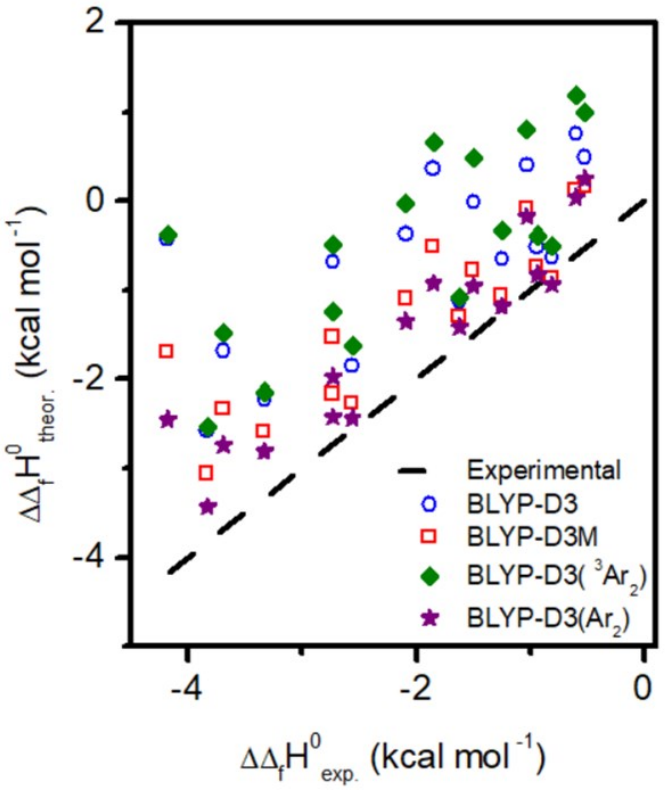


Figure S10. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the BLYP functional and the following dispersion corrections: D3 (blue circles), D3M (red squares), D3($^3Ar_2$) (green diamons), and D3(Ar_2) (purple stars).

BLYP - D3: $\Delta\Delta_f H°_{theor.} = 0.549\Delta\Delta_f H°_{exp.} + 0.393$ ($R^2 = 0.499$)

BLYP - D3M: $\Delta\Delta_f H°_{theor.} = 0.690\Delta\Delta_f H°_{exp.} + 0.139$ ($R^2 = 0.7719$)

BLYP - D3(3Ar2): $\Delta\Delta_f H°_{theor.} = 0.596\Delta\Delta_f H°_{exp.} + 0.718$ ($R^2 = 0.486$)

BLYP - D3(Ar2): $\Delta\Delta_f H°_{theor.} = 0.823\Delta\Delta_f H°_{exp.} + 0.183$ ($R^2 = 0.872$)

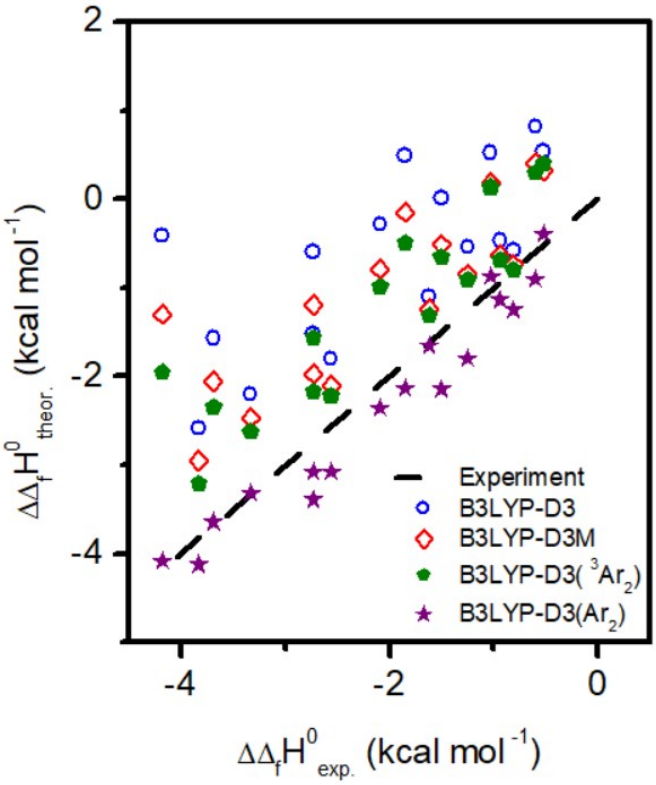


Figure S11. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the B3LYP functional and the following dispersion corrections: D3 (blue circles), D3M (red squares), D3($^3Ar_2$) (green diamons), and D3(Ar_2) (purple stars).

