

Electronic supporting Information for:

**Lanthanide complexes of DOTA-nitroxide conjugates
for redox imaging: Spectro-electrochemistry, CEST,
relaxivity and cytotoxicity.**

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Content :

Fig. S1-S22.....	S2-13
Details of the calculations.....	S14-102

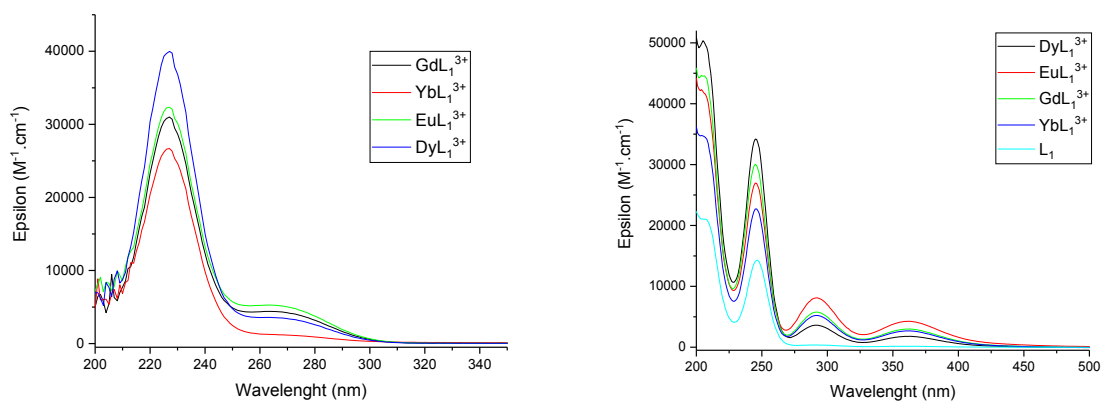


Fig. S1 UV-Vis spectra of 0.5 mM solution of YbL_1^{3+} , DyL_1^{3+} , EuL_1^{3+} and GdL_1^{3+} (Left : in Water, Right : in MeCN)

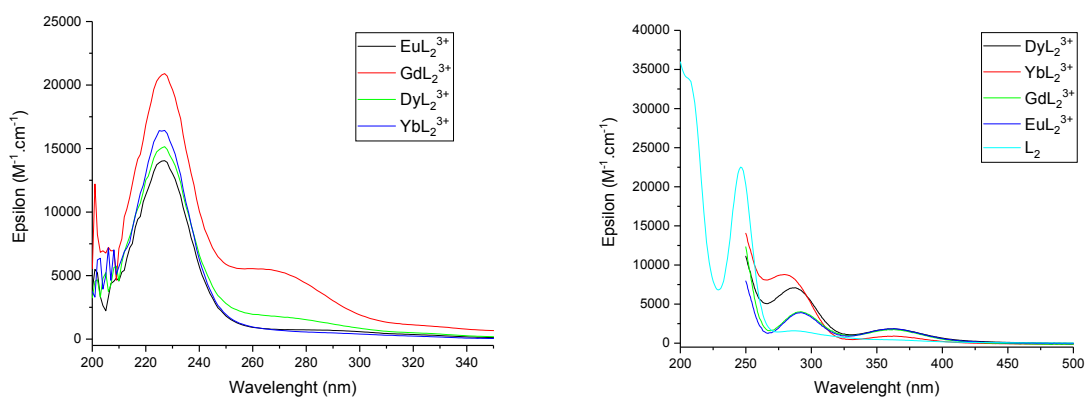


Fig. S2 UV-Vis spectra of 0.5 mM solution of YbL_2^{3+} , DyL_2^{3+} , EuL_2^{3+} and GdL_2^{3+} (Left : in Water, Right : in MeCN)

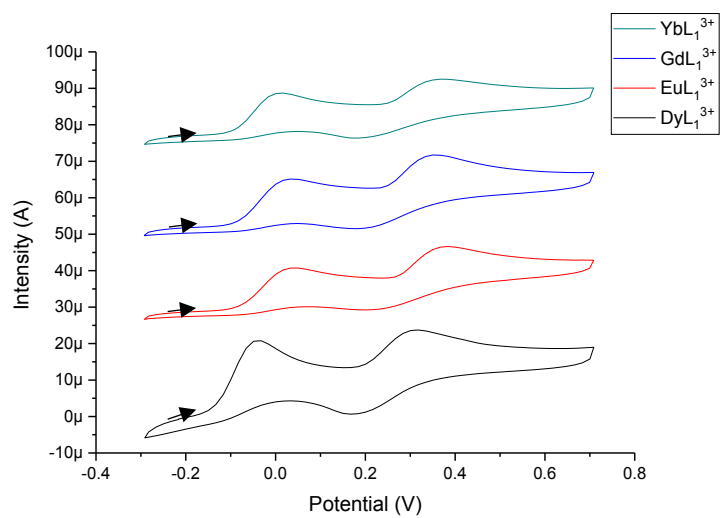


Fig. S3 CV curves of 0.5 mM solution of YbL_1^{3+} , DyL_1^{3+} , EuL_1^{3+} and GdL_1^{3+} in CH_3CN containing TBAP. Scan rate = 0.1 V/sec; Ref:Fc⁺/Fc.

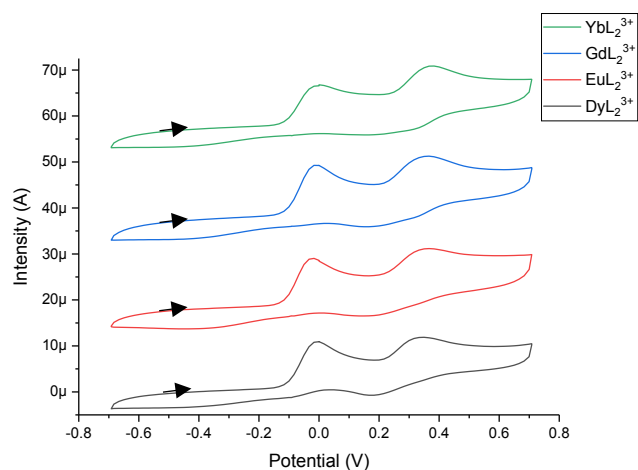


Fig. S4 CV curves of 0.5 mM solution of YbL_2^{3+} , DyL_2^{3+} , EuL_2^{3+} and GdL_2^{3+} in CH_3CN containing TBAP. Scan rate = 0.1 V/sec; Ref:Fc⁺/Fc.

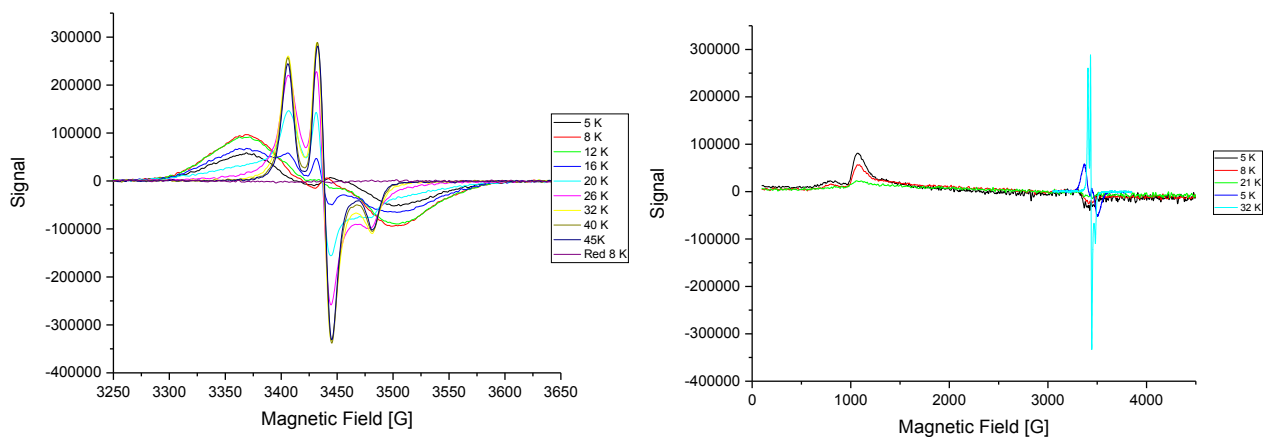


Fig. S5 Low temperature evolution of the EPR spectrum of a 0.45 mM aqueous solution (containing 10% glycerol) of $[\text{Yb}(\text{L}_1)]^{3+}$. Microwave Freq; 9.63 GHz, power 0.2 mW; Mod. Freq. 100 KHz, Amp. 0.4 mT.

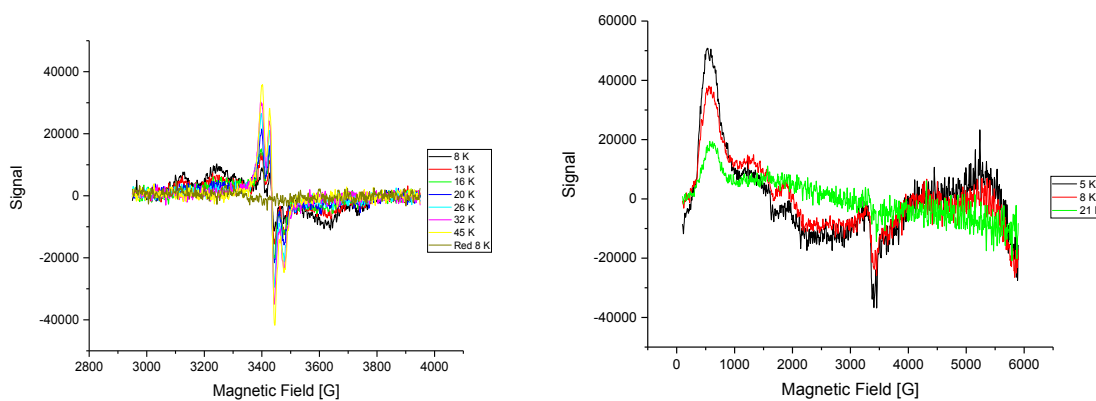


Fig. S6 Low temperature evolution of the EPR spectrum of a 0.45 mM aqueous solution (containing 10% glycerol) of $[\text{Dy}(\text{L}_1)]^{3+}$. Microwave Freq; 9.63 GHz, power 4 mW; Mod. Freq. 100 KHz, Amp. 0.4 mT.

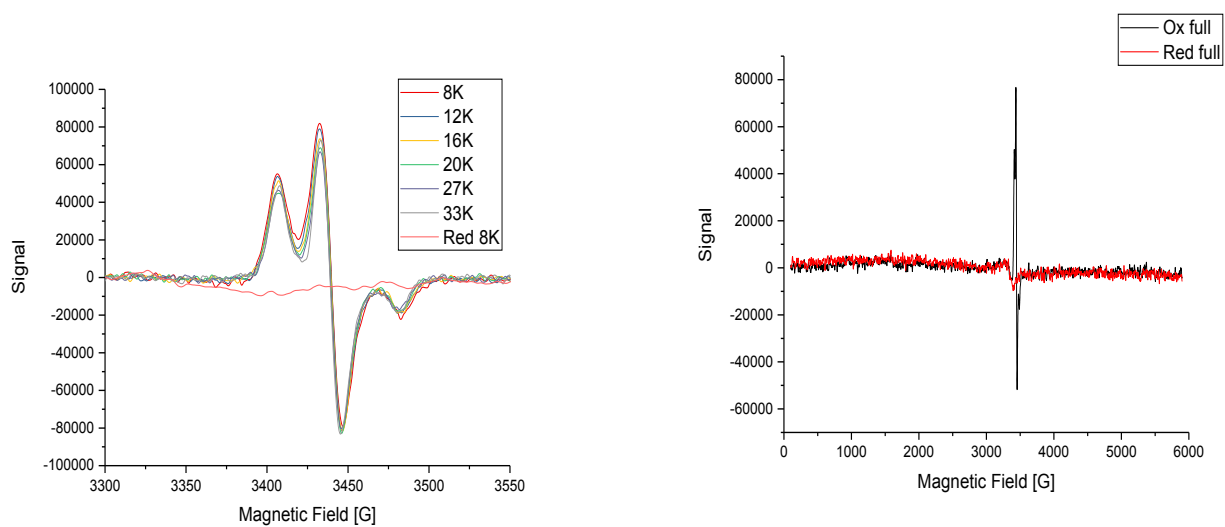


Fig. S7 Low temperature evolution of the EPR spectrum of a 0.45 mM aqueous solution (containing 10% glycerol) of $[\text{Eu}(\text{L}_1)]^{3+}$. Microwave Freq; 9.63 GHz, power 0.2 mW; Mod. Freq. 100 KHz, Amp. 0.4 mT.

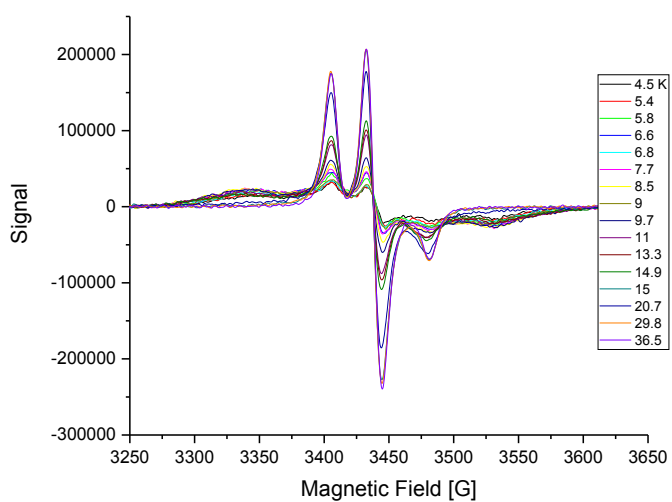


Fig. S8 Low temperature evolution of the EPR spectrum of a 0.45 mM aqueous solution (containing 10% glycerol) of $[\text{Yb}(\text{L}_2)]^{3+}$. Microwave Freq; 9.63 GHz, power 2 mW; Mod. Freq. 100 KHz, Amp. 0.4 mT.

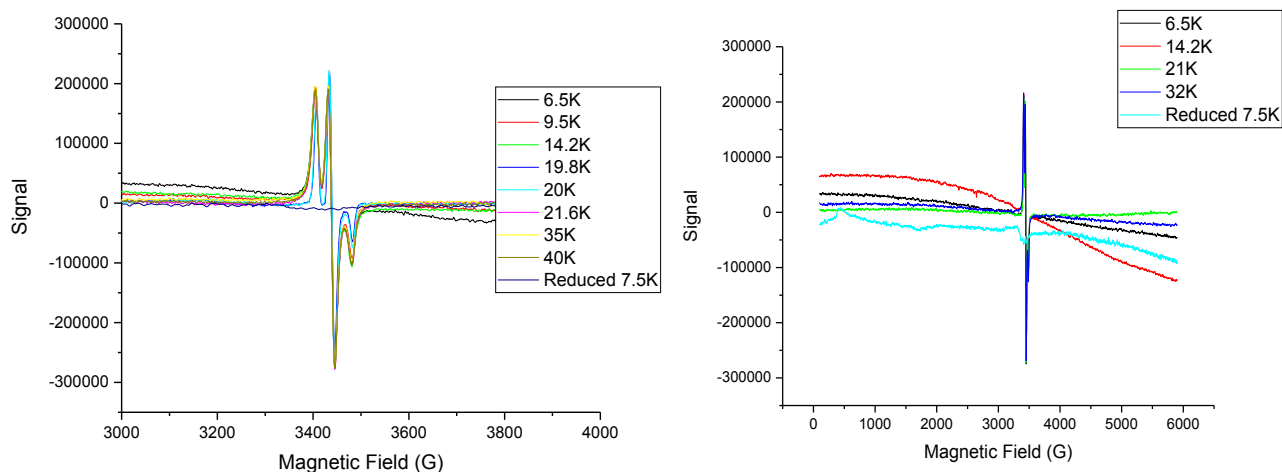


Fig. S9 Low temperature evolution of the EPR spectrum of a 0.45 mM aqueous solution (containing 10% glycerol) of $[\text{Dy}(\text{L}_2)]^{3+}$. Microwave Freq; 9.63 GHz, power 2 mW (left), 4 mW (right); Mod. Freq. 100 KHz, Amp. 0.4 mT.

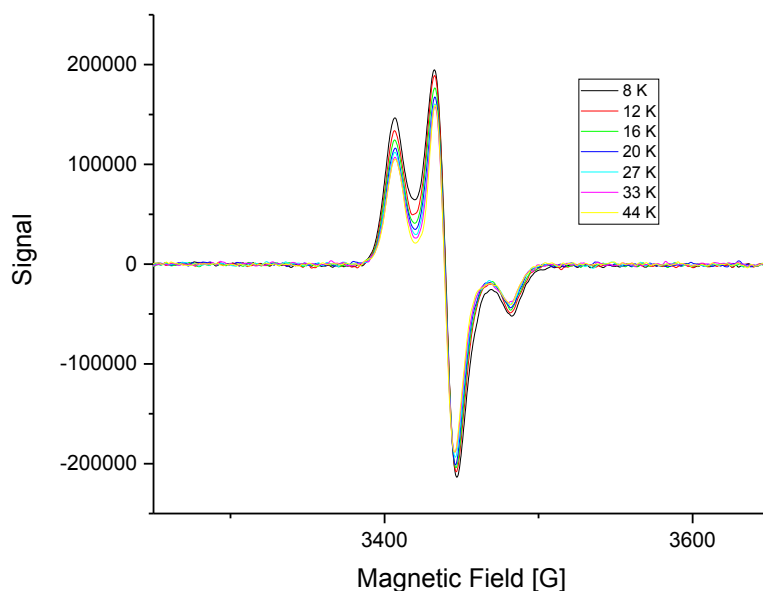


Fig. S10 Low temperature evolution of the EPR spectrum of a 0.45 mM aqueous solution (containing 10% glycerol) of $[\text{Eu}(\text{L}_2)]^{3+}$. Microwave Freq; 9.63 GHz, power 0.2 mW; Mod. Freq. 100 KHz, Amp. 0.4 mT.