B3LYP - D3: $\Delta\Delta_f H°_{theor.} = 0.553\Delta\Delta_f H°_{exp.} + 0.458$ ($R^2 = 0.492$)

BLYP - D3M: $\Delta\Delta_f H°_{theor.} = 0.658\Delta\Delta_f H°_{exp.} + 0.288$ ($R^2 = 0.691$)

BLYP - D3(3Ar2): $\Delta\Delta_f H°_{theor.} = 0.764\Delta\Delta_f H°_{exp.} + 0.325$ ($R^2 = 0.802$)

BLYP - D3(Ar2): $\Delta\Delta_f H°_{theor.} = 0.993\Delta\Delta_f H°_{exp.} - 0.241$ ($R^2 = 0.956$)

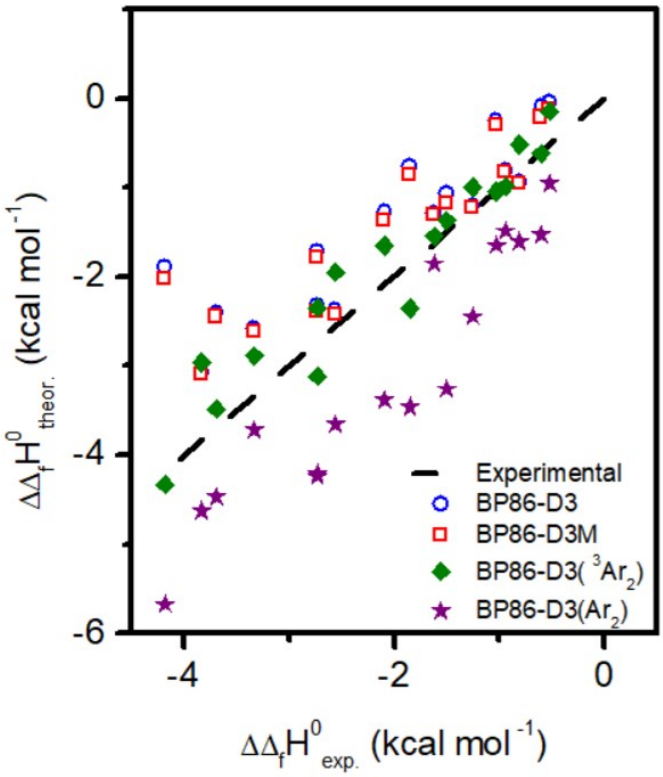


Figure S12. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the BP86 functional and the following dispersion corrections: D3 (blue circles), D3M (red squares), D3($^3Ar_2$) (green diamons), and D3(Ar_2) (purple stars).

BP86 - D3: $\Delta\Delta_f H°_{theor.} = 0.680\Delta\Delta_f H°_{exp.} - 0.006$ ($R^2 = 0.811$)

BP86 - D3M: $\Delta\Delta_f H°_{theor.} = 0.688\Delta\Delta_f H°_{exp.} - 0.052$ ($R^2 = 0.833$)

BP86 - D3(3Ar2): $\Delta\Delta_f H°_{theor.} = 0.937\Delta\Delta_f H°_{exp.} + 0.042$ ($R^2 = 0.927$)

BP86 - D3(Ar2): $\Delta\Delta_f H°_{theor.} = 1.148\Delta\Delta_f H°_{exp.} - 0.652$ ($R^2 = 0.956$)