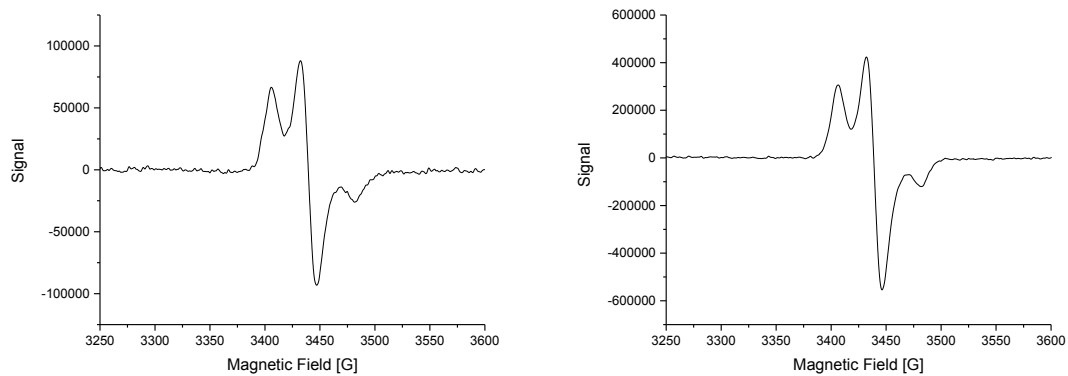


Fig. S11 X-Band EPR spectra of 0.45 mM aqueous solutions (containing 10% glycerol) of L_1 (left) and L_2 (right). Microwave Freq; 9.63 GHz, power 2 mW; Mod. Freq. 100 KHz, Amp. 0.4 mT. $T = 8.8$ K (left), 10.7 K (right).

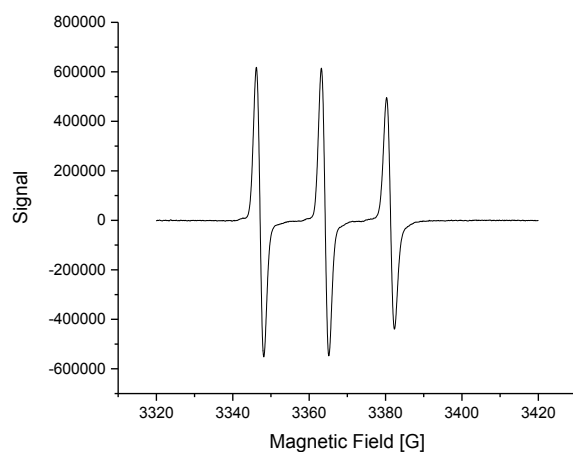


Fig. S12 X-Band EPR spectrum of a 0.5 mM solution of L_2 in water with HEPES buffer at pH 7.9. Microwave Freq; 9.42 GHz, power 3.5 mW; Mod. Freq. 100 KHz, Amp. 0.2 mT. $T = 293$ K.

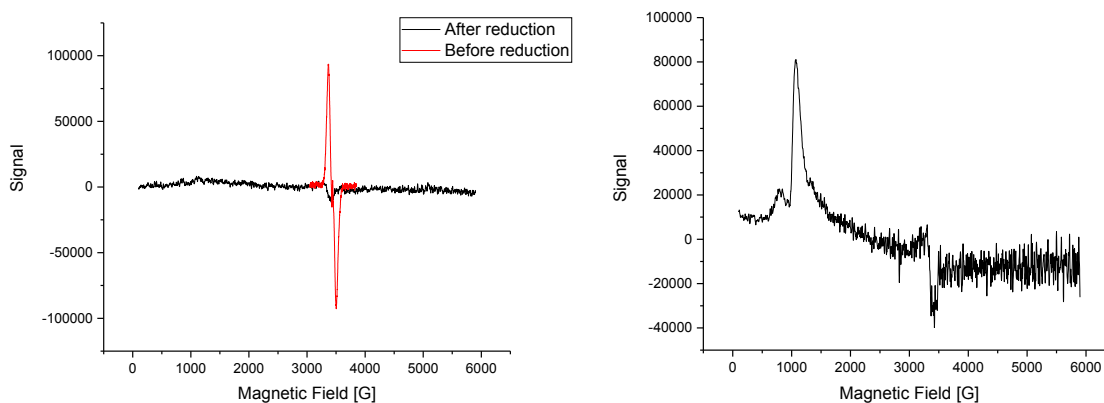


Fig. S13 X-Band EPR spectrum of $[\text{Yb}(\text{L}_1)]^{3+}$ after addition of 2 molar equiv. of ascorbate. Microwave Freq; 9.63 GHz, power 0.2 mW (left), 2 mW (right); Mod. Freq. 100 KHz, Amp. 0.4 mT (left), 1 mT (right). T = 7K (left), 5K (right).

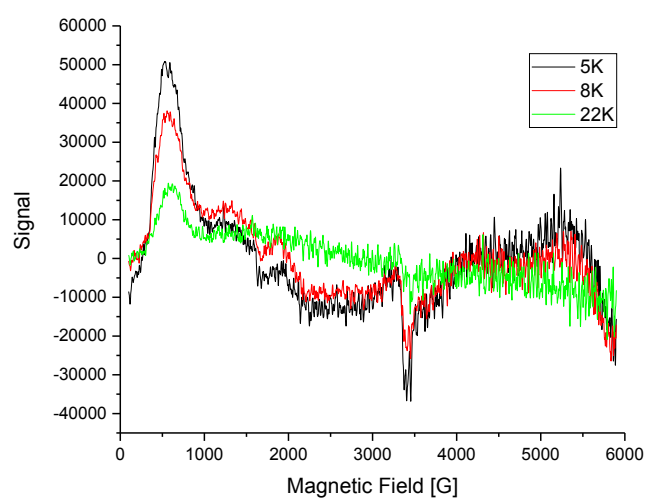


Fig. S14 Low temperature evolution of the X-Band EPR spectrum of $[\text{Dy}(\text{L}_1)]^{3+}$ after addition of 2 molar equiv. of ascorbate. Microwave Freq; 9.63 GHz, power 2 mW; Mod. Freq. 100 KHz, Amp. 1 mT.

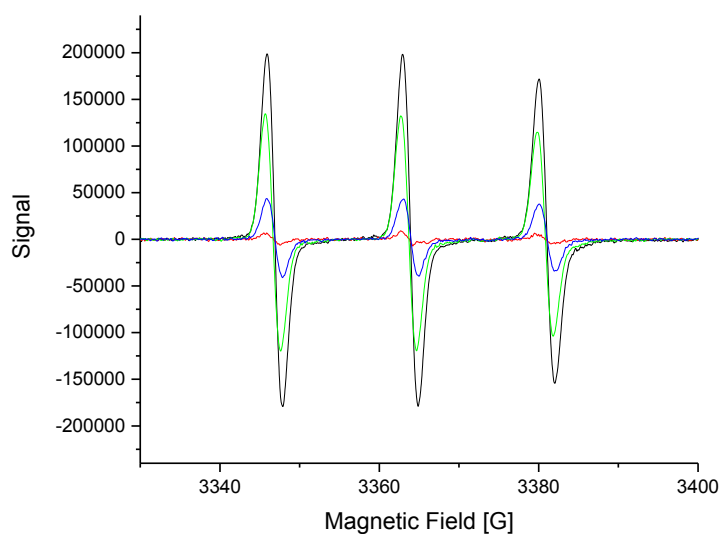


Fig. S15 X-Band EPR spectrum of a 0.5 mM solution of $[\text{Gd}(\text{L}_2)]^{3+}$ in water with HEPES buffer at pH 7. (black) initial; (red) after addition of 1 molar equivalent of ascorbate; (green) after addition of 1 molar equivalent of ascorbate followed by addition of NaIO_4 in excess and 30 min reaction; (blue) after addition of 1 molar equivalent of ascorbate followed by increase of pH to 13 and dioxygen bubbling during 30 min. Microwave Freq; 9.42 GHz, power 3.5 mW; Mod. Freq. 100 KHz, Amp. 0.2 mT. $T = 293$ K.

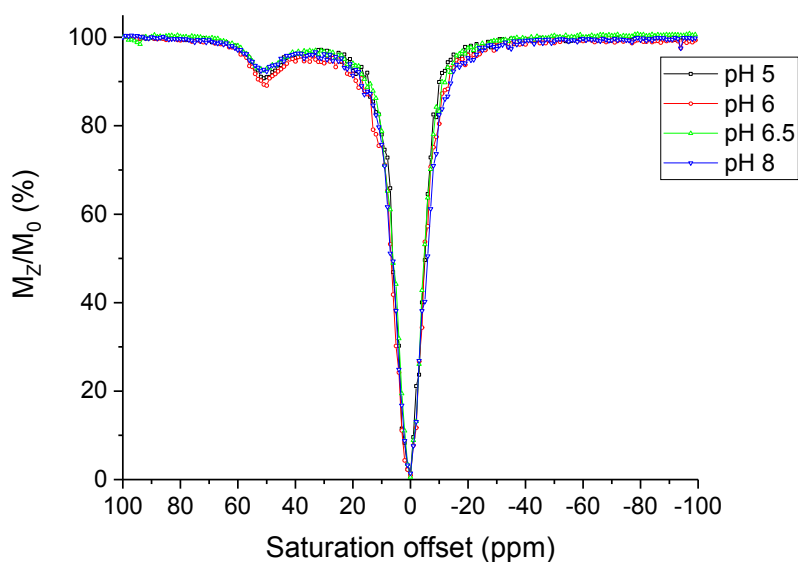


Fig. S16 PARACEST spectra of $[\text{Eu}(\text{L}_1)]^{3+}$ as a function of the pH. CEST at +51 ppm coming from the coordinated water molecules of the hydroxylamine Eu^{3+} complexes recorded at 11.7 T, 298 K, $B_1 = 1064$ Hz (25 μT), concentration = 12 mM (66% H_2O -HEPES buffer 0.1M in CD_3CN) and irradiation time = 3 s.

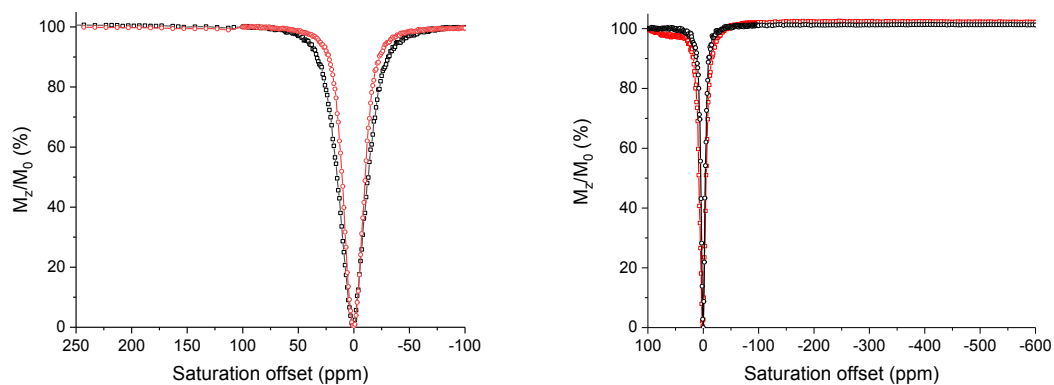


Fig. S17 CEST spectra of 13 mM solution of $[\text{Yb}(\text{L}_1)]^{3+}$ (Left) and $[\text{Dy}(\text{L}_1)]^{3+}$ (Right) in oxidized (black) and reduced (red) forms using 2 eq of sodium ascorbate. Recorded at 11.7 T, 298 K, in mixture of 0.1M HEPES buffer pH 7.4 and CD_3CN (2/1), $B_1 = 25 \mu\text{T}$, and irradiation time of 3 s.

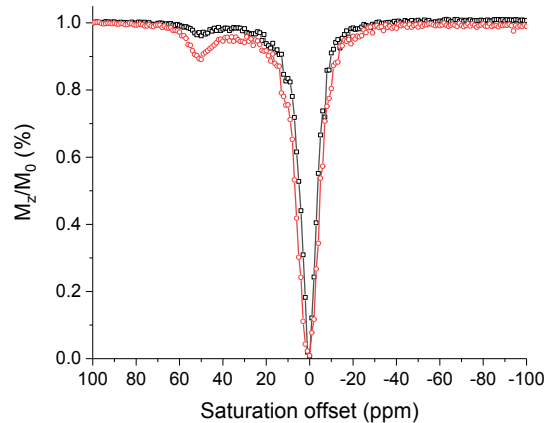


Fig. S18 CEST spectra of 14 mM solution of $[\text{Eu}(\text{L}_1)]^{3+}$ in oxidized (black) and reduced (red) forms using sodium ascorbate. Recorded at 11.7 T, 298 K, in mixture of 0.1M HEPES buffer pH 7.4 and CD_3CN (2/1), $B_1 = 25 \mu\text{T}$, and irradiation time of 3 s.

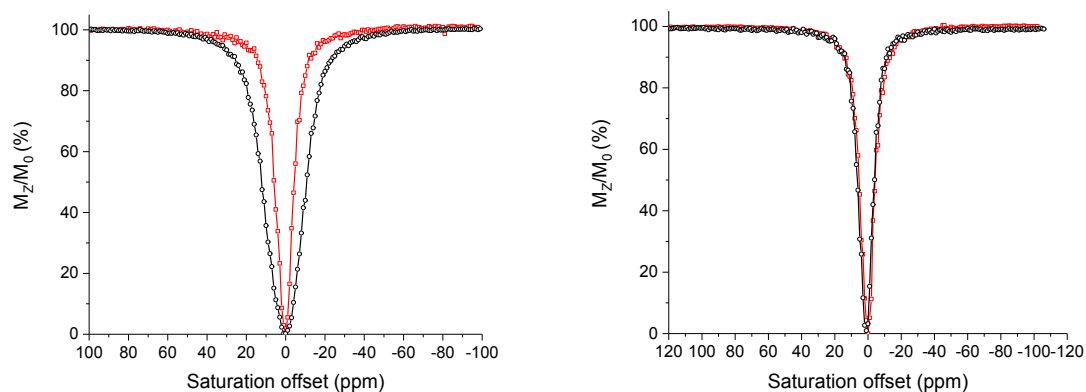


Fig. S19 CEST spectra of 20 mM solution of $[\text{Yb}(\text{L}_2)]^{3+}$ (Left) and $[\text{Dy}(\text{L}_2)]^{3+}$ (Right) in oxidized (black) and reduced (red) forms using 2 eq of sodium ascorbate. Recorded at 11.7 T, 298 K, in mixture of 0.1M HEPES buffer pH 7.4 and CD_3CN (2/1), $B_1 = 25 \mu\text{T}$, and irradiation time of 3 s.

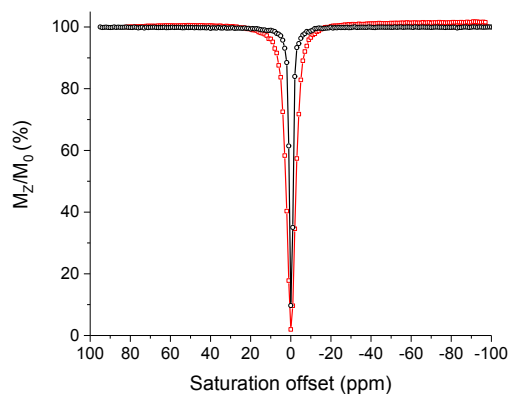


Fig. S20 CEST spectra of 20 mM solution of $[\text{Eu}(\text{L}_2)]^{3+}$ in oxidized (black) and reduced (red) forms using 2 eq of sodium ascorbate. Recorded at 11.7 T, 298 K, in mixture of 0.1M HEPES buffer pH 7.4 and CD_3CN (2/1), $B_1 = 25 \mu\text{T}$, and irradiation time of 3 s.

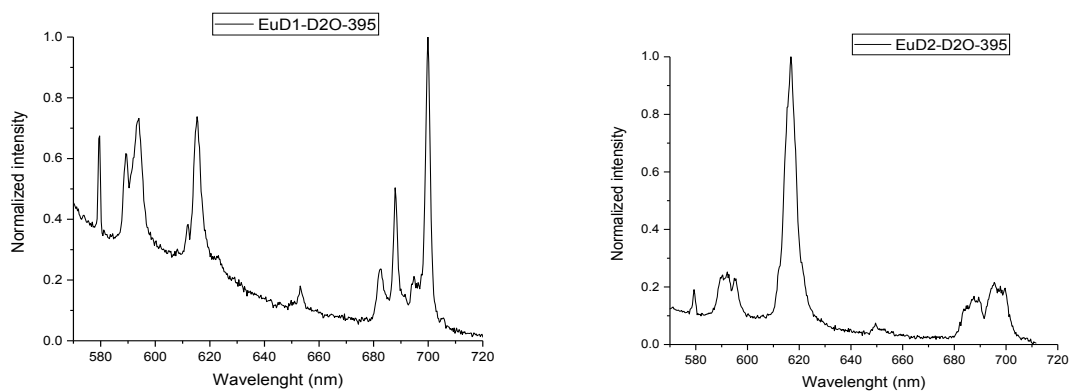


Fig. S21 Luminescence spectra of $[\text{Eu}(\text{L}_1)]^{3+}$ (left) and $[\text{Eu}(\text{L}_2)]^{3+}$ (right) in D_2O

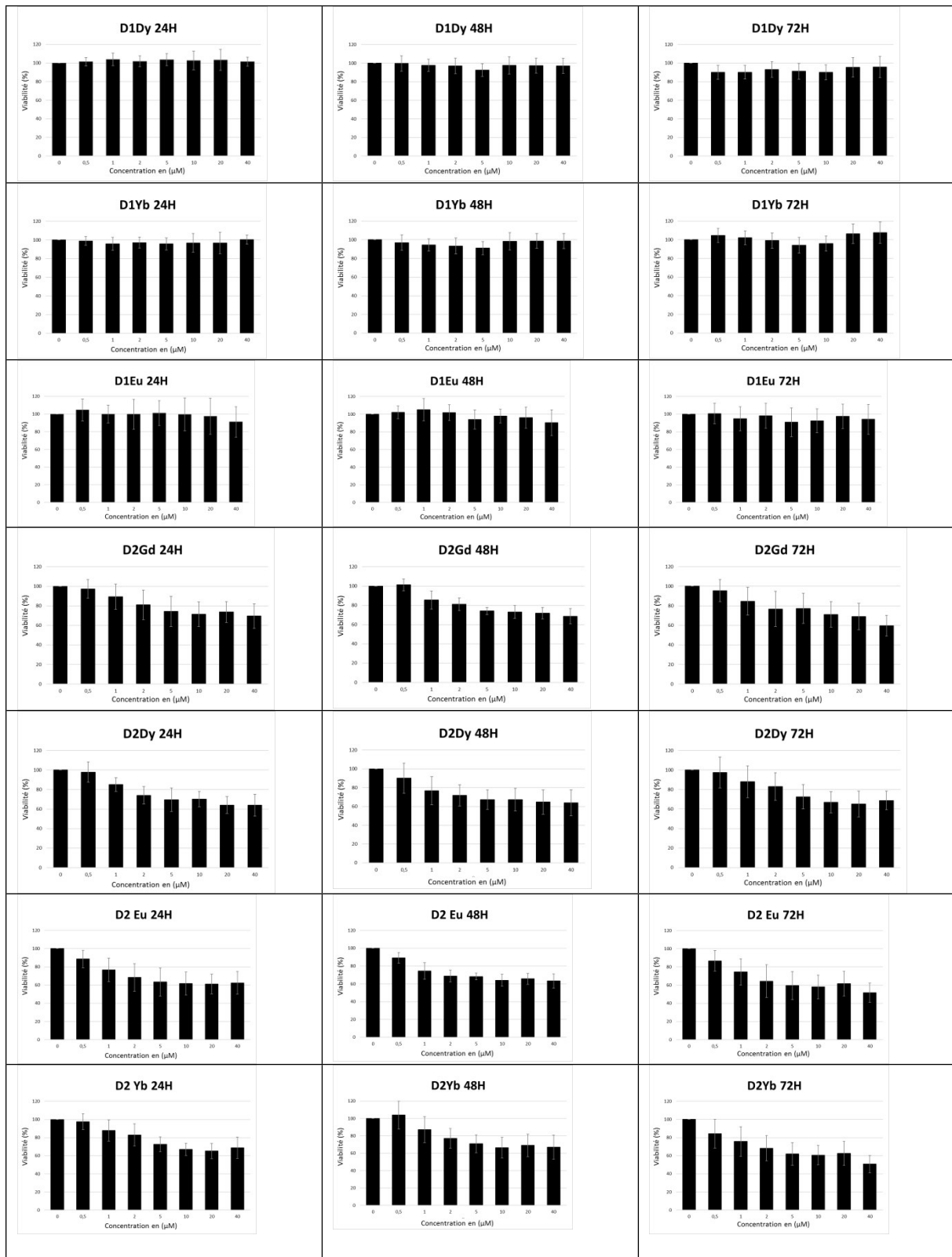


Fig. S22 Cytotoxicity of D1 complexes tested in this study. M21 cells were incubated with different complexes at different time and concentration. Their viability was analysed using MTT assay.

XYZ coordinates (B3LYP/6-31g*-LANL2DZ for Y/PCM)

- $[Y(L_1)]^{3+}$ as a function of the dihedral angle O(amide)-Y-O(water)-H(water):

-15°

Y	1.508060000	0.059608000	0.339153000
O	-0.763018000	0.363506000	-0.148712000
O	0.802212000	-2.005156000	1.235769000
O	-7.305693000	-0.323625000	1.029375000
O	1.454688000	2.397298000	0.708447000
N	-6.222369000	0.068112000	0.458582000
N	1.077193000	1.177982000	-2.052005000
N	3.691176000	1.341361000	-0.508940000
N	-2.509008000	1.221658000	-1.314110000
H	-2.793969000	1.806052000	-2.093345000
N	0.944253000	-1.797086000	-1.504187000
N	3.558311000	-1.637177000	0.048418000
N	2.374771000	4.451218000	0.900396000
H	1.492818000	4.851353000	1.199547000
H	3.175770000	5.065325000	0.830401000
N	-0.227680000	-4.013991000	1.166615000
H	-0.137060000	-4.128530000	2.169526000
H	-0.686926000	-4.748250000	0.643715000
C	-0.237038000	1.857289000	-1.959623000
H	-0.662814000	2.062884000	-2.950133000
H	-0.097562000	2.818571000	-1.455846000
C	-3.568864000	0.614023000	-0.493361000
H	-3.052758000	-0.070374000	0.181033000
C	-1.209516000	1.078796000	-1.086685000
C	0.219565000	-2.906898000	0.586929000
C	3.817205000	2.570553000	0.307293000
H	4.467417000	3.314767000	-0.170095000
H	4.270060000	2.310261000	1.269006000
C	2.455526000	3.152796000	0.641306000
C	-5.422379000	1.094754000	1.210556000
C	-4.552679000	-0.146606000	-1.384829000
H	-5.014396000	0.563404000	-2.083459000
H	-4.024514000	-0.895278000	-1.984832000
C	-4.324666000	1.685076000	0.299729000
H	-3.630555000	2.258943000	0.923037000
H	-4.782285000	2.387369000	-0.408836000
C	-5.661493000	-0.859171000	-0.582632000
C	2.150693000	2.173209000	-2.349622000
H	1.911103000	3.101643000	-1.830371000
H	2.164690000	2.415797000	-3.420988000
C	-0.037527000	-2.724734000	-0.898580000
H	-0.066868000	-3.689726000	-1.421417000
H	-1.035564000	-2.282115000	-0.973941000
C	0.351700000	-1.158068000	-2.716185000
H	-0.702485000	-0.962133000	-2.516121000
H	0.381744000	-1.847463000	-3.571031000

C	-4.822590000	0.447586000	2.477941000
H	-5.614630000	-0.051673000	3.043282000
H	-4.375899000	1.220822000	3.112066000
H	-4.047558000	-0.289174000	2.248183000
C	-6.387489000	2.218748000	1.623735000
H	-6.882368000	2.647925000	0.746184000
H	-5.826537000	3.012335000	2.128141000
H	-7.152373000	1.841209000	2.305062000
C	3.990525000	-2.005284000	1.414659000
H	5.014058000	-2.401356000	1.428046000
H	3.330509000	-2.791087000	1.794341000
C	-6.809546000	-1.228680000	-1.536830000
H	-6.422341000	-1.857663000	-2.345025000
H	-7.251523000	-0.329467000	-1.978644000
H	-7.591399000	-1.776684000	-1.007707000
C	4.899996000	0.485237000	-0.315818000
H	5.204937000	0.558220000	0.728836000
H	5.741211000	0.866255000	-0.910667000
C	4.666408000	-0.972447000	-0.700371000
H	4.439862000	-1.041904000	-1.764983000
H	5.605121000	-1.524134000	-0.549703000
C	-5.134984000	-2.138836000	0.102173000
H	-4.878453000	-2.885823000	-0.656636000
H	-5.913019000	-2.553518000	0.749349000
H	-4.243366000	-1.956579000	0.709589000
C	3.110991000	-2.850648000	-0.699323000
H	2.608094000	-3.519351000	-0.000002000
H	3.976655000	-3.405245000	-1.086200000
C	3.542469000	1.682132000	-1.956094000
H	3.799647000	0.794109000	-2.535101000
H	4.273052000	2.454049000	-2.236803000
C	3.837726000	-0.841839000	2.381775000
C	2.195391000	-2.521319000	-1.876897000
H	2.731135000	-1.909397000	-2.603421000
H	1.945349000	-3.459705000	-2.391941000
C	1.061703000	0.130759000	-3.116638000
H	2.095559000	-0.083837000	-3.390948000
H	0.580195000	0.524387000	-4.022812000
O	2.983521000	0.053494000	2.162430000
O	0.242236000	0.513652000	2.399148000
H	0.664332000	1.183912000	2.963583000
H	-0.631530000	0.873823000	2.165951000
N	4.595431000	-0.833872000	3.469911000
H	5.293981000	-1.544597000	3.645254000
H	4.464229000	-0.112422000	4.169796000

-25°

Y	1.504994000	0.059635000	0.337668000
O	-0.761039000	0.370503000	-0.145325000
O	0.810317000	-2.013959000	1.228496000
O	-7.303892000	-0.332996000	1.027843000

O	1.444587000	2.399781000	0.699925000
N	-6.221239000	0.062112000	0.458079000
N	1.076000000	1.184229000	-2.052448000
N	3.687057000	1.344451000	-0.502903000
N	-2.508806000	1.226416000	-1.309520000
H	-2.794775000	1.809841000	-2.089100000
N	0.943843000	-1.791487000	-1.509613000
N	3.558348000	-1.634891000	0.043684000
N	2.365523000	4.452166000	0.906092000
H	1.481949000	4.852521000	1.199997000
H	3.167848000	5.065327000	0.843903000
N	-0.222286000	-4.021354000	1.152655000
H	-0.128529000	-4.141276000	2.154623000
H	-0.683933000	-4.752347000	0.627345000
C	-0.238208000	1.863089000	-1.958536000
H	-0.665923000	2.067137000	-2.948558000
H	-0.098495000	2.824989000	-1.456167000
C	-3.567583000	0.616687000	-0.489153000
H	-3.049870000	-0.063297000	0.188472000
C	-1.208804000	1.084650000	-1.083197000
C	0.224376000	-2.911513000	0.577348000
C	3.809797000	2.571638000	0.316809000
H	4.463513000	3.316261000	-0.155166000
H	4.256926000	2.308518000	1.280455000
C	2.446390000	3.154207000	0.643400000
C	-5.427249000	1.094189000	1.208963000
C	-4.546104000	-0.150774000	-1.380811000
H	-5.008414000	0.555210000	-2.083102000
H	-4.013269000	-0.899234000	-1.976948000
C	-4.330089000	1.686657000	0.298947000
H	-3.640012000	2.265549000	0.922063000
H	-4.789233000	2.384843000	-0.412706000
C	-5.654484000	-0.865290000	-0.579825000
C	2.150220000	2.179522000	-2.346771000
H	1.909214000	3.107898000	-1.828278000
H	2.167433000	2.422258000	-3.418077000
C	-0.037217000	-2.721390000	-0.906415000
H	-0.069128000	-3.683451000	-1.434474000
H	-1.034905000	-2.277076000	-0.976673000
C	0.350537000	-1.150190000	-2.720059000
H	-0.703426000	-0.954065000	-2.518672000
H	0.379427000	-1.838287000	-3.575989000
C	-4.827563000	0.452762000	2.479315000
H	-5.618830000	-0.048075000	3.044324000
H	-4.385100000	1.229388000	3.112271000
H	-4.049211000	-0.281557000	2.253021000
C	-6.398050000	2.215142000	1.616967000
H	-6.892037000	2.640548000	0.737070000
H	-5.841831000	3.012051000	2.121398000
H	-7.163442000	1.835909000	2.296761000
C	3.989551000	-2.008342000	1.408824000
H	5.013868000	-2.402379000	1.421810000

H	3.330489000	-2.797024000	1.784047000
C	-6.798944000	-1.240857000	-1.535986000
H	-6.407636000	-1.870082000	-2.342037000
H	-7.243031000	-0.344091000	-1.980648000
H	-7.580106000	-1.790587000	-1.007625000
C	4.897080000	0.490120000	-0.310012000
H	5.199166000	0.559715000	0.735750000
H	5.739070000	0.875157000	-0.901180000
C	4.666829000	-0.966367000	-0.700803000
H	4.442250000	-1.032220000	-1.766072000
H	5.606101000	-1.517227000	-0.550535000
C	-5.125030000	-2.141566000	0.109050000
H	-4.864975000	-2.889619000	-0.647510000
H	-5.902678000	-2.557117000	0.756110000
H	-4.234860000	-1.954795000	0.717199000
C	3.112703000	-2.845911000	-0.709179000
H	2.611876000	-3.518854000	-0.012562000
H	3.979162000	-3.396980000	-1.099314000
C	3.541070000	1.688413000	-1.949851000
H	3.800070000	0.801641000	-2.529931000
H	4.272092000	2.461183000	-2.227089000
C	3.833197000	-0.850591000	2.381945000
C	2.195674000	-2.513624000	-1.884829000
H	2.730496000	-1.898902000	-2.609693000
H	1.946123000	-3.450607000	-2.402659000
C	1.060581000	0.139175000	-3.118853000
H	2.094381000	-0.074787000	-3.393973000
H	0.578670000	0.534104000	-4.024278000
O	2.975466000	0.043042000	2.167617000
O	0.263010000	0.505173000	2.409606000
H	0.773652000	1.025822000	3.053256000
H	-0.548385000	1.012374000	2.234480000
N	4.590819000	-0.845646000	3.469909000
H	5.291688000	-1.555053000	3.641406000
H	4.457317000	-0.128336000	4.173631000

-35°

Y	1.502382000	0.059538000	0.335583000
O	-0.760009000	0.376145000	-0.143707000
O	0.812514000	-2.015507000	1.225106000
O	-7.303023000	-0.340722000	1.026381000
O	1.439476000	2.399910000	0.699022000
N	-6.220697000	0.057241000	0.457970000
N	1.074115000	1.190136000	-2.052276000
N	3.683989000	1.345807000	-0.499979000
N	-2.509494000	1.231877000	-1.305471000
H	-2.796399000	1.815304000	-2.084679000
N	0.941593000	-1.786617000	-1.513526000
N	3.557544000	-1.634943000	0.037823000
N	2.361402000	4.451086000	0.913627000
H	1.477411000	4.851411000	1.206288000

H	3.164408000	5.063722000	0.855340000
N	-0.220339000	-4.022653000	1.145584000
H	-0.124988000	-4.145275000	2.147078000
H	-0.682779000	-4.752283000	0.619075000
C	-0.239746000	1.869664000	-1.956660000
H	-0.668497000	2.074008000	-2.946167000
H	-0.099141000	2.831363000	-1.454244000
C	-3.567161000	0.619406000	-0.485819000
H	-3.047979000	-0.058415000	0.192850000
C	-1.209000000	1.090530000	-1.080391000
C	0.225342000	-2.911278000	0.572548000
C	3.805718000	2.570969000	0.322940000
H	4.461068000	3.316218000	-0.145745000
H	4.250570000	2.305156000	1.286942000
C	2.441838000	3.153748000	0.647487000
C	-5.430709000	1.091898000	1.209519000
C	-4.542213000	-0.151623000	-1.378312000
H	-5.005444000	0.552513000	-2.081840000
H	-4.006282000	-0.898928000	-1.973127000
C	-4.334113000	1.687316000	0.300697000
H	-3.646709000	2.268662000	0.924460000
H	-4.794491000	2.383756000	-0.411875000
C	-5.649856000	-0.868883000	-0.578806000
C	2.149111000	2.185133000	-2.344491000
H	1.908005000	3.113170000	-1.825461000
H	2.167813000	2.428890000	-3.415535000
C	-0.038957000	-2.717151000	-0.910349000
H	-0.073029000	-3.677819000	-1.440768000
H	-1.036323000	-2.271557000	-0.977390000
C	0.347011000	-1.142962000	-2.722238000
H	-0.706540000	-0.946452000	-2.519087000
H	0.374316000	-1.829885000	-3.579144000
C	-4.830805000	0.452548000	2.480818000
H	-5.621380000	-0.050268000	3.045040000
H	-4.391187000	1.230599000	3.114003000
H	-4.050175000	-0.279703000	2.255700000
C	-6.405347000	2.210079000	1.615933000
H	-6.899197000	2.634036000	0.735257000
H	-5.852234000	3.008617000	2.121202000
H	-7.170720000	1.828686000	2.294546000
C	3.990077000	-2.013586000	1.401067000
H	5.014910000	-2.406325000	1.411919000
H	3.332347000	-2.804709000	1.773462000
C	-6.791907000	-1.247821000	-1.536530000
H	-6.397771000	-1.876298000	-2.341792000
H	-7.237715000	-0.352387000	-1.982161000
H	-7.572411000	-1.799412000	-1.009124000
C	4.894505000	0.491754000	-0.308723000
H	5.195397000	0.558171000	0.737609000
H	5.736765000	0.879512000	-0.897717000
C	4.665524000	-0.963538000	-0.704689000
H	4.440934000	-1.026079000	-1.770154000

H	5.605188000	-1.514239000	-0.556320000
C	-5.118041000	-2.143549000	0.111227000
H	-4.855388000	-2.891301000	-0.644726000
H	-5.895352000	-2.560686000	0.757678000
H	-4.228969000	-1.954309000	0.720195000
C	3.111398000	-2.843607000	-0.718625000
H	2.611639000	-3.519093000	-0.023687000
H	3.977557000	-3.393092000	-1.111638000
C	3.539305000	1.693082000	-1.946499000
H	3.798754000	0.807411000	-2.528036000
H	4.270929000	2.466202000	-2.221166000
C	3.832606000	-0.860910000	2.379617000
C	2.192797000	-2.508165000	-1.892065000
H	2.726802000	-1.891662000	-2.616043000
H	1.942362000	-3.443801000	-2.411902000
C	1.057365000	0.146668000	-3.120124000
H	2.090785000	-0.067156000	-3.396850000
H	0.574538000	0.542880000	-4.024489000
O	2.971859000	0.031526000	2.170504000
O	0.286330000	0.506780000	2.421742000
H	0.873488000	0.884022000	3.099764000
H	-0.440786000	1.142636000	2.307582000
N	4.591325000	-0.858908000	3.466538000
H	5.294212000	-1.567340000	3.633907000
H	4.457110000	-0.145033000	4.173645000

-45°

Y	1.500929000	0.059859000	0.333231000
O	-0.760169000	0.376242000	-0.145553000
O	0.813372000	-2.013309000	1.224059000
O	-7.302832000	-0.345496000	1.027530000
O	1.431687000	2.399348000	0.699314000
N	-6.221005000	0.053567000	0.458924000
N	1.071933000	1.193569000	-2.053188000
N	3.679612000	1.348553000	-0.498155000
N	-2.511254000	1.232497000	-1.304551000
H	-2.799038000	1.816479000	-2.083005000
N	0.941929000	-1.784272000	-1.516079000
N	3.558744000	-1.634005000	0.033333000
N	2.352717000	4.450318000	0.919833000
H	1.468095000	4.849770000	1.211824000
H	3.155616000	5.063351000	0.864139000
N	-0.220409000	-4.019836000	1.144374000
H	-0.125709000	-4.142080000	2.145982000
H	-0.682784000	-4.749539000	0.617897000
C	-0.242483000	1.871952000	-1.957231000
H	-0.671703000	2.075726000	-2.946658000
H	-0.102790000	2.833826000	-1.454953000
C	-3.567937000	0.619119000	-0.484439000
H	-3.047605000	-0.056313000	0.195741000
C	-1.210364000	1.091419000	-1.080705000