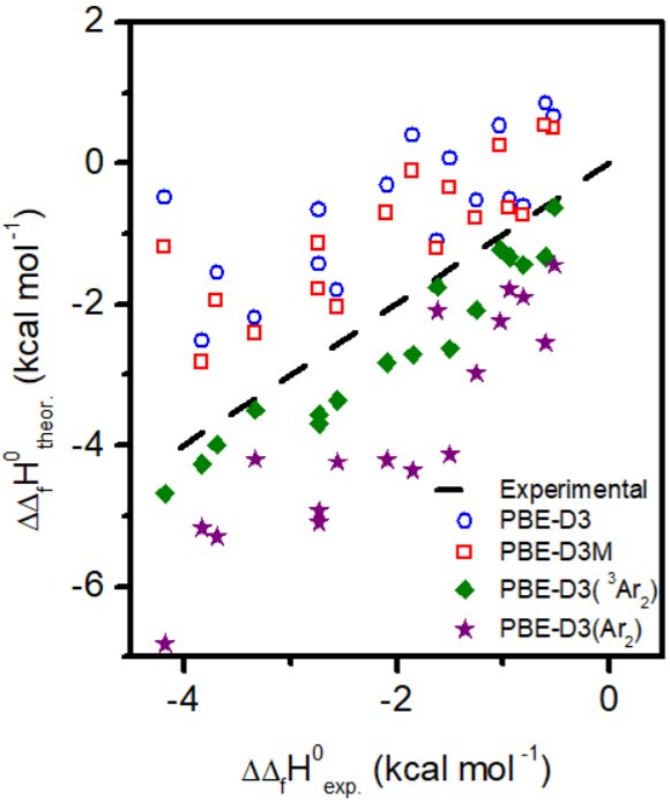


Figure S13. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the PBE functional and the following dispersion corrections: D3 (blue circles), D3M (red squares), D3($^3Ar_2$) (green diamons), and D3(Ar_2) (purple stars).

PBE - D3: $\Delta\Delta_f H°_{theor.} = 0.559\Delta\Delta_f H°_{exp.} + 0.474$ ($R^2 = 0.508$)

PBE - D3M: $\Delta\Delta_f H°_{theor.} = 0.645\Delta\Delta_f H°_{exp.} + 0.340$ ($R^2 = 0.669$)

PBE - D3(3Ar2): $\Delta\Delta_f H°_{theor.} = 1.036\Delta\Delta_f H°_{exp.} - 0.468$ ($R^2 = 0.937$)

PBE - D3(Ar2): $\Delta\Delta_f H°_{theor.} = 1.264\Delta\Delta_f H°_{exp.} - 1.047$ ($R^2 = 0.837$)

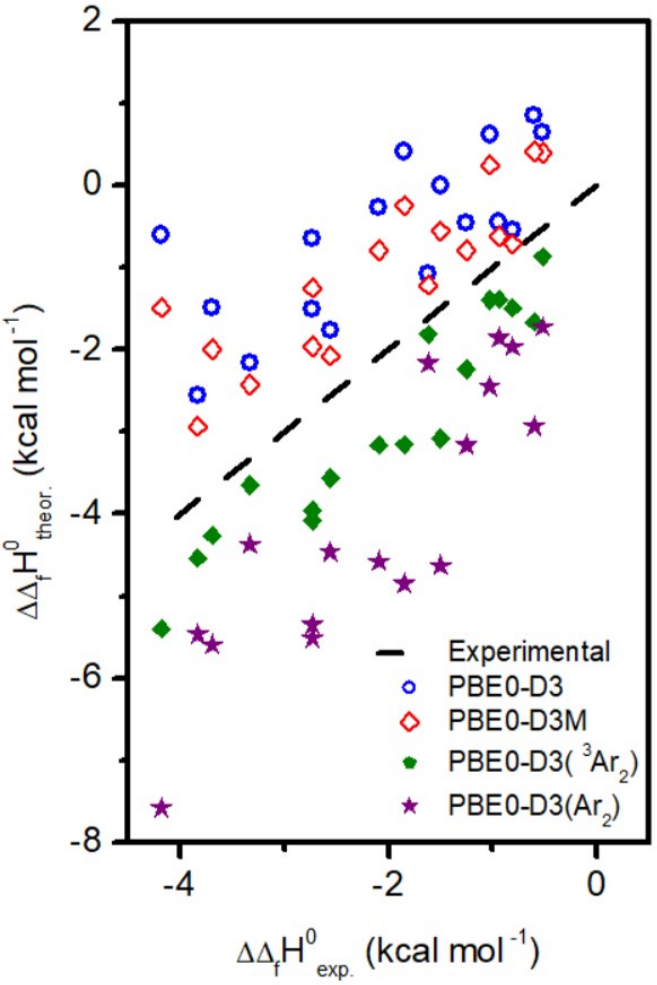


Figure S14. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the PBE functional and the following dispersion corrections: D3 (blue circles), D3M (red squares), D3($^3Ar_2$) (green diamonds), and D3(Ar_2) (purple stars).