C	0.226184000	-2.909007000	0.571171000
C	3.798854000	2.571984000	0.327904000
H	4.454834000	3.318619000	-0.137609000
H	4.241835000	2.304015000	1.292201000
C	2.434089000	3.153675000	0.651223000
C	-5.433363000	1.091054000	1.209013000
C	-4.541019000	-0.155483000	-1.376064000
H	-5.004930000	0.546412000	-2.081369000
H	-4.003285000	-0.902982000	-1.969016000
C	-4.337484000	1.686911000	0.299670000
H	-3.651514000	2.270788000	0.922641000
H	-4.798900000	2.381118000	-0.414429000
C	-5.648021000	-0.873202000	-0.576084000
C	2.146210000	2.189722000	-2.343637000
H	1.903615000	3.117186000	-1.824250000
H	2.166040000	2.434250000	-3.414481000
C	-0.037528000	-2.715596000	-0.912133000
H	-0.070434000	-3.676696000	-1.441832000
H	-1.035406000	-2.271231000	-0.979689000
C	0.346171000	-1.139757000	-2.723920000
H	-0.707320000	-0.943822000	-2.519998000
H	0.373253000	-1.826049000	-3.581326000
C	-4.832825000	0.455081000	2.481700000
H	-5.622672000	-0.048346000	3.046393000
H	-4.395022000	1.235100000	3.113722000
H	-4.050563000	-0.275930000	2.258193000
C	-6.410363000	2.208082000	1.612923000
H	-6.904405000	2.629653000	0.731204000
H	-5.859087000	3.008510000	2.117220000
H	-7.175498000	1.826420000	2.291648000
C	3.993996000	-2.016554000	1.394544000
H	5.019373000	-2.407942000	1.402596000
H	3.338030000	-2.809839000	1.765469000
C	-6.788940000	-1.255472000	-1.533847000
H	-6.393372000	-1.884586000	-2.337918000
H	-7.235904000	-0.361439000	-1.981128000
H	-7.568880000	-1.807476000	-1.006032000
C	4.891508000	0.495850000	-0.308445000
H	5.191972000	0.560175000	0.738124000
H	5.733245000	0.886581000	-0.896192000
C	4.664883000	-0.958812000	-0.708443000
H	4.439518000	-1.018793000	-1.773888000
H	5.605680000	-1.508196000	-0.562435000
C	-5.114560000	-2.145914000	0.116265000
H	-4.850672000	-2.894571000	-0.638364000
H	-5.891400000	-2.563078000	0.763261000
H	-4.225881000	-1.954301000	0.725047000
C	3.112868000	-2.841488000	-0.725169000
H	2.613930000	-3.518446000	-0.030989000
H	3.979051000	-3.389830000	-1.119751000
C	3.536264000	1.698703000	-1.944340000
H	3.797539000	0.814440000	-2.527173000

H	4.267504000	2.473106000	-2.216317000
C	3.836287000	-0.867842000	2.377183000
C	2.193037000	-2.504824000	-1.897043000
H	2.726004000	-1.887077000	-2.620729000
H	1.942360000	-3.439775000	-2.417976000
C	1.055826000	0.150574000	-3.121452000
H	2.089331000	-0.062393000	-3.398616000
H	0.572431000	0.546701000	-4.025550000
O	2.973209000	0.023621000	2.172084000
O	0.306874000	0.508639000	2.433387000
H	0.945926000	0.751728000	3.126305000
H	-0.314658000	1.253508000	2.366171000
N	4.596354000	-0.867905000	3.462939000
H	5.300747000	-1.575645000	3.627002000
H	4.462081000	-0.156410000	4.172459000

-55°

Y	1.499933000	0.060600000	0.330302000
O	-0.760031000	0.370269000	-0.154412000
O	0.808323000	-2.005328000	1.226249000
O	-7.300420000	-0.345599000	1.031953000
O	1.427104000	2.398804000	0.700264000
N	-6.219406000	0.053187000	0.461592000
N	1.071700000	1.193857000	-2.055485000
N	3.676825000	1.349181000	-0.496963000
N	-2.512240000	1.231354000	-1.308011000
H	-2.800804000	1.817882000	-2.084247000
N	0.942864000	-1.784605000	-1.516947000
N	3.558569000	-1.635371000	0.032417000
N	2.348335000	4.449330000	0.923984000
H	1.463516000	4.848500000	1.215873000
H	3.151352000	5.062391000	0.869844000
N	-0.227402000	-4.010689000	1.149674000
H	-0.136199000	-4.129359000	2.152050000
H	-0.688703000	-4.741908000	0.624340000
C	-0.243567000	1.870873000	-1.961778000
H	-0.671749000	2.073417000	-2.951914000
H	-0.105926000	2.833367000	-1.460114000
C	-3.567866000	0.617708000	-0.486763000
H	-3.046667000	-0.058790000	0.191680000
C	-1.211031000	1.088703000	-1.086295000
C	0.222438000	-2.902680000	0.573941000
C	3.794855000	2.571548000	0.331091000
H	4.451646000	3.318758000	-0.132262000
H	4.236355000	2.302028000	1.295666000
C	2.429916000	3.153309000	0.653808000
C	-5.429435000	1.089330000	1.211120000
C	-4.543381000	-0.155235000	-1.377121000
H	-5.008351000	0.547737000	-2.080658000
H	-4.007470000	-0.902485000	-1.972041000
C	-4.334998000	1.685230000	0.300067000

H	-3.647237000	2.267941000	0.922155000
H	-4.797427000	2.380457000	-0.412391000
C	-5.649147000	-0.873016000	-0.575473000
C	2.145395000	2.191005000	-2.344261000
H	1.901136000	3.117997000	-1.824750000
H	2.166582000	2.436033000	-3.414965000
C	-0.036789000	-2.714695000	-0.911145000
H	-0.067212000	-3.678068000	-1.436863000
H	-1.035054000	-2.271956000	-0.982959000
C	0.347828000	-1.140565000	-2.725599000
H	-0.705929000	-0.945040000	-2.523016000
H	0.376248000	-1.827118000	-3.582729000
C	-4.826805000	0.451643000	2.481969000
H	-5.615954000	-0.051458000	3.047932000
H	-4.386792000	1.230655000	3.113692000
H	-4.045779000	-0.279957000	2.256140000
C	-6.404729000	2.206679000	1.618245000
H	-6.900433000	2.629461000	0.738044000
H	-5.851713000	3.006199000	2.122076000
H	-7.168621000	1.824939000	2.298336000
C	3.996099000	-2.019843000	1.392230000
H	5.022009000	-2.409870000	1.398315000
H	3.341882000	-2.814882000	1.762569000
C	-6.792280000	-1.253778000	-1.531199000
H	-6.398701000	-1.882365000	-2.336655000
H	-7.239674000	-0.359094000	-1.976745000
H	-7.571424000	-1.805837000	-1.002275000
C	4.888981000	0.496419000	-0.307454000
H	5.188893000	0.559638000	0.739329000
H	5.730790000	0.888267000	-0.894304000
C	4.663158000	-0.957901000	-0.709599000
H	4.436627000	-1.016250000	-1.774868000
H	5.604695000	-1.506553000	-0.565629000
C	-5.115014000	-2.146667000	0.114621000
H	-4.852890000	-2.894719000	-0.641231000
H	-5.890846000	-2.564091000	0.762663000
H	-4.225105000	-1.956092000	0.721933000
C	3.112701000	-2.842679000	-0.726257000
H	2.612840000	-3.519082000	-0.032063000
H	3.978771000	-3.391679000	-1.120205000
C	3.535304000	1.701153000	-1.943134000
H	3.798550000	0.817940000	-2.526637000
H	4.266190000	2.476640000	-2.212813000
C	3.837562000	-0.873537000	2.376983000
C	2.193335000	-2.505992000	-1.898124000
H	2.726505000	-1.888857000	-2.622157000
H	1.941994000	-3.440963000	-2.418694000
C	1.057735000	0.149920000	-3.122936000
H	2.091755000	-0.062922000	-3.398345000
H	0.575576000	0.545143000	-4.028099000
O	2.972565000	0.016695000	2.173587000
O	0.310985000	0.523477000	2.436328000

H	0.976422000	0.644692000	3.137354000
H	-0.186454000	1.358648000	2.397524000
N	4.597797000	-0.874215000	3.462429000
H	5.303399000	-1.581113000	3.625051000
H	4.462896000	-0.163934000	4.173066000

-65°

Y	1.499544000	0.061184000	0.328547000
O	-0.760266000	0.364488000	-0.161408000
O	0.804072000	-1.996973000	1.230009000
O	-7.300158000	-0.346954000	1.033733000
O	1.424480000	2.397848000	0.705549000
N	-6.219570000	0.052067000	0.462724000
N	1.070385000	1.194762000	-2.056402000
N	3.674315000	1.349780000	-0.497468000
N	-2.513762000	1.231438000	-1.308877000
H	-2.802849000	1.820927000	-2.082659000
N	0.942989000	-1.784733000	-1.516779000
N	3.559032000	-1.637133000	0.029601000
N	2.346116000	4.448212000	0.928516000
H	1.461690000	4.847074000	1.222157000
H	3.148907000	5.061534000	0.873314000
N	-0.233548000	-4.001169000	1.157008000
H	-0.145264000	-4.116221000	2.160088000
H	-0.693856000	-4.734037000	0.633065000
C	-0.245354000	1.870852000	-1.963693000
H	-0.672875000	2.073258000	-2.954169000
H	-0.109111000	2.833463000	-1.461838000
C	-3.568676000	0.617106000	-0.487353000
H	-3.046841000	-0.059350000	0.190641000
C	-1.212229000	1.086713000	-1.089476000
C	0.219193000	-2.896037000	0.578495000
C	3.792092000	2.570980000	0.332576000
H	4.448835000	3.318943000	-0.129525000
H	4.233686000	2.299830000	1.296687000
C	2.427589000	3.152732000	0.657453000
C	-5.429259000	1.088256000	1.211836000
C	-4.544666000	-0.155972000	-1.377115000
H	-5.010122000	0.546957000	-2.080366000
H	-4.009009000	-0.903119000	-1.972400000
C	-4.335527000	1.684343000	0.300114000
H	-3.647394000	2.267130000	0.921725000
H	-4.798558000	2.379540000	-0.412000000
C	-5.649875000	-0.873929000	-0.574841000
C	2.143295000	2.192793000	-2.344514000
H	1.898207000	3.119170000	-1.824175000
H	2.164516000	2.438777000	-3.414999000
C	-0.036374000	-2.713533000	-0.908209000
H	-0.064698000	-3.679242000	-1.429735000
H	-1.035103000	-2.272516000	-0.983648000
C	0.347448000	-1.140749000	-2.725432000

H	-0.706360000	-0.945682000	-2.523081000
H	0.376316000	-1.827332000	-3.582500000
C	-4.825697000	0.450550000	2.482241000
H	-5.614432000	-0.052513000	3.048814000
H	-4.385134000	1.229551000	3.113597000
H	-4.044855000	-0.281057000	2.255807000
C	-6.404452000	2.205423000	1.619702000
H	-6.900789000	2.628230000	0.739867000
H	-5.851207000	3.004965000	2.123250000
H	-7.167850000	1.823517000	2.300254000
C	4.000042000	-2.023573000	1.387553000
H	5.025932000	-2.413712000	1.390561000
H	3.346841000	-2.819215000	1.758486000
C	-6.793617000	-1.254663000	-1.529846000
H	-6.400505000	-1.883105000	-2.335646000
H	-7.241375000	-0.359958000	-1.974985000
H	-7.572376000	-1.806864000	-1.000501000
C	4.886860000	0.496778000	-0.309603000
H	5.187664000	0.558970000	0.736954000
H	5.728002000	0.889605000	-0.896710000
C	4.661316000	-0.957256000	-0.713605000
H	4.432698000	-1.013998000	-1.778501000
H	5.603773000	-1.505097000	-0.572528000
C	-5.115211000	-2.147617000	0.114782000
H	-4.853363000	-2.895513000	-0.641323000
H	-5.890646000	-2.565268000	0.763155000
H	-4.225022000	-1.956992000	0.721664000
C	3.112331000	-2.844095000	-0.728885000
H	2.612135000	-3.519960000	-0.034235000
H	3.977807000	-3.393861000	-1.123121000
C	3.533352000	1.703762000	-1.943356000
H	3.797715000	0.821589000	-2.527897000
H	4.263792000	2.480189000	-2.211393000
C	3.843292000	-0.878687000	2.373678000
C	2.192274000	-2.507037000	-1.899731000
H	2.724966000	-1.890334000	-2.624465000
H	1.939578000	-3.441825000	-2.419958000
C	1.057247000	0.149961000	-3.123104000
H	2.091445000	-0.062785000	-3.397965000
H	0.575336000	0.544427000	-4.028728000
O	2.976300000	0.010297000	2.172997000
O	0.315826000	0.537169000	2.439550000
H	0.983351000	0.528887000	3.149205000
H	-0.042395000	1.442100000	2.431519000
N	4.606359000	-0.879022000	3.457071000
H	5.313340000	-1.585086000	3.617376000
H	4.472649000	-0.169139000	4.168344000

-75°

Y	1.499858000	0.061712000	0.327734000
O	-0.760991000	0.354752000	-0.170169000

O	0.799675000	-1.987494000	1.236667000
O	-7.301698000	-0.344932000	1.035341000
O	1.424048000	2.396489000	0.712963000
N	-6.221121000	0.052787000	0.463378000
N	1.069106000	1.193061000	-2.057423000
N	3.672647000	1.350308000	-0.500414000
N	-2.515598000	1.228638000	-1.311107000
H	-2.804878000	1.821605000	-2.082141000
N	0.944048000	-1.787298000	-1.514206000
N	3.560264000	-1.638235000	0.028335000
N	2.345236000	4.447587000	0.929724000
H	1.461664000	4.845893000	1.226837000
H	3.147247000	5.061655000	0.870831000
N	-0.236966000	-3.992068000	1.168693000
H	-0.151677000	-4.102594000	2.172566000
H	-0.695495000	-4.727470000	0.646696000
C	-0.247398000	1.867775000	-1.966395000
H	-0.673817000	2.069913000	-2.957422000
H	-0.113111000	2.830539000	-1.464250000
C	-3.570262000	0.615031000	-0.488838000
H	-3.048335000	-0.061249000	0.189267000
C	-1.213828000	1.081280000	-1.093990000
C	0.217031000	-2.889602000	0.586615000
C	3.790660000	2.571196000	0.330187000
H	4.445933000	3.320018000	-0.132523000
H	4.234279000	2.299740000	1.293305000
C	2.426906000	3.152341000	0.659502000
C	-5.429635000	1.089061000	1.211110000
C	-4.547403000	-0.158033000	-1.377334000
H	-5.012736000	0.544694000	-2.080866000
H	-4.012727000	-0.906069000	-1.972384000
C	-4.335928000	1.683393000	0.298272000
H	-3.647004000	2.266241000	0.918937000
H	-4.798864000	2.378305000	-0.414200000
C	-5.652694000	-0.874476000	-0.573790000
C	2.140470000	2.192358000	-2.346259000
H	1.894629000	3.118154000	-1.825046000
H	2.160483000	2.439018000	-3.416614000
C	-0.035017000	-2.714074000	-0.901835000
H	-0.061498000	-3.682551000	-1.418270000
H	-1.034101000	-2.274615000	-0.981014000
C	0.348092000	-1.144675000	-2.723573000
H	-0.705970000	-0.950606000	-2.522161000
H	0.378231000	-1.831925000	-3.580046000
C	-4.825924000	0.452126000	2.481812000
H	-5.614779000	-0.049647000	3.049374000
H	-4.384233000	1.231369000	3.112076000
H	-4.045879000	-0.280404000	2.255642000
C	-6.403730000	2.207395000	1.618430000
H	-6.900140000	2.629805000	0.738443000
H	-5.849578000	3.006944000	2.120966000
H	-7.167127000	1.826754000	2.299700000

C	4.005092000	-2.023912000	1.385111000
H	5.030912000	-2.414244000	1.385526000
H	3.352935000	-2.819298000	1.758533000
C	-6.797254000	-1.255204000	-1.527817000
H	-6.405046000	-1.884637000	-2.333281000
H	-7.244584000	-0.360553000	-1.973502000
H	-7.576135000	-1.806351000	-0.997555000
C	4.885586000	0.497178000	-0.314017000
H	5.188176000	0.559561000	0.731972000
H	5.725663000	0.890055000	-0.902574000
C	4.659859000	-0.957084000	-0.717707000
H	4.428424000	-1.013680000	-1.781993000
H	5.603216000	-1.504064000	-0.579290000
C	-5.118516000	-2.147955000	0.116581000
H	-4.857640000	-2.896677000	-0.639044000
H	-5.893838000	-2.564519000	0.765795000
H	-4.227824000	-1.957409000	0.722749000
C	3.112985000	-2.846320000	-0.727740000
H	2.612661000	-3.520525000	-0.031404000
H	3.977986000	-3.397327000	-1.121339000
C	3.531193000	1.704869000	-1.946145000
H	3.796378000	0.823323000	-2.531248000
H	4.260727000	2.482204000	-2.213880000
C	3.850632000	-0.877897000	2.369839000
C	2.192093000	-2.510947000	-1.898018000
H	2.724142000	-1.895751000	-2.624468000
H	1.938159000	-3.446428000	-2.416388000
C	1.057246000	0.146302000	-3.122397000
H	2.091755000	-0.066223000	-3.396309000
H	0.575641000	0.539035000	-4.028949000
O	2.982050000	0.009577000	2.170099000
O	0.313726000	0.551461000	2.438200000
H	0.951094000	0.412918000	3.162034000
H	0.104102000	1.502134000	2.463282000
N	4.616981000	-0.875651000	3.450993000
H	5.325062000	-1.580792000	3.610482000
H	4.484870000	-0.164518000	4.161307000

-85°

Y	1.500445000	0.061764000	0.328965000
O	-0.762068000	0.345101000	-0.178982000
O	0.796379000	-1.980260000	1.244736000
O	-7.304060000	-0.343455000	1.034541000
O	1.428374000	2.392978000	0.727456000
N	-6.223276000	0.054035000	0.462806000
N	1.067616000	1.192447000	-2.056871000
N	3.672762000	1.349959000	-0.505430000
N	-2.517413000	1.229667000	-1.311071000
H	-2.806501000	1.827703000	-2.078226000
N	0.943785000	-1.789134000	-1.510559000
N	3.560915000	-1.640088000	0.026214000

N	2.348669000	4.445429000	0.932351000
H	1.466830000	4.842838000	1.235921000
H	3.149193000	5.060740000	0.865979000
N	-0.240219000	-3.984688000	1.179749000
H	-0.156896000	-4.092288000	2.184131000
H	-0.697997000	-4.721532000	0.659078000
C	-0.248951000	1.866807000	-1.966867000
H	-0.674147000	2.069969000	-2.958274000
H	-0.115709000	2.829226000	-1.463675000
C	-3.572088000	0.615477000	-0.489467000
H	-3.050277000	-0.061681000	0.187859000
C	-1.215388000	1.077841000	-1.096998000
C	0.214798000	-2.884095000	0.595353000
C	3.792564000	2.570297000	0.325774000
H	4.444748000	3.320467000	-0.139030000
H	4.240794000	2.298495000	1.286665000
C	2.430350000	3.150189000	0.663784000
C	-5.430917000	1.089044000	1.211365000
C	-4.549972000	-0.156266000	-1.378362000
H	-5.014895000	0.547402000	-2.081227000
H	-4.015896000	-0.904111000	-1.974196000
C	-4.337058000	1.683458000	0.298815000
H	-3.647667000	2.265435000	0.919777000
H	-4.799766000	2.379236000	-0.412982000
C	-5.655646000	-0.872654000	-0.575320000
C	2.137720000	2.192440000	-2.347152000
H	1.892561000	3.117291000	-1.823672000
H	2.154966000	2.440940000	-3.417153000
C	-0.035555000	-2.713122000	-0.894161000
H	-0.062549000	-3.683599000	-1.406765000
H	-1.034376000	-2.273437000	-0.974947000
C	0.347164000	-1.147282000	-2.720217000
H	-0.707025000	-0.954055000	-2.519311000
H	0.378155000	-1.834949000	-3.576300000
C	-4.827253000	0.450454000	2.481266000
H	-5.616332000	-0.051020000	3.048784000
H	-4.384455000	1.228728000	3.111954000
H	-4.048044000	-0.282647000	2.254071000
C	-6.404110000	2.207645000	1.620103000
H	-6.900502000	2.631308000	0.740708000
H	-5.849240000	3.006295000	2.123281000
H	-7.167561000	1.826856000	2.301232000
C	4.009784000	-2.023845000	1.382005000
H	5.034719000	-2.416562000	1.379589000
H	3.357179000	-2.816935000	1.759581000
C	-6.800652000	-1.251694000	-1.529472000
H	-6.409043000	-1.880677000	-2.335579000
H	-7.247396000	-0.356310000	-1.974279000
H	-7.579866000	-1.802743000	-0.999593000
C	4.885532000	0.495772000	-0.321902000
H	5.191869000	0.558908000	0.722869000
H	5.723914000	0.887335000	-0.913734000

C	4.657711000	-0.958820000	-0.723837000
H	4.422499000	-1.015725000	-1.787276000
H	5.601623000	-1.505676000	-0.588550000
C	-5.122232000	-2.147118000	0.113841000
H	-4.861827000	-2.895296000	-0.642491000
H	-5.897783000	-2.563817000	0.762697000
H	-4.231396000	-1.957654000	0.720153000
C	3.112132000	-2.849255000	-0.726722000
H	2.612077000	-3.521608000	-0.028251000
H	3.976131000	-3.401861000	-1.120368000
C	3.529346000	1.705389000	-1.950551000
H	3.793931000	0.824406000	-2.536789000
H	4.258081000	2.483232000	-2.218948000
C	3.860898000	-0.873974000	2.362984000
C	2.189714000	-2.515206000	-1.895906000
H	2.721038000	-1.901961000	-2.624522000
H	1.933466000	-3.451270000	-2.412078000
C	1.055862000	0.143871000	-3.120206000
H	2.090393000	-0.068847000	-3.393860000
H	0.574168000	0.535276000	-4.027304000
O	2.992818000	0.013209000	2.163029000
O	0.303187000	0.558260000	2.431967000
H	0.858590000	0.280854000	3.182208000
H	0.242805000	1.527836000	2.506353000
N	4.632320000	-0.868269000	3.440944000
H	5.340122000	-1.573665000	3.600324000
H	4.504286000	-0.153918000	4.148721000

-95°

Y	1.500509000	0.062408000	0.330693000
O	-0.763594000	0.335900000	-0.188170000
O	0.789754000	-1.972841000	1.251834000
O	-7.305823000	-0.339048000	1.034404000
O	1.438149000	2.388102000	0.742639000
N	-6.224772000	0.057955000	0.462812000
N	1.067015000	1.191969000	-2.055524000
N	3.675607000	1.348065000	-0.511699000
N	-2.518693000	1.232089000	-1.311782000
H	-2.807263000	1.835793000	-2.074643000
N	0.941623000	-1.790853000	-1.507287000
N	3.559483000	-1.642611000	0.024443000
N	2.358251000	4.441212000	0.937777000
H	1.478636000	4.837546000	1.249199000
H	3.157224000	5.057680000	0.863558000
N	-0.247119000	-3.976998000	1.189224000
H	-0.165590000	-4.082222000	2.194026000
H	-0.703896000	-4.715180000	0.669518000
C	-0.249185000	1.866964000	-1.966368000
H	-0.672601000	2.072644000	-2.958068000
H	-0.116280000	2.828268000	-1.460845000
C	-3.573602000	0.617065000	-0.491242000

H	-3.052265000	-0.063551000	0.182964000
C	-1.216582000	1.075382000	-1.100261000
C	0.209261000	-2.878236000	0.602886000
C	3.799245000	2.567874000	0.319559000
H	4.447263000	3.319363000	-0.148893000
H	4.254198000	2.296014000	1.277239000
C	2.439183000	3.146218000	0.668799000
C	-5.429067000	1.088450000	1.214034000
C	-4.554398000	-0.149526000	-1.381314000
H	-5.018954000	0.557595000	-2.080962000
H	-4.022755000	-0.896328000	-1.980626000
C	-4.335258000	1.683762000	0.301968000
H	-3.643763000	2.262131000	0.923952000
H	-4.797564000	2.382959000	-0.406739000
C	-5.660328000	-0.866464000	-0.579109000
C	2.136415000	2.192085000	-2.347455000
H	1.893108000	3.115787000	-1.820814000
H	2.150037000	2.443032000	-3.416956000
C	-0.039141000	-2.711131000	-0.887575000
H	-0.067710000	-3.683338000	-1.396765000
H	-1.037177000	-2.270017000	-0.969805000
C	0.345578000	-1.149048000	-2.717381000
H	-0.708767000	-0.956115000	-2.517650000
H	0.377542000	-1.836792000	-3.573355000
C	-4.824930000	0.443953000	2.480745000
H	-5.614342000	-0.057373000	3.047944000
H	-4.378980000	1.218912000	3.113294000
H	-4.048049000	-0.290398000	2.249735000
C	-6.399132000	2.207671000	1.628454000
H	-6.896391000	2.635338000	0.751498000
H	-5.841524000	3.003431000	2.133180000
H	-7.162003000	1.826254000	2.309899000
C	4.011935000	-2.023702000	1.379681000
H	5.035669000	-2.419573000	1.374874000
H	3.358292000	-2.813733000	1.761937000
C	-6.807364000	-1.240213000	-1.532903000
H	-6.417988000	-1.867178000	-2.341650000
H	-7.253078000	-0.342529000	-1.974103000
H	-7.586874000	-1.791617000	-1.003826000
C	4.886954000	0.491191000	-0.331559000
H	5.197987000	0.555137000	0.711695000
H	5.723837000	0.879725000	-0.927507000
C	4.654413000	-0.963581000	-0.730495000
H	4.414802000	-1.021060000	-1.792909000
H	5.597884000	-1.511997000	-0.598352000
C	-5.128416000	-2.144174000	0.105185000
H	-4.870042000	-2.890225000	-0.653946000
H	-5.904037000	-2.561751000	0.753405000
H	-4.236629000	-1.958333000	0.711240000
C	3.108182000	-2.853154000	-0.724399000
H	2.607535000	-3.522536000	-0.023385000
H	3.970844000	-3.408477000	-1.117233000

C	3.528988000	1.704187000	-1.956014000
H	3.791588000	0.823498000	-2.543634000
H	4.257206000	2.481948000	-2.226048000
C	3.869869000	-0.869157000	2.356263000
C	2.185038000	-2.520467000	-1.893173000
H	2.716382000	-1.909945000	-2.624036000
H	1.926096000	-3.457230000	-2.406737000
C	1.054828000	0.141942000	-3.117626000
H	2.089296000	-0.071636000	-3.390777000
H	0.573655000	0.532844000	-4.025240000
O	3.004498000	0.019543000	2.155244000
O	0.291551000	0.557289000	2.424874000
H	0.733744000	0.140993000	3.185343000
H	0.366956000	1.516440000	2.578275000
N	4.645626000	-0.861538000	3.431615000
H	5.351768000	-1.568468000	3.591260000
H	4.522803000	-0.143586000	4.136602000

-105°

Y	1.500820000	0.062879000	0.332810000
O	-0.765073000	0.325476000	-0.197759000
O	0.788405000	-1.970741000	1.256062000
O	-7.308807000	-0.334283000	1.034315000
O	1.442589000	2.379719000	0.760774000
N	-6.227443000	0.061338000	0.462346000
N	1.066044000	1.192037000	-2.054504000
N	3.676330000	1.350926000	-0.517238000
N	-2.520648000	1.231516000	-1.313314000
H	-2.808782000	1.840275000	-2.072283000
N	0.943729000	-1.792703000	-1.505045000
N	3.561450000	-1.639766000	0.023512000
N	2.355278000	4.436703000	0.944969000
H	1.476786000	4.829048000	1.264500000
H	3.150390000	5.057015000	0.861913000
N	-0.245656000	-3.976216000	1.193405000
H	-0.165122000	-4.080554000	2.198407000
H	-0.700910000	-4.715439000	0.673797000
C	-0.250862000	1.865488000	-1.967008000
H	-0.672546000	2.072310000	-2.959266000
H	-0.120014000	2.826309000	-1.459903000
C	-3.575799000	0.616971000	-0.492983000
H	-3.054933000	-0.064646000	0.180583000
C	-1.218353000	1.070753000	-1.104244000
C	0.209908000	-2.877578000	0.606647000
C	3.799670000	2.570403000	0.314483000
H	4.440054000	3.325941000	-0.157914000
H	4.263310000	2.300061000	1.268342000
C	2.439667000	3.141851000	0.675942000
C	-5.429949000	1.090524000	1.213448000
C	-4.558227000	-0.147990000	-1.382678000
H	-5.022161000	0.560015000	-2.081846000

H	-4.027976000	-0.895320000	-1.982575000
C	-4.335636000	1.684343000	0.301101000
H	-3.642996000	2.261531000	0.922911000
H	-4.797210000	2.384466000	-0.407195000
C	-5.664721000	-0.863608000	-0.580062000
C	2.133048000	2.194201000	-2.347470000
H	1.889895000	3.116110000	-1.817315000
H	2.142911000	2.448056000	-3.416353000
C	-0.037346000	-2.711828000	-0.884185000
H	-0.066346000	-3.684671000	-1.392112000
H	-1.035112000	-2.270225000	-0.966778000
C	0.348047000	-1.151460000	-2.715718000
H	-0.706874000	-0.960584000	-2.517593000
H	0.382556000	-1.838966000	-3.571783000
C	-4.826223000	0.444911000	2.479784000
H	-5.616130000	-0.055273000	3.047306000
H	-4.378733000	1.219080000	3.112214000
H	-4.050597000	-0.290594000	2.248219000
C	-6.398175000	2.211116000	1.628505000
H	-6.895226000	2.639633000	0.751842000
H	-5.839136000	3.005995000	2.133040000
H	-7.161277000	1.830754000	2.310283000
C	4.017031000	-2.016967000	1.378746000
H	5.039706000	-2.415639000	1.372293000
H	3.362394000	-2.803802000	1.765946000
C	-6.812738000	-1.235685000	-1.533320000
H	-6.424592000	-1.863014000	-2.342372000
H	-7.257478000	-0.337333000	-1.974150000
H	-7.592722000	-1.786144000	-1.003956000
C	4.888117000	0.494233000	-0.339915000
H	5.203534000	0.559910000	0.701802000
H	5.722764000	0.881292000	-0.939978000
C	4.653904000	-0.961253000	-0.735571000
H	4.410804000	-1.020040000	-1.797115000
H	5.597788000	-1.509547000	-0.605674000
C	-5.134129000	-2.142123000	0.103764000
H	-4.876880000	-2.888316000	-0.655610000
H	-5.910032000	-2.558925000	0.752150000
H	-4.241918000	-1.957460000	0.709567000
C	3.110536000	-2.852647000	-0.721387000
H	2.610540000	-3.520162000	-0.018065000
H	3.973232000	-3.408788000	-1.113066000
C	3.527077000	1.707683000	-1.960686000
H	3.789449000	0.827830000	-2.549706000
H	4.253687000	2.486587000	-2.231802000
C	3.881075000	-0.857039000	2.350031000
C	2.186573000	-2.523301000	-1.890368000
H	2.717233000	-1.914582000	-2.623222000
H	1.927268000	-3.461367000	-2.401371000
C	1.055815000	0.140697000	-3.115517000
H	2.090748000	-0.071959000	-3.387571000
H	0.574974000	0.530299000	-4.023899000

O	3.019526000	0.033695000	2.145702000
O	0.278697000	0.530391000	2.420559000
H	0.575794000	-0.027686000	3.159924000
H	0.461198000	1.447187000	2.692815000
N	4.659482000	-0.847246000	3.423964000
H	5.363237000	-1.556031000	3.585600000
H	4.540966000	-0.125267000	4.125501000

-115°

Y	1.501393000	0.063882000	0.333726000
O	-0.765549000	0.319835000	-0.203133000
O	0.784850000	-1.971146000	1.255447000
O	-7.311047000	-0.331081000	1.033302000
O	1.444259000	2.372383000	0.774565000
N	-6.229171000	0.063960000	0.461887000
N	1.065870000	1.195222000	-2.052803000
N	3.676673000	1.354881000	-0.518657000
N	-2.521534000	1.233091000	-1.312560000
H	-2.809441000	1.845662000	-2.068520000
N	0.945825000	-1.791762000	-1.506581000
N	3.562558000	-1.636355000	0.021527000
N	2.349948000	4.432417000	0.955823000
H	1.471601000	4.820858000	1.280424000
H	3.141900000	5.056110000	0.868299000
N	-0.245024000	-3.978560000	1.188482000
H	-0.165886000	-4.083854000	2.193524000
H	-0.697844000	-4.718235000	0.667352000
C	-0.251839000	1.866881000	-1.965881000
H	-0.672676000	2.074587000	-2.958353000
H	-0.122778000	2.827299000	-1.457481000
C	-3.576911000	0.618035000	-0.493022000
H	-3.056428000	-0.064938000	0.179453000
C	-1.219113000	1.069459000	-1.105439000
C	0.209400000	-2.878708000	0.603633000
C	3.798681000	2.573060000	0.315185000
H	4.433409000	3.332467000	-0.158627000
H	4.268106000	2.302802000	1.266158000
C	2.437915000	3.138033000	0.684754000
C	-5.430602000	1.091378000	1.214228000
C	-4.560237000	-0.144967000	-1.383410000
H	-5.023624000	0.564311000	-2.081652000
H	-4.030797000	-0.892072000	-1.984315000
C	-4.335593000	1.685053000	0.302626000
H	-3.642268000	2.260641000	0.925156000
H	-4.796383000	2.386637000	-0.404744000
C	-5.667294000	-0.860461000	-0.581457000
C	2.131020000	2.199529000	-2.344799000
H	1.887416000	3.119498000	-1.811305000
H	2.138745000	2.456561000	-3.412958000
C	-0.035759000	-2.711344000	-0.887280000
H	-0.064620000	-3.683693000	-1.396155000

H	-1.033364000	-2.269407000	-0.970007000
C	0.350923000	-1.149088000	-2.716992000
H	-0.704426000	-0.959742000	-2.519953000
H	0.387300000	-1.835251000	-3.574052000
C	-4.827590000	0.443682000	2.479841000
H	-5.618031000	-0.056239000	3.046857000
H	-4.379198000	1.216657000	3.113095000
H	-4.052784000	-0.292417000	2.247417000
C	-6.397612000	2.212545000	1.630564000
H	-6.894396000	2.642416000	0.754412000
H	-5.837633000	3.006364000	2.135724000
H	-7.160971000	1.832360000	2.312160000
C	4.020007000	-2.012646000	1.376388000
H	5.041944000	-2.413242000	1.368537000
H	3.364598000	-2.797749000	1.765860000
C	-6.815672000	-1.230645000	-1.535011000
H	-6.428083000	-1.857525000	-2.344677000
H	-7.259651000	-0.331492000	-1.974975000
H	-7.596126000	-1.780937000	-1.006164000
C	4.888867000	0.498390000	-0.343956000
H	5.207078000	0.564185000	0.696820000
H	5.722057000	0.885160000	-0.946252000
C	4.653631000	-0.957117000	-0.739173000
H	4.408391000	-1.015405000	-1.800236000
H	5.597679000	-1.505613000	-0.611264000
C	-5.137764000	-2.140077000	0.101119000
H	-4.881039000	-2.885717000	-0.658976000
H	-5.914046000	-2.556917000	0.749033000
H	-4.245450000	-1.956725000	0.707181000
C	3.112640000	-2.850163000	-0.722321000
H	2.612801000	-3.517245000	-0.018416000
H	3.975753000	-3.406238000	-1.113205000
C	3.526046000	1.713997000	-1.961101000
H	3.788937000	0.835649000	-2.552169000
H	4.251342000	2.494355000	-2.231584000
C	3.888237000	-0.850223000	2.345464000
C	2.188705000	-2.522214000	-1.891676000
H	2.719110000	-1.913823000	-2.624986000
H	1.929781000	-3.460758000	-2.401992000
C	1.057774000	0.144379000	-3.114459000
H	2.093177000	-0.067086000	-3.385587000
H	0.577515000	0.534226000	-4.023066000
O	3.030320000	0.042898000	2.139118000
O	0.274594000	0.491403000	2.422529000
H	0.435241000	-0.191066000	3.096811000
H	0.544490000	1.334976000	2.825324000
N	4.667419000	-0.841116000	3.419192000
H	5.368810000	-1.551967000	3.581807000
H	4.551913000	-0.117218000	4.119206000