PBE0 - D3: $\Delta\Delta_f H°_{theor.} = 0.575\Delta\Delta_f H°_{exp.} + 0.515$ ($R^2 = 0.536$)

PBE0 - D3M: $\Delta\Delta_f H°_{theor.} = 0.677\Delta\Delta_f H°_{exp.} + 0.324$ ($R^2 = 0.729$)

PBE0 - D3(3Ar2): $\Delta\Delta_f H°_{theor.} = 1.113\Delta\Delta_f H°_{exp.} - 0.580$ ($R^2 = 0.911$)

PBE0 - D3(Ar2): $\Delta\Delta_f H°_{theor.} = 1.343\Delta\Delta_f H°_{exp.} - 1.183$ ($R^2 = 0.799$)

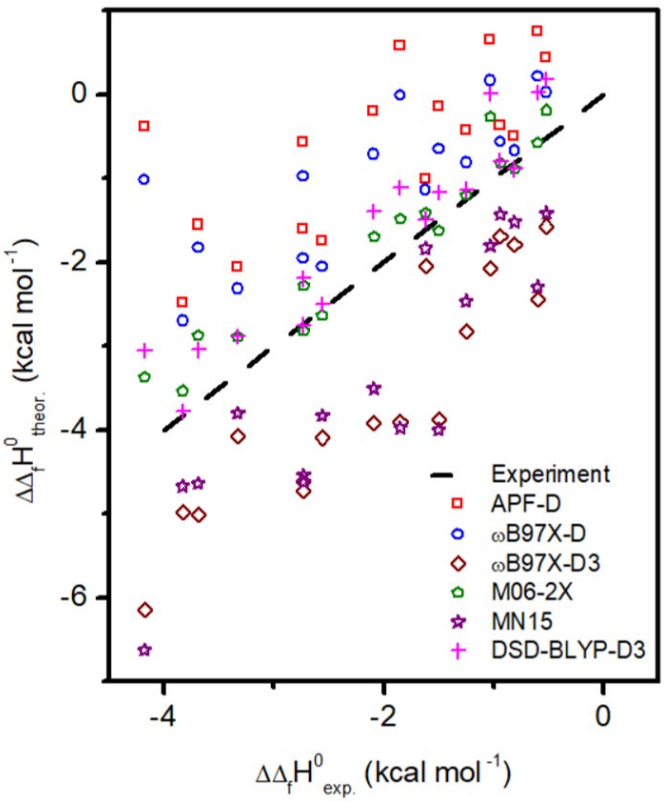


Figure S15. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the following functionals: APF-D (red squares), ωB97X-D (blue circles), ωB97X-D3 (brown diamons), M06-2X (green pentangon), MN15 (purple stars), and DSD-BLYP-D3 (pink cross). The slopes and R^2 are provided in the table below:

$$\text{APF - D: } \Delta\Delta_f H°_{theor.} = 0.540\Delta\Delta_f H°_{exp.} + 0.464 \qquad (R^2 = 0.493)$$

$$\omega\text{B97X - D: } \Delta\Delta_f H°_{theor.} = 0.566\Delta\Delta_f H°_{exp.} + 0.164 \qquad (R^2 = 0.624)$$

$$\omega\text{B97X - D3: } \Delta\Delta_f H°_{theor.} = 1.169\Delta\Delta_f H°_{exp.} - 1.033 \qquad (R^2 = 0.856)$$

$$\text{M06 - 2X: } \Delta\Delta_f H°_{theor.} = 0.877\Delta\Delta_f H°_{exp.} + 0.019 \qquad (R^2 = 0.943)$$

$$\text{MN15: } \Delta\Delta_f H°_{theor.} = 1.194\Delta\Delta_f H°_{exp.} - 0.828 \qquad (R^2 = 0.819)$$

$$\text{DSD - BLYP - D3: } \Delta\Delta_f H°_{theor.} = 0.940\Delta\Delta_f H°_{exp.} + 0.287 \qquad (R^2 = 0.912)$$