-125°

Y	1.501953000	0.065117000	0.333608000
O	-0.765187000	0.316800000	-0.205749000
O	0.776750000	-1.972137000	1.252744000
O	-7.311133000	-0.327203000	1.033336000
O	1.446041000	2.369098000	0.779232000
N	-6.228991000	0.067280000	0.462033000
N	1.067455000	1.196546000	-2.052117000
N	3.678141000	1.356413000	-0.518144000
N	-2.520687000	1.234580000	-1.312258000
H	-2.808189000	1.849235000	-2.066671000
N	0.946700000	-1.791363000	-1.508823000
N	3.561294000	-1.634452000	0.022660000
N	2.348517000	4.430335000	0.961253000
H	1.470085000	4.816836000	1.287869000
H	3.139306000	5.055407000	0.873271000
N	-0.248717000	-3.981636000	1.180922000
H	-0.172128000	-4.087669000	2.186107000
H	-0.698928000	-4.721642000	0.657970000
C	-0.250713000	1.867370000	-1.965303000
H	-0.671100000	2.075666000	-2.957856000
H	-0.122355000	2.827469000	-1.456109000
C	-3.576446000	0.619708000	-0.493151000
H	-3.056493000	-0.064361000	0.178597000
C	-1.218319000	1.068879000	-1.106083000
C	0.205080000	-2.880593000	0.598278000
C	3.799575000	2.574278000	0.316247000
H	4.431652000	3.335292000	-0.158526000
H	4.271626000	2.304544000	1.266013000
C	2.438230000	3.136183000	0.688784000
C	-5.429282000	1.093368000	1.215012000
C	-4.560740000	-0.141664000	-1.383859000
H	-5.023760000	0.568614000	-2.081333000
H	-4.032142000	-0.888717000	-1.985578000
C	-4.333944000	1.686735000	0.303639000
H	-3.639889000	2.261119000	0.926464000
H	-4.794228000	2.389350000	-0.403042000
C	-5.668123000	-0.856869000	-0.582106000
C	2.132116000	2.201719000	-2.343052000
H	1.888359000	3.120801000	-1.808063000
H	2.139322000	2.460297000	-3.410849000
C	-0.036055000	-2.711791000	-0.892905000
H	-0.063655000	-3.683567000	-1.402938000
H	-1.033562000	-2.269925000	-0.977283000
C	0.353808000	-1.147446000	-2.719552000
H	-0.701911000	-0.958558000	-2.524053000
H	0.391817000	-1.832635000	-3.577325000
C	-4.826537000	0.444114000	2.479959000
H	-5.617333000	-0.055299000	3.046925000
H	-4.377002000	1.216132000	3.113572000
H	-4.052670000	-0.292704000	2.246703000
C	-6.395086000	2.215147000	1.632554000
H	-6.891833000	2.646095000	0.756913000

H	-5.834145000	3.008089000	2.138027000
H	-7.158493000	1.835185000	2.314216000
C	4.017400000	-2.010087000	1.378330000
H	5.038214000	-2.413539000	1.371176000
H	3.359676000	-2.792868000	1.768640000
C	-6.817048000	-1.225502000	-1.535597000
H	-6.430142000	-1.852060000	-2.345837000
H	-7.260492000	-0.325698000	-1.974769000
H	-7.597751000	-1.775617000	-1.006936000
C	4.889889000	0.499412000	-0.343631000
H	5.208983000	0.565776000	0.696797000
H	5.722919000	0.885055000	-0.946882000
C	4.653505000	-0.956286000	-0.737677000
H	4.408878000	-1.015098000	-1.798849000
H	5.596959000	-1.505546000	-0.608761000
C	-5.139405000	-2.137385000	0.099431000
H	-4.883258000	-2.882623000	-0.661258000
H	-5.915912000	-2.554188000	0.747099000
H	-4.246903000	-1.955131000	0.705555000
C	3.112237000	-2.848890000	-0.720842000
H	2.611079000	-3.515159000	-0.017090000
H	3.975893000	-3.405514000	-1.109698000
C	3.527384000	1.716143000	-1.960317000
H	3.790284000	0.838132000	-2.551906000
H	4.252460000	2.496761000	-2.230637000
C	3.888761000	-0.845627000	2.345488000
C	2.190366000	-2.521424000	-1.891979000
H	2.721838000	-1.912819000	-2.624337000
H	1.932661000	-3.460053000	-2.402744000
C	1.060790000	0.146620000	-3.114642000
H	2.096516000	-0.064355000	-3.384879000
H	0.581398000	0.537208000	-4.023407000
O	3.034342000	0.050095000	2.136540000
O	0.271836000	0.464393000	2.424257000
H	0.310788000	-0.306730000	3.016461000
H	0.625397000	1.213880000	2.933465000
N	4.667260000	-0.837288000	3.419773000
H	5.365903000	-1.550383000	3.584333000
H	4.553433000	-0.111986000	4.118598000

-135°

Y	1.502161000	0.065861000	0.331880000
O	-0.764093000	0.317079000	-0.205723000
O	0.769389000	-1.976111000	1.246445000
O	-7.309131000	-0.322817000	1.035647000
O	1.443760000	2.367371000	0.778877000
N	-6.227308000	0.070317000	0.462807000
N	1.070228000	1.197184000	-2.052540000
N	3.678580000	1.358852000	-0.514568000
N	-2.518976000	1.232841000	-1.314741000
H	-2.806251000	1.846413000	-2.070135000

N	0.949354000	-1.791156000	-1.512734000
N	3.560192000	-1.630988000	0.026405000
N	2.342245000	4.430074000	0.963944000
H	1.462644000	4.814743000	1.289511000
H	3.132204000	5.056470000	0.878132000
N	-0.253282000	-3.986882000	1.168989000
H	-0.179588000	-4.094031000	2.174301000
H	-0.700747000	-4.726991000	0.643797000
C	-0.248946000	1.866309000	-1.966835000
H	-0.668912000	2.073644000	-2.959746000
H	-0.121975000	2.826851000	-1.458128000
C	-3.575065000	0.620092000	-0.494321000
H	-3.055313000	-0.062219000	0.179359000
C	-1.216734000	1.067907000	-1.107495000
C	0.201102000	-2.884946000	0.589033000
C	3.797564000	2.576873000	0.319958000
H	4.428530000	3.339002000	-0.154519000
H	4.269581000	2.308091000	1.269967000
C	2.434646000	3.136053000	0.690960000
C	-5.427739000	1.098881000	1.212524000
C	-4.559353000	-0.143774000	-1.382891000
H	-5.022485000	0.564429000	-2.082376000
H	-4.030761000	-0.892551000	-1.982473000
C	-4.332469000	1.689508000	0.299337000
H	-3.638368000	2.265729000	0.920405000
H	-4.792806000	2.390056000	-0.409367000
C	-5.666587000	-0.856735000	-0.578835000
C	2.134400000	2.203614000	-2.341224000
H	1.889182000	3.122078000	-1.805875000
H	2.142806000	2.462917000	-3.408823000
C	-0.034576000	-2.713921000	-0.902423000
H	-0.059087000	-3.684772000	-1.414385000
H	-1.032409000	-2.273282000	-0.989601000
C	0.359431000	-1.146222000	-2.724378000
H	-0.696820000	-0.957786000	-2.531038000
H	0.399659000	-1.830523000	-3.582754000
C	-4.824950000	0.453691000	2.479512000
H	-5.615653000	-0.044290000	3.047861000
H	-4.375800000	1.227799000	3.110842000
H	-4.050764000	-0.283528000	2.248569000
C	-6.393735000	2.221848000	1.626425000
H	-6.890356000	2.650012000	0.749345000
H	-5.832967000	3.016432000	2.129518000
H	-7.157235000	1.843929000	2.309107000
C	4.012905000	-2.005850000	1.383665000
H	5.033214000	-2.410526000	1.378966000
H	3.353291000	-2.787469000	1.773156000
C	-6.815713000	-1.228198000	-1.530988000
H	-6.428955000	-1.857062000	-2.339515000
H	-7.259326000	-0.329692000	-1.972628000
H	-7.596234000	-1.776855000	-1.000550000
C	4.890414000	0.502478000	-0.338141000

H	5.208275000	0.569603000	0.702610000
H	5.724116000	0.887831000	-0.940651000
C	4.654687000	-0.953468000	-0.731592000
H	4.412680000	-1.012910000	-1.793314000
H	5.597549000	-1.503042000	-0.599934000
C	-5.137645000	-2.135254000	0.106236000
H	-4.881883000	-2.882753000	-0.652361000
H	-5.913867000	-2.550127000	0.755479000
H	-4.244871000	-1.951241000	0.711409000
C	3.113627000	-2.846191000	-0.717762000
H	2.610657000	-3.512075000	-0.014964000
H	3.978711000	-3.402683000	-1.103510000
C	3.529545000	1.718702000	-1.956889000
H	3.793816000	0.840980000	-2.548293000
H	4.254456000	2.499832000	-2.226146000
C	3.883756000	-0.840266000	2.349590000
C	2.195259000	-2.519617000	-1.892037000
H	2.728409000	-1.910322000	-2.622580000
H	1.940372000	-3.458480000	-2.403742000
C	1.066510000	0.148555000	-3.116382000
H	2.102927000	-0.061447000	-3.384685000
H	0.588735000	0.539995000	-4.025627000
O	3.030748000	0.056344000	2.137962000
O	0.270773000	0.433815000	2.428994000
H	0.209743000	-0.402725000	2.922954000
H	0.702023000	1.068618000	3.026378000
N	4.660231000	-0.831593000	3.425228000
H	5.357467000	-1.545530000	3.592134000
H	4.545699000	-0.105544000	4.123182000

-5°

Y	1.511140000	0.060575000	0.339150000
O	-0.764444000	0.352375000	-0.157377000
O	0.786504000	-1.988165000	1.246280000
O	-7.306205000	-0.308332000	1.035439000
O	1.464973000	2.396136000	0.714170000
N	-6.222152000	0.078394000	0.462617000
N	1.078682000	1.170030000	-2.053234000
N	3.695052000	1.335745000	-0.515956000
N	-2.509162000	1.215150000	-1.321559000
H	-2.793179000	1.802958000	-2.098542000
N	0.943298000	-1.804233000	-1.497962000
N	3.556158000	-1.642975000	0.053346000
N	2.388546000	4.449172000	0.896016000
H	1.508900000	4.850322000	1.200706000
H	3.189700000	5.062508000	0.820619000
N	-0.243163000	-3.997069000	1.187679000
H	-0.158577000	-4.102633000	2.192128000
H	-0.699026000	-4.736109000	0.668502000
C	-0.235582000	1.849814000	-1.963468000
H	-0.658867000	2.056550000	-2.954784000

H	-0.096801000	2.810634000	-1.458464000
C	-3.569607000	0.608864000	-0.500583000
H	-3.055825000	-0.087368000	0.163345000
C	-1.210025000	1.070644000	-1.093574000
C	0.208032000	-2.895701000	0.600847000
C	3.825708000	2.566318000	0.297504000
H	4.474020000	3.309299000	-0.184309000
H	4.283061000	2.307482000	1.257465000
C	2.466761000	3.150667000	0.638627000
C	-5.407664000	1.089351000	1.220336000
C	-4.565968000	-0.133608000	-1.393129000
H	-5.026223000	0.587712000	-2.081131000
H	-4.048621000	-0.880739000	-2.004393000
C	-4.310219000	1.678639000	0.308492000
H	-3.606708000	2.239444000	0.933187000
H	-4.765590000	2.392332000	-0.390044000
C	-5.675606000	-0.844276000	-0.590368000
C	2.151694000	2.164981000	-2.354098000
H	1.913324000	3.093578000	-1.834390000
H	2.162948000	2.407102000	-3.425584000
C	-0.040224000	-2.727226000	-0.887919000
H	-0.065498000	-3.697433000	-1.401204000
H	-1.038612000	-2.287263000	-0.972742000
C	0.352541000	-1.168060000	-2.712410000
H	-0.701922000	-0.971649000	-2.514848000
H	0.384159000	-1.859359000	-3.565652000
C	-4.806046000	0.423418000	2.477113000
H	-5.599331000	-0.073356000	3.042908000
H	-4.347168000	1.185619000	3.115884000
H	-4.040181000	-0.318906000	2.234877000
C	-6.359160000	2.218128000	1.651633000
H	-6.857063000	2.659893000	0.782102000
H	-5.786845000	3.001822000	2.158719000
H	-7.121950000	1.841342000	2.335747000
C	3.990933000	-2.006046000	1.420028000
H	5.013398000	-2.404920000	1.432515000
H	3.330012000	-2.788553000	1.805056000
C	-6.832460000	-1.195645000	-1.540734000
H	-6.455234000	-1.820291000	-2.356944000
H	-7.269743000	-0.288891000	-1.971675000
H	-7.615514000	-1.742163000	-1.011880000
C	4.901766000	0.476267000	-0.322970000
H	5.210265000	0.552486000	0.720335000
H	5.742227000	0.852276000	-0.922016000
C	4.663273000	-0.982485000	-0.701078000
H	4.433329000	-1.055118000	-1.764720000
H	5.601311000	-1.535532000	-0.551315000
C	-5.155724000	-2.134458000	0.079666000
H	-4.907696000	-2.875865000	-0.687408000
H	-5.934242000	-2.549692000	0.725923000
H	-4.260377000	-1.964866000	0.685294000
C	3.105830000	-2.859069000	-0.688051000

H	2.599285000	-3.521734000	0.014611000
H	3.970008000	-3.419081000	-1.070445000
C	3.544210000	1.673963000	-1.963330000
H	3.799973000	0.784891000	-2.541376000
H	4.274421000	2.445182000	-2.246793000
C	3.843688000	-0.836707000	2.380837000
C	2.192486000	-2.532695000	-1.867884000
H	2.729877000	-1.924921000	-2.596609000
H	1.940533000	-3.472532000	-2.379332000
C	1.063617000	0.119588000	-3.115001000
H	2.097684000	-0.096487000	-3.387239000
H	0.583589000	0.511273000	-4.022790000
O	2.994239000	0.061254000	2.155968000
O	0.228169000	0.539473000	2.389872000
H	0.547507000	1.346222000	2.830266000
H	-0.686738000	0.736520000	2.119815000
N	4.601804000	-0.826287000	3.468913000
H	5.296653000	-1.539571000	3.648389000
H	4.474079000	-0.100232000	4.164622000

5°

Y	1.513234000	0.061762000	0.337847000
O	-0.765945000	0.335826000	-0.168928000
O	0.773641000	-1.969939000	1.260031000
O	-7.309109000	-0.292802000	1.041055000
O	1.473342000	2.395940000	0.721409000
N	-6.224050000	0.088017000	0.466189000
N	1.078797000	1.160102000	-2.055807000
N	3.696909000	1.332106000	-0.524929000
N	-2.510501000	1.206001000	-1.328574000
H	-2.793705000	1.797923000	-2.102680000
N	0.944342000	-1.813248000	-1.489657000
N	3.555922000	-1.647429000	0.058537000
N	2.399484000	4.448568000	0.891690000
H	1.522462000	4.850326000	1.203273000
H	3.200104000	5.061755000	0.808922000
N	-0.252291000	-3.980751000	1.213251000
H	-0.173160000	-4.076824000	2.219136000
H	-0.703367000	-4.725743000	0.698314000
C	-0.236267000	1.838712000	-1.969364000
H	-0.657501000	2.044507000	-2.961768000
H	-0.099518000	2.800189000	-1.464876000
C	-3.571642000	0.602229000	-0.506817000
H	-3.060290000	-0.103153000	0.149240000
C	-1.211439000	1.058280000	-1.101581000
C	0.200662000	-2.884624000	0.618694000
C	3.831509000	2.564635000	0.285120000
H	4.476561000	3.306853000	-0.202119000
H	4.294765000	2.308192000	1.242889000
C	2.475486000	3.150242000	0.635500000
C	-5.396583000	1.085694000	1.227438000

C	-4.578887000	-0.125328000	-1.399259000
H	-5.036750000	0.604969000	-2.079413000
H	-4.071218000	-0.872300000	-2.018800000
C	-4.299135000	1.672242000	0.313914000
H	-3.587813000	2.222998000	0.938715000
H	-4.752287000	2.394418000	-0.377325000
C	-5.690342000	-0.832212000	-0.595567000
C	2.149962000	2.155859000	-2.360760000
H	1.911825000	3.084514000	-1.840796000
H	2.157894000	2.397136000	-3.432452000
C	-0.040262000	-2.730877000	-0.873060000
H	-0.062592000	-3.706467000	-1.376058000
H	-1.038892000	-2.293255000	-0.966139000
C	0.354506000	-1.181861000	-2.707250000
H	-0.700479000	-0.986058000	-2.512545000
H	0.388665000	-1.875950000	-3.558101000
C	-4.794015000	0.404852000	2.475738000
H	-5.588662000	-0.088551000	3.042582000
H	-4.324188000	1.157878000	3.117434000
H	-4.036633000	-0.342943000	2.223732000
C	-6.335625000	2.219434000	1.672789000
H	-6.835138000	2.671629000	0.809576000
H	-5.753392000	2.994539000	2.181750000
H	-7.097343000	1.844332000	2.359038000
C	3.994572000	-2.003889000	1.425521000
H	5.016199000	-2.405004000	1.436800000
H	3.333476000	-2.783099000	1.817073000
C	-6.854606000	-1.167885000	-1.542506000
H	-6.486398000	-1.790220000	-2.364559000
H	-7.286559000	-0.254830000	-1.965449000
H	-7.639509000	-1.711514000	-1.013436000
C	4.902303000	0.470299000	-0.331809000
H	5.214629000	0.550539000	0.709960000
H	5.741477000	0.841698000	-0.935472000
C	4.660302000	-0.989928000	-0.702704000
H	4.426088000	-1.066310000	-1.765129000
H	5.598629000	-1.542968000	-0.554618000
C	-5.177946000	-2.131074000	0.063428000
H	-4.937451000	-2.868649000	-0.709707000
H	-5.957685000	-2.545313000	0.708870000
H	-4.279755000	-1.972516000	0.667828000
C	3.103857000	-2.867251000	-0.675089000
H	2.595093000	-3.523952000	0.031809000
H	3.966977000	-3.431859000	-1.053176000
C	3.543783000	1.666839000	-1.972697000
H	3.799217000	0.776760000	-2.549352000
H	4.272695000	2.438074000	-2.259271000
C	3.852394000	-0.828065000	2.378893000
C	2.191504000	-2.546074000	-1.856722000
H	2.729630000	-1.943490000	-2.589153000
H	1.937494000	-3.488240000	-2.362833000
C	1.065397000	0.104964000	-3.113358000

H	2.099972000	-0.112015000	-3.382852000
H	0.586728000	0.493099000	-4.023384000
O	3.005850000	0.070663000	2.148367000
O	0.224560000	0.572110000	2.381493000
H	0.436640000	1.477666000	2.669716000
H	-0.715086000	0.601397000	2.126060000
N	4.611989000	-0.812795000	3.466124000
H	5.304769000	-1.527022000	3.649691000
H	4.487399000	-0.081534000	4.156896000

15°

Y	1.513970000	0.062056000	0.338171000
O	-0.765078000	0.329287000	-0.175388000
O	0.763741000	-1.958616000	1.268550000
O	-7.309767000	-0.301903000	1.036324000
O	1.474071000	2.394180000	0.728077000
N	-6.225621000	0.082391000	0.462027000
N	1.078093000	1.158997000	-2.056039000
N	3.696131000	1.332029000	-0.528679000
N	-2.511249000	1.210345000	-1.325065000
H	-2.794290000	1.805271000	-2.096923000
N	0.944509000	-1.815509000	-1.485638000
N	3.556319000	-1.649497000	0.058421000
N	2.401125000	4.446217000	0.898127000
H	1.525437000	4.847175000	1.214574000
H	3.201221000	5.059842000	0.813087000
N	-0.255822000	-3.972498000	1.224815000
H	-0.180172000	-4.064455000	2.231390000
H	-0.702587000	-4.720960000	0.711081000
C	-0.237167000	1.837301000	-1.970938000
H	-0.658209000	2.041401000	-2.963819000
H	-0.101004000	2.799746000	-1.468116000
C	-3.572521000	0.606926000	-0.503461000
H	-3.060003000	-0.089112000	0.161688000
C	-1.211679000	1.056696000	-1.102706000
C	0.196207000	-2.877673000	0.627706000
C	3.831280000	2.564078000	0.282139000
H	4.473842000	3.307651000	-0.206258000
H	4.297835000	2.307287000	1.238206000
C	2.476364000	3.148774000	0.638973000
C	-5.409039000	1.093306000	1.217478000
C	-4.570639000	-0.135272000	-1.394394000
H	-5.029493000	0.585840000	-2.083546000
H	-4.054815000	-0.884335000	-2.004591000
C	-4.311355000	1.679261000	0.303922000
H	-3.606935000	2.240584000	0.927087000
H	-4.766272000	2.392138000	-0.395787000
C	-5.681589000	-0.842461000	-0.590353000
C	2.148093000	2.155322000	-2.362584000
H	1.910112000	3.083612000	-1.841710000
H	2.154300000	2.397066000	-3.434194000

C	-0.040586000	-2.730415000	-0.865554000
H	-0.062110000	-3.708385000	-1.363831000
H	-1.039130000	-2.293385000	-0.962077000
C	0.354378000	-1.184978000	-2.703796000
H	-0.700639000	-0.989343000	-2.509556000
H	0.389002000	-1.879802000	-3.554014000
C	-4.807467000	0.428547000	2.474925000
H	-5.600836000	-0.067158000	3.041541000
H	-4.347986000	1.191237000	3.112666000
H	-4.042054000	-0.314468000	2.233274000
C	-6.358516000	2.224198000	1.647739000
H	-6.856249000	2.665509000	0.777877000
H	-5.784651000	3.007704000	2.153365000
H	-7.121478000	1.849559000	2.332838000
C	3.999046000	-2.004838000	1.424219000
H	5.019686000	-2.408587000	1.432596000
H	3.337475000	-2.781789000	1.819583000
C	-6.839707000	-1.192208000	-1.539782000
H	-6.464300000	-1.818529000	-2.355549000
H	-7.275068000	-0.284875000	-1.971462000
H	-7.623787000	-1.736375000	-1.010022000
C	4.901401000	0.469323000	-0.337282000
H	5.216722000	0.550606000	0.703388000
H	5.739141000	0.839409000	-0.943710000
C	4.657998000	-0.991388000	-0.706386000
H	4.420502000	-1.068102000	-1.768044000
H	5.597009000	-1.544040000	-0.561067000
C	-5.164161000	-2.132990000	0.080850000
H	-4.917682000	-2.875632000	-0.685533000
H	-5.943313000	-2.546106000	0.727692000
H	-4.268358000	-1.964384000	0.686108000
C	3.102972000	-2.870362000	-0.672268000
H	2.593680000	-3.524781000	0.036580000
H	3.965207000	-3.436935000	-1.049515000
C	3.542464000	1.667293000	-1.976171000
H	3.798230000	0.777644000	-2.553367000
H	4.270686000	2.439164000	-2.262727000
C	3.862705000	-0.825926000	2.374316000
C	2.189923000	-2.550659000	-1.853443000
H	2.727689000	-1.950111000	-2.587782000
H	1.933983000	-3.493438000	-2.357416000
C	1.065227000	0.101609000	-3.111446000
H	2.099968000	-0.115806000	-3.379982000
H	0.586954000	0.487932000	-4.022477000
O	3.018503000	0.073976000	2.142098000
O	0.236759000	0.589482000	2.383382000
H	0.341014000	1.543437000	2.551373000
H	-0.710866000	0.466191000	2.196200000
N	4.625066000	-0.809226000	3.459881000
H	5.316091000	-1.524875000	3.644372000
H	4.504215000	-0.075176000	4.148317000

25°

Y	1.513996000	0.062194000	0.339284000
O	-0.764705000	0.323452000	-0.181887000
O	0.759768000	-1.953300000	1.272967000
O	-7.311176000	-0.305400000	1.034479000
O	1.468395000	2.390761000	0.733987000
N	-6.227097000	0.079871000	0.460682000
N	1.076550000	1.160838000	-2.056167000
N	3.692952000	1.335268000	-0.530620000
N	-2.512662000	1.211956000	-1.323527000
H	-2.796044000	1.810023000	-2.092793000
N	0.946207000	-1.815516000	-1.484519000
N	3.558609000	-1.648364000	0.055486000
N	2.393073000	4.443371000	0.907559000
H	1.517487000	4.842162000	1.227037000
H	3.191786000	5.058659000	0.821448000
N	-0.254972000	-3.969406000	1.228768000
H	-0.181294000	-4.059953000	2.235645000
H	-0.698635000	-4.719710000	0.714986000
C	-0.239447000	1.837376000	-1.972392000
H	-0.660345000	2.039862000	-2.965734000
H	-0.105184000	2.800675000	-1.470696000
C	-3.573407000	0.607919000	-0.502069000
H	-3.059936000	-0.084780000	0.165875000
C	-1.212527000	1.054961000	-1.104383000
C	0.195966000	-2.874577000	0.631272000
C	3.825356000	2.565834000	0.283062000
H	4.464952000	3.312552000	-0.204379000
H	4.294145000	2.307990000	1.237725000
C	2.469708000	3.146901000	0.644459000
C	-5.413739000	1.094374000	1.214737000
C	-4.568510000	-0.139120000	-1.392498000
H	-5.027314000	0.579029000	-2.084752000
H	-4.049953000	-0.888872000	-1.999533000
C	-4.316264000	1.680538000	0.301183000
H	-3.614254000	2.245534000	0.923722000
H	-4.772066000	2.390302000	-0.401143000
C	-5.679727000	-0.846271000	-0.588825000
C	2.144511000	2.158924000	-2.362869000
H	1.905441000	3.086275000	-1.840661000
H	2.149585000	2.401896000	-3.434239000
C	-0.038541000	-2.729768000	-0.862757000
H	-0.059419000	-3.708721000	-1.359072000
H	-1.037204000	-2.293327000	-0.960603000
C	0.355406000	-1.185010000	-2.702596000
H	-0.699784000	-0.990477000	-2.508628000
H	0.390963000	-1.879733000	-3.552847000
C	-4.812210000	0.433770000	2.474404000
H	-5.605174000	-0.062353000	3.041216000
H	-4.355083000	1.198897000	3.110918000
H	-4.044938000	-0.308166000	2.235237000

C	-6.366245000	2.224174000	1.641163000
H	-6.863414000	2.662730000	0.769575000
H	-5.794835000	3.009894000	2.146148000
H	-7.129606000	1.849375000	2.325716000
C	4.005618000	-2.004439000	1.419576000
H	5.025548000	-2.410112000	1.424446000
H	3.344058000	-2.780140000	1.817513000
C	-6.835722000	-1.199985000	-1.539391000
H	-6.457985000	-1.827396000	-2.353254000
H	-7.271851000	-0.294267000	-1.973691000
H	-7.619796000	-1.744306000	-1.009768000
C	4.899557000	0.473697000	-0.341694000
H	5.217408000	0.555012000	0.698079000
H	5.735439000	0.844808000	-0.950045000
C	4.657056000	-0.987267000	-0.711421000
H	4.416764000	-1.063013000	-1.772510000
H	5.597394000	-1.538561000	-0.569342000
C	-5.161151000	-2.134405000	0.086034000
H	-4.913140000	-2.878642000	-0.678305000
H	-5.940166000	-2.546956000	0.733394000
H	-4.265950000	-1.962944000	0.691384000
C	3.105479000	-2.869722000	-0.674111000
H	2.597137000	-3.523888000	0.035803000
H	3.967547000	-3.436239000	-1.051915000
C	3.539544000	1.672954000	-1.977460000
H	3.797111000	0.784846000	-2.556248000
H	4.266526000	2.446632000	-2.262281000
C	3.874405000	-0.824157000	2.368317000
C	2.190791000	-2.551122000	-1.854001000
H	2.727347000	-1.951160000	-2.589690000
H	1.933921000	-3.494228000	-2.356875000
C	1.065388000	0.102240000	-3.110417000
H	2.100517000	-0.114616000	-3.377972000
H	0.587428000	0.487154000	-4.022249000
O	3.031984000	0.076829000	2.135885000
O	0.251504000	0.587111000	2.389969000
H	0.240569000	1.556829000	2.482462000
H	-0.680880000	0.324988000	2.295952000
N	4.639409000	-0.807385000	3.452283000
H	5.329100000	-1.524343000	3.636538000
H	4.521839000	-0.071780000	4.139591000

35°

Y	1.513127000	0.063069000	0.339661000
O	-0.763873000	0.320439000	-0.189227000
O	0.754364000	-1.949898000	1.272921000
O	-7.309001000	-0.307413000	1.035923000
O	1.460164000	2.387074000	0.737989000
N	-6.225348000	0.078384000	0.461666000
N	1.076558000	1.165599000	-2.056247000
N	3.689626000	1.338642000	-0.527614000

N	-2.513045000	1.213630000	-1.325183000
H	-2.797256000	1.814469000	-2.091936000
N	0.948037000	-1.812828000	-1.487086000
N	3.559451000	-1.647253000	0.052204000
N	2.382200000	4.440123000	0.918727000
H	1.505797000	4.836904000	1.238437000
H	3.180180000	5.056670000	0.835061000
N	-0.255130000	-3.968366000	1.224409000
H	-0.183763000	-4.059339000	2.231438000
H	-0.695495000	-4.719599000	0.709125000
C	-0.240229000	1.840465000	-1.974290000
H	-0.660221000	2.042231000	-2.968196000
H	-0.108192000	2.804002000	-1.472516000
C	-3.572429000	0.607928000	-0.503413000
H	-3.057410000	-0.085096000	0.162985000
C	-1.212429000	1.055380000	-1.107871000
C	0.194792000	-2.872393000	0.628626000
C	3.818173000	2.566620000	0.290734000
H	4.457136000	3.316359000	-0.192843000
H	4.285740000	2.306048000	1.245229000
C	2.460767000	3.144405000	0.652091000
C	-5.411361000	1.092151000	1.216037000
C	-4.568420000	-0.138681000	-1.393220000
H	-5.028284000	0.579918000	-2.084310000
H	-4.050392000	-0.887745000	-2.001568000
C	-4.314782000	1.679281000	0.302010000
H	-3.612170000	2.243677000	0.924428000
H	-4.771394000	2.389783000	-0.399056000
C	-5.678529000	-0.846874000	-0.588938000
C	2.143449000	2.165368000	-2.360279000
H	1.902515000	3.091521000	-1.836730000
H	2.149661000	2.410205000	-3.431242000
C	-0.036886000	-2.727350000	-0.865977000
H	-0.056984000	-3.706400000	-1.362121000
H	-1.035565000	-2.291181000	-0.964920000
C	0.357866000	-1.180729000	-2.704837000
H	-0.697564000	-0.986990000	-2.511753000
H	0.394662000	-1.874417000	-3.555871000
C	-4.808739000	0.430309000	2.474504000
H	-5.601275000	-0.065857000	3.041887000
H	-4.350440000	1.194711000	3.111047000
H	-4.042146000	-0.311819000	2.233863000
C	-6.363540000	2.221421000	1.644542000
H	-6.861784000	2.660682000	0.773927000
H	-5.791629000	3.006769000	2.149536000
H	-7.126078000	1.845994000	2.329688000
C	4.008833000	-2.006586000	1.414555000
H	5.028454000	-2.413134000	1.416663000
H	3.347457000	-2.782498000	1.812427000
C	-6.835308000	-1.200578000	-1.538536000
H	-6.458048000	-1.827319000	-2.353130000
H	-7.272326000	-0.294832000	-1.971884000

H	-7.618605000	-1.745602000	-1.008481000
C	4.897301000	0.478056000	-0.340676000
H	5.215758000	0.557617000	0.698963000
H	5.732360000	0.851411000	-0.948773000
C	4.656259000	-0.982467000	-0.713949000
H	4.415054000	-1.055655000	-1.775007000
H	5.597492000	-1.532865000	-0.574239000
C	-5.158815000	-2.135237000	0.084655000
H	-4.911146000	-2.878874000	-0.680378000
H	-5.937099000	-2.548539000	0.732432000
H	-4.263174000	-1.963788000	0.689340000
C	3.107142000	-2.867769000	-0.679003000
H	2.598904000	-3.522936000	0.030201000
H	3.969395000	-3.433671000	-1.057383000
C	3.538352000	1.680564000	-1.973711000
H	3.798203000	0.794508000	-2.554623000
H	4.264874000	2.456022000	-2.254865000
C	3.880425000	-0.827309000	2.364548000
C	2.192200000	-2.548184000	-1.858103000
H	2.728474000	-1.947348000	-2.593287000
H	1.935067000	-3.490706000	-2.361942000
C	1.067775000	0.107380000	-3.110796000
H	2.103405000	-0.108662000	-3.377128000
H	0.590766000	0.492188000	-4.023213000
O	3.039089000	0.074535000	2.133398000
O	0.258770000	0.577884000	2.395119000
H	0.125012000	1.541678000	2.438263000
H	-0.632048000	0.187041000	2.389957000
N	4.647214000	-0.812244000	3.447531000
H	5.336178000	-1.530241000	3.630319000
H	4.531749000	-0.076819000	4.135353000

45°

Y	1.513578000	0.064348000	0.341019000
O	-0.763407000	0.320438000	-0.191457000
O	0.753162000	-1.950438000	1.270588000
O	-7.309591000	-0.314180000	1.033125000
O	1.452298000	2.383015000	0.744020000
N	-6.225951000	0.073875000	0.460358000
N	1.075300000	1.173711000	-2.054207000
N	3.686436000	1.343639000	-0.523529000
N	-2.514093000	1.217974000	-1.321632000
H	-2.799140000	1.821364000	-2.086055000
N	0.949692000	-1.807170000	-1.491433000
N	3.561707000	-1.644852000	0.045665000
N	2.370745000	4.436845000	0.932854000
H	1.493292000	4.831139000	1.252705000
H	3.167745000	5.054980000	0.851881000
N	-0.250724000	-3.971404000	1.214458000
H	-0.179929000	-4.065426000	2.221267000
H	-0.688813000	-4.722138000	0.696499000

C	-0.242201000	1.846679000	-1.971667000
H	-0.662397000	2.048914000	-2.965445000
H	-0.111778000	2.809932000	-1.468968000
C	-3.572546000	0.609578000	-0.500808000
H	-3.056133000	-0.081323000	0.166738000
C	-1.213019000	1.058632000	-1.106467000
C	0.196793000	-2.872565000	0.622460000
C	3.811165000	2.568132000	0.300756000
H	4.449563000	3.321325000	-0.178142000
H	4.277404000	2.303802000	1.254845000
C	2.451761000	3.141959000	0.662159000
C	-5.416063000	1.090669000	1.215073000
C	-4.565252000	-0.140652000	-1.391345000
H	-5.025806000	0.575999000	-2.083981000
H	-4.044248000	-0.888951000	-1.998096000
C	-4.319038000	1.679499000	0.302667000
H	-3.618830000	2.245937000	0.925956000
H	-4.775937000	2.388522000	-0.399718000
C	-5.674857000	-0.850981000	-0.588330000
C	2.140979000	2.175478000	-2.354779000
H	1.898481000	3.099862000	-1.828787000
H	2.147849000	2.423423000	-3.425057000
C	-0.034612000	-2.723388000	-0.871881000
H	-0.055066000	-3.701175000	-1.370509000
H	-1.033301000	-2.286801000	-0.969052000
C	0.358800000	-1.172041000	-2.707398000
H	-0.696681000	-0.979408000	-2.513686000
H	0.395816000	-1.863640000	-3.560111000
C	-4.814388000	0.431889000	2.475590000
H	-5.606817000	-0.065712000	3.041851000
H	-4.359462000	1.198258000	3.112188000
H	-4.045283000	-0.308404000	2.237383000
C	-6.372011000	2.218054000	1.640171000
H	-6.869373000	2.655111000	0.767939000
H	-5.803220000	3.005410000	2.145573000
H	-7.135164000	1.841493000	2.324004000
C	4.014076000	-2.009705000	1.405501000
H	5.033403000	-2.417046000	1.403747000
H	3.353044000	-2.786514000	1.802219000
C	-6.829098000	-1.208706000	-1.539512000
H	-6.448829000	-1.835271000	-2.352851000
H	-7.267757000	-0.304543000	-1.974503000
H	-7.611876000	-1.755244000	-1.010243000
C	4.895742000	0.484494000	-0.340413000
H	5.215292000	0.561059000	0.699044000
H	5.729484000	0.861345000	-0.948153000
C	4.656518000	-0.975124000	-0.719115000
H	4.414093000	-1.044406000	-1.780160000
H	5.598834000	-1.524535000	-0.582783000
C	-5.152902000	-2.137262000	0.087503000
H	-4.902394000	-2.881197000	-0.676317000
H	-5.931016000	-2.551725000	0.734741000