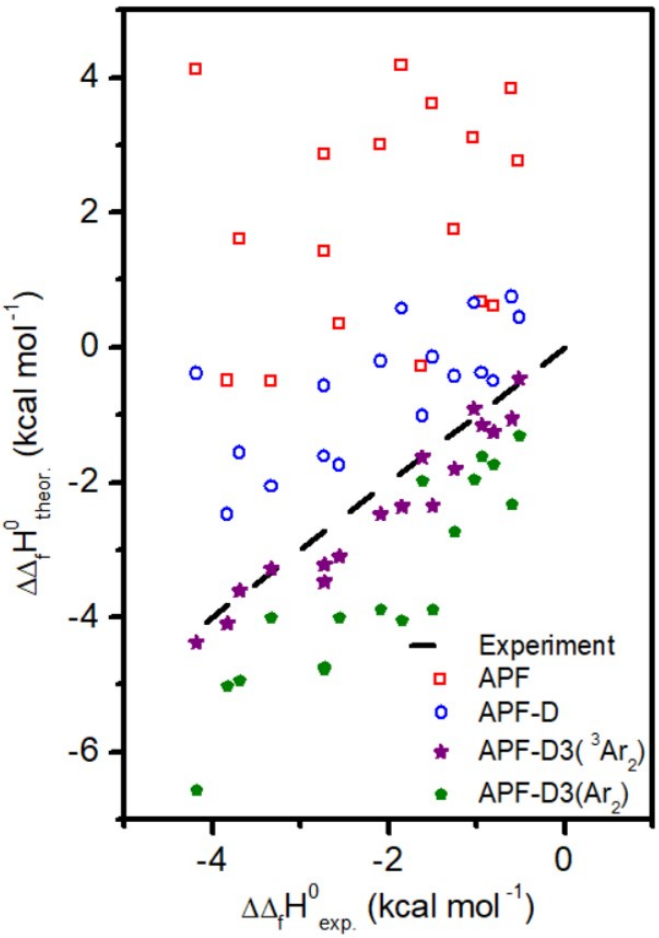


Figure S16. The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the following functionals: APF (red squares), APF-D (blue circles), APF-D3($^3Ar_2$) (purple stars), and APF-D3(Ar_2) (green pentagon).

$$\text{APF: } \Delta\Delta_f H°_{theor.} = 0.095\Delta\Delta_f H°_{exp.} + 1.990 \qquad (R^2 = 0.005)$$

$$\text{APF - D: } \Delta\Delta_f H°_{theor.} = 0.540\Delta\Delta_f H°_{exp.} + 0.464 \qquad (R^2 = 0.493)$$

APF - D3(3Ar2): $\Delta\Delta_f H°_{theor.} = 1.001\Delta\Delta_f H°_{exp.} + 0.295$ $(R^2 = 0.946)$

APF - D3$(Ar2)$: $\Delta\Delta_f H°_{theor.} = 1.232\Delta\Delta_f H°_{exp.} - 0.891$ $(R^2 = 0.850)$

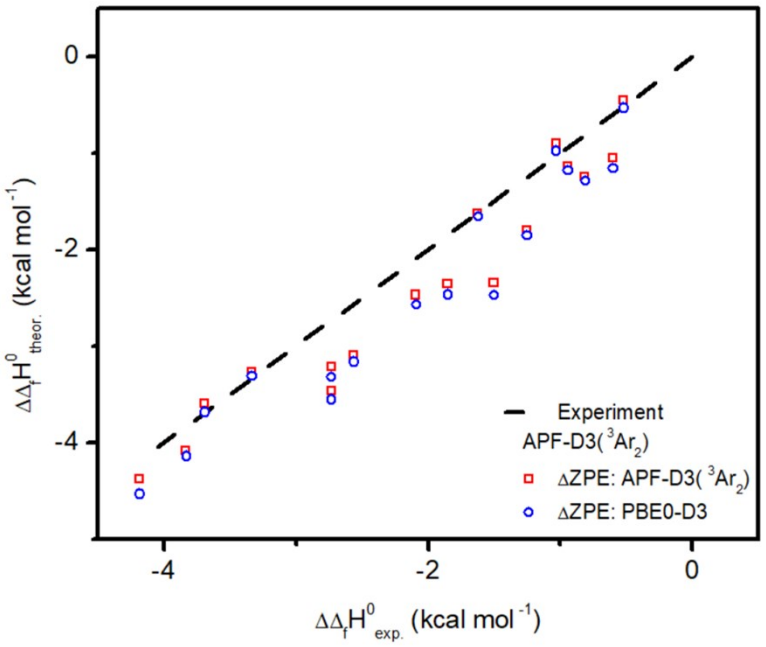


Figure S17. $\Delta\Delta_f H°_{theor.}$ for the APF-D3(3Ar$_2$) functional is plotted for APF-D3(3Ar$_2$) and PBE0-D3 $\Delta\Delta_{trv}H°$ thermal corrections.The relationship between the calculated and experimental $\Delta\Delta H°_f$ for the isomers of octane for the following functionals: APF-D3(^{3}Ar$_2$) (red squares) and PBE0-D3 (blue circles). The $\Delta\Delta_{trv}H°$ data from the APF-D3(3Ar$_2$) and PBE0-D3 level of theory are provided in the Table below. Note: the average deviation between the functionals is 0.0725 kcal mol^{-1}.

$\Delta\Delta_{trv}H°$ [APF - D3$(3Ar2)$]: $\Delta\Delta_f H°_{theor.} = 1.001\Delta\Delta_f H°_{exp.} - 0.2946$ $(R^2 = 0.946)$

$\Delta\Delta_{trv}H°$ [PBE0 - D3]: $\Delta\Delta_f H°_{theor.} = 1.014\Delta\Delta_f H°_{exp.} - 0.3422$ $(R^2 = 0.941)$

Compound	APF-D3($^3Ar_2$): $\Delta\Delta_{trv}H°$ (kcal mol^{-1})	PBE0-D3: $\Delta\Delta_{trv}H°$ (kcal mol^{-1})	$\Delta\Delta_{trv}H^{°PBE0\text{-}D3} - \Delta\Delta_{trv}H^{°APF\text{-}D3(3Ar2)}$ (kcal mol^{-1})
n-octane	0	0	0
3-ethyl-hexane	0.0351	-0.03451305	-0.06965361
3-Ethyl-2-Methyl-Pentane	-0.1443273	-0.24535641	-0.10102911
4-Methyl-Heptane	-0.19076304	-0.22841364	-0.0376506
3-Methyl-Heptane	-0.20582328	-0.24096384	-0.03514056
3,4-Dimethyl-Hexane	-0.3012048	-0.37525098	-0.07404618
2,3-Dimethyl-Hexane	-0.38717367	-0.43486443	-0.04769076
3-Ethyl-3-Methyl-Pentane	-0.38717367	-0.51393069	-0.12675702
2-Methyl-Heptane	-0.26480922	-0.29304717	-0.02823795
2,3,3-Trimethyl-Pentane	-0.67959333	-0.78940758	-0.10981425
2,3,4-Trimethyl-Pentane	-0.51581322	-0.61119474	-0.09538152
2,4-Dimethyl-Hexane	-0.44866965	-0.51267567	-0.06400602
2,2,3-Trimethyl-Pentane	-0.79819272	-0.90110436	-0.10291164
3,3-Dimethyl-Hexane	-0.56413149	-0.64696281	-0.08283132
2,5-Dimethyl-Hexane	-0.55785639	-0.59299695	-0.03514056
2,2,4-Trimethyl-Pentane	-0.93059733	-1.01593869	-0.08534136
2,2-Dimethyl-Hexane	-0.71661642	-0.76807224	-0.05145582
2,2,3,3-Tetramethyl-Butane	-1.16905113	-1.32718365	-0.15813252