H	-4.258479000	-1.962853000	0.693137000
C	3.109979000	-2.863383000	-0.689063000
H	2.602959000	-3.521196000	0.018659000
H	3.972353000	-3.427445000	-1.069958000
C	3.536072000	1.691484000	-1.968398000
H	3.798055000	0.808272000	-2.552681000
H	4.261755000	2.469215000	-2.245405000
C	3.888577000	-0.833157000	2.358877000
C	2.193530000	-2.541224000	-1.866037000
H	2.728688000	-1.938118000	-2.600178000
H	1.936115000	-3.482476000	-2.372099000
C	1.068030000	0.117501000	-3.110534000
H	2.103904000	-0.097171000	-3.377088000
H	0.590943000	0.503422000	-4.022481000
O	3.047075000	0.069129000	2.131550000
O	0.267191000	0.556294000	2.403506000
H	0.004672000	1.493499000	2.417172000
H	-0.557137000	0.045697000	2.477156000
N	4.658240000	-0.820841000	3.440045000
H	5.347274000	-1.539590000	3.619477000
H	4.544803000	-0.086936000	4.129804000

55°

Y	1.514523000	0.065254000	0.343078000
O	-0.763008000	0.326775000	-0.186850000
O	0.757006000	-1.955456000	1.265574000
O	-7.310831000	-0.322868000	1.029078000
O	1.444613000	2.378995000	0.750649000
N	-6.227166000	0.068238000	0.458411000
N	1.073377000	1.184740000	-2.050343000
N	3.683349000	1.349176000	-0.518512000
N	-2.515070000	1.222883000	-1.316086000
H	-2.800905000	1.826755000	-2.079838000
N	0.949701000	-1.798574000	-1.497362000
N	3.564235000	-1.642154000	0.035859000
N	2.359977000	4.433080000	0.950454000
H	1.481350000	4.824838000	1.270133000
H	3.155990000	5.052828000	0.872478000
N	-0.244768000	-3.977153000	1.199706000
H	-0.172575000	-4.076571000	2.205917000
H	-0.683301000	-4.725337000	0.678427000
C	-0.244412000	1.856572000	-1.964727000
H	-0.665667000	2.061296000	-2.957559000
H	-0.114364000	2.818457000	-1.459404000
C	-3.572941000	0.611557000	-0.496759000
H	-3.055454000	-0.076762000	0.172645000
C	-1.213657000	1.065360000	-1.100847000
C	0.200599000	-2.874793000	0.613023000
C	3.804523000	2.569524000	0.312515000
H	4.442489000	3.326350000	-0.161184000
H	4.269477000	2.300719000	1.265974000

C	2.443162000	3.139335000	0.674176000
C	-5.422524000	1.088516000	1.213962000
C	-4.561111000	-0.142917000	-1.388844000
H	-5.022006000	0.571472000	-2.083566000
H	-4.036237000	-0.890298000	-1.993377000
C	-4.324917000	1.679802000	0.303817000
H	-3.628071000	2.249049000	0.928310000
H	-4.782199000	2.386757000	-0.400401000
C	-5.670613000	-0.855825000	-0.588035000
C	2.138248000	2.188237000	-2.347167000
H	1.894910000	3.110661000	-1.818134000
H	2.145484000	2.439943000	-3.416582000
C	-0.033528000	-2.717422000	-0.880085000
H	-0.056160000	-3.692542000	-1.383845000
H	-1.032068000	-2.279324000	-0.972339000
C	0.356870000	-1.158747000	-2.709994000
H	-0.698230000	-0.966508000	-2.513798000
H	0.392111000	-1.847461000	-3.565103000
C	-4.822087000	0.433004000	2.476767000
H	-5.614473000	-0.066281000	3.041602000
H	-4.370980000	1.201462000	3.113560000
H	-4.050248000	-0.305279000	2.241240000
C	-6.383141000	2.213361000	1.635205000
H	-6.879025000	2.648341000	0.761087000
H	-5.818341000	3.002781000	2.141868000
H	-7.147363000	1.835007000	2.316846000
C	4.019511000	-2.014771000	1.392565000
H	5.038629000	-2.422634000	1.386432000
H	3.358910000	-2.793227000	1.786745000
C	-6.821403000	-1.217916000	-1.541746000
H	-6.437300000	-1.844178000	-2.353525000
H	-7.261634000	-0.315472000	-1.978720000
H	-7.603907000	-1.766206000	-1.013868000
C	4.894423000	0.491495000	-0.340315000
H	5.214876000	0.563692000	0.699129000
H	5.726866000	0.872875000	-0.947011000
C	4.657290000	-0.966702000	-0.726439000
H	4.413981000	-1.030896000	-1.787621000
H	5.600628000	-1.515271000	-0.593823000
C	-5.146387000	-2.139856000	0.090322000
H	-4.892709000	-2.884100000	-0.672144000
H	-5.924422000	-2.555532000	0.736873000
H	-4.253373000	-1.962217000	0.697091000
C	3.112411000	-2.857246000	-0.704441000
H	2.607733000	-3.519432000	0.000921000
H	3.974584000	-3.418380000	-1.090127000
C	3.533378000	1.704003000	-1.961830000
H	3.796629000	0.823867000	-2.550164000
H	4.258638000	2.483670000	-2.234480000
C	3.896584000	-0.842804000	2.351576000
C	2.193062000	-2.530466000	-1.877745000
H	2.726361000	-1.923685000	-2.610228000

H	1.935035000	-3.469584000	-2.387454000
C	1.065689000	0.132144000	-3.109919000
H	2.101280000	-0.081281000	-3.378656000
H	0.587318000	0.520619000	-4.020128000
O	3.054312000	0.060001000	2.130033000
O	0.278260000	0.528914000	2.415652000
H	-0.113801000	1.419328000	2.403117000
H	-0.458797000	-0.088883000	2.560623000
N	4.669290000	-0.834782000	3.430681000
H	5.358837000	-1.554231000	3.605206000
H	4.557621000	-0.103835000	4.123855000

65°

Y	1.515401000	0.066359000	0.343589000
O	-0.762024000	0.334507000	-0.181786000
O	0.761026000	-1.963030000	1.257480000
O	-7.310728000	-0.330146000	1.026458000
O	1.435853000	2.376434000	0.755765000
N	-6.227153000	0.063355000	0.457265000
N	1.072709000	1.196232000	-2.046585000
N	3.680240000	1.355588000	-0.509893000
N	-2.515362000	1.226801000	-1.312027000
H	-2.802075000	1.830228000	-2.075824000
N	0.951701000	-1.789657000	-1.505063000
N	3.566764000	-1.638293000	0.027561000
N	2.347796000	4.430889000	0.967568000
H	1.467413000	4.820377000	1.285103000
H	3.143321000	5.051848000	0.894868000
N	-0.238276000	-3.985588000	1.179834000
H	-0.164668000	-4.091436000	2.185306000
H	-0.676120000	-4.731217000	0.654314000
C	-0.245876000	1.866145000	-1.959021000
H	-0.667814000	2.072311000	-2.951253000
H	-0.116996000	2.827178000	-1.451836000
C	-3.572623000	0.613006000	-0.493718000
H	-3.054219000	-0.073263000	0.177077000
C	-1.213729000	1.072231000	-1.096108000
C	0.205144000	-2.879228000	0.599631000
C	3.797348000	2.571651000	0.328087000
H	4.436545000	3.331436000	-0.139138000
H	4.258765000	2.297891000	1.281858000
C	2.433565000	3.138069000	0.686690000
C	-5.426799000	1.086743000	1.213119000
C	-4.557202000	-0.145103000	-1.386770000
H	-5.018732000	0.567282000	-2.083109000
H	-4.029246000	-0.891729000	-1.989548000
C	-4.328964000	1.679932000	0.304497000
H	-3.634793000	2.251608000	0.929743000
H	-4.786687000	2.385049000	-0.401274000
C	-5.666223000	-0.860195000	-0.587262000
C	2.136889000	2.201926000	-2.337863000
H	1.891566000	3.122197000	-1.806071000

H	2.145955000	2.457470000	-3.406364000
C	-0.030781000	-2.712155000	-0.892087000
H	-0.054854000	-3.683924000	-1.402214000
H	-1.029252000	-2.272842000	-0.979795000
C	0.357936000	-1.144788000	-2.714679000
H	-0.697007000	-0.953241000	-2.516790000
H	0.392249000	-1.830213000	-3.572446000
C	-4.827076000	0.434338000	2.477870000
H	-5.619230000	-0.066332000	3.041791000
H	-4.379186000	1.204753000	3.114574000
H	-4.052861000	-0.302171000	2.244645000
C	-6.391330000	2.209485000	1.631002000
H	-6.886352000	2.642269000	0.755302000
H	-5.829812000	3.000930000	2.138157000
H	-7.156114000	1.829788000	2.311256000
C	4.023305000	-2.018626000	1.381711000
H	5.043092000	-2.424782000	1.372649000
H	3.364140000	-2.800476000	1.771513000
C	-6.814337000	-1.226354000	-1.542649000
H	-6.427169000	-1.852471000	-2.353092000
H	-7.256178000	-0.325537000	-1.981344000
H	-7.596325000	-1.776141000	-1.015562000
C	4.893141000	0.499693000	-0.335527000
H	5.212694000	0.566742000	0.704544000
H	5.725154000	0.886404000	-0.939416000
C	4.658890000	-0.956648000	-0.730543000
H	4.415905000	-1.014986000	-1.792146000
H	5.603121000	-1.504395000	-0.600973000
C	-5.139740000	-2.142123000	0.093337000
H	-4.883309000	-2.886690000	-0.667890000
H	-5.917568000	-2.558876000	0.739433000
H	-4.247923000	-1.961536000	0.700983000
C	3.116446000	-2.849991000	-0.719258000
H	2.613628000	-3.517047000	-0.017148000
H	3.979252000	-3.407479000	-1.108809000
C	3.531822000	1.717808000	-1.951827000
H	3.797430000	0.841079000	-2.544139000
H	4.256582000	2.499780000	-2.219073000
C	3.898782000	-0.852702000	2.347589000
C	2.195454000	-2.518799000	-1.889950000
H	2.727485000	-1.908044000	-2.620062000
H	1.937761000	-3.455784000	-2.403700000
C	1.066336000	0.147800000	-3.110031000
H	2.102057000	-0.063824000	-3.379727000
H	0.587630000	0.539120000	-4.018849000
O	3.053930000	0.049123000	2.131960000
O	0.280856000	0.493146000	2.425188000
H	-0.248006000	1.308514000	2.386721000
H	-0.345339000	-0.225616000	2.619700000
N	4.672616000	-0.848772000	3.425872000
H	5.364486000	-1.567215000	3.595273000
H	4.560160000	-0.121819000	4.123114000

75°

Y	1.515903000	0.067288000	0.341535000
O	-0.761016000	0.339592000	-0.179328000
O	0.769281000	-1.974135000	1.247473000
O	-7.307868000	-0.333956000	1.027542000
O	1.426292000	2.374895000	0.755734000
N	-6.224919000	0.060741000	0.458006000
N	1.073948000	1.205349000	-2.044698000
N	3.677438000	1.362490000	-0.498877000
N	-2.514576000	1.228008000	-1.311910000
H	-2.802031000	1.830775000	-2.075993000
N	0.955960000	-1.781954000	-1.512955000
N	3.569437000	-1.632627000	0.023322000
N	2.333379000	4.429836000	0.983983000
H	1.450415000	4.816336000	1.297902000
H	3.128335000	5.052370000	0.919303000
N	-0.229477000	-3.996674000	1.158116000
H	-0.154143000	-4.109333000	2.162734000
H	-0.668216000	-4.738821000	0.628411000
C	-0.245713000	1.872958000	-1.956013000
H	-0.667712000	2.080714000	-2.947868000
H	-0.118558000	2.833006000	-1.446590000
C	-3.571309000	0.612972000	-0.493615000
H	-3.052301000	-0.072989000	0.176992000
C	-1.213026000	1.076518000	-1.094803000
C	0.212299000	-2.886292000	0.584673000
C	3.789608000	2.575736000	0.343954000
H	4.429857000	3.337935000	-0.117842000
H	4.247356000	2.299146000	1.298695000
C	2.422854000	3.138353000	0.697336000
C	-5.425529000	1.085092000	1.213586000
C	-4.555238000	-0.146045000	-1.386544000
H	-5.017800000	0.565815000	-2.082708000
H	-4.026694000	-0.892162000	-1.989426000
C	-4.328430000	1.679266000	0.304730000
H	-3.634664000	2.251567000	0.929851000
H	-4.786908000	2.383943000	-0.400968000
C	-5.663196000	-0.862330000	-0.586548000
C	2.137816000	2.213172000	-2.329637000
H	1.889485000	3.131838000	-1.796590000
H	2.150491000	2.471354000	-3.397456000
C	-0.025969000	-2.708537000	-0.905316000
H	-0.051479000	-3.676429000	-1.422655000
H	-1.024293000	-2.267826000	-0.988104000
C	0.362476000	-1.133625000	-2.720941000
H	-0.692749000	-0.943433000	-2.522933000
H	0.397580000	-1.816429000	-3.580742000
C	-4.824955000	0.433596000	2.478401000
H	-5.616503000	-0.067842000	3.042486000
H	-4.377905000	1.204655000	3.114918000

H	-4.049943000	-0.302099000	2.245285000
C	-6.391119000	2.206962000	1.631367000
H	-6.886732000	2.639035000	0.755655000
H	-5.830318000	2.999090000	2.138251000
H	-7.155393000	1.826642000	2.311846000
C	4.023806000	-2.018601000	1.376782000
H	5.045591000	-2.419668000	1.368367000
H	3.367346000	-2.805801000	1.760158000
C	-6.811161000	-1.229966000	-1.541549000
H	-6.423505000	-1.855824000	-2.351955000
H	-7.254160000	-0.329743000	-1.980284000
H	-7.592351000	-1.780530000	-1.014093000
C	4.892107000	0.508986000	-0.325018000
H	5.207679000	0.571258000	0.716644000
H	5.725207000	0.901256000	-0.923792000
C	4.662425000	-0.945671000	-0.728633000
H	4.422527000	-0.999226000	-1.791210000
H	5.607306000	-1.492256000	-0.599136000
C	-5.135138000	-2.143561000	0.094127000
H	-4.877975000	-2.887953000	-0.667021000
H	-5.912415000	-2.561090000	0.740387000
H	-4.243468000	-1.961936000	0.701665000
C	3.122706000	-2.841802000	-0.730022000
H	2.621580000	-3.513907000	-0.031628000
H	3.987267000	-3.394819000	-1.121988000
C	3.532132000	1.729704000	-1.940223000
H	3.800651000	0.855345000	-2.534643000
H	4.256745000	2.513435000	-2.202578000
C	3.891112000	-0.859560000	2.349694000
C	2.201522000	-2.507531000	-1.899697000
H	2.732970000	-1.892865000	-2.626974000
H	1.945735000	-3.442882000	-2.417320000
C	1.069999000	0.160847000	-3.111766000
H	2.106148000	-0.048483000	-3.381702000
H	0.591281000	0.554498000	-4.019568000
O	3.041496000	0.039211000	2.138700000
O	0.269046000	0.459695000	2.428050000
H	-0.397725000	1.161589000	2.334191000
H	-0.225810000	-0.345315000	2.662315000
N	4.662823000	-0.858308000	3.429331000
H	5.358490000	-1.573919000	3.595236000
H	4.545110000	-0.136501000	4.131061000

85°

Y	1.516076000	0.067233000	0.338514000
O	-0.760426000	0.347292000	-0.175513000
O	0.781546000	-1.988762000	1.235983000
O	-7.303187000	-0.337959000	1.030539000
O	1.415905000	2.374531000	0.753812000
N	-6.221523000	0.057814000	0.459344000
N	1.075766000	1.212736000	-2.043682000

N	3.674288000	1.370114000	-0.486389000
N	-2.513688000	1.227832000	-1.314121000
H	-2.801884000	1.827971000	-2.080056000
N	0.962228000	-1.775437000	-1.520485000
N	3.572934000	-1.625467000	0.021889000
N	2.316776000	4.430599000	0.997576000
H	1.430738000	4.813976000	1.306539000
H	3.110894000	5.054969000	0.941207000
N	-0.217234000	-4.011115000	1.135116000
H	-0.138840000	-4.131398000	2.138628000
H	-0.656693000	-4.749744000	0.601084000
C	-0.245291000	1.877830000	-1.955622000
H	-0.666962000	2.085182000	-2.947648000
H	-0.120294000	2.837934000	-1.445809000
C	-3.569802000	0.612754000	-0.494770000
H	-3.049969000	-0.071421000	0.176992000
C	-1.212419000	1.080750000	-1.094759000
C	0.222559000	-2.896450000	0.568710000
C	3.780825000	2.581615000	0.359796000
H	4.422189000	3.345730000	-0.097250000
H	4.234583000	2.303626000	1.316071000
C	2.410807000	3.140279000	0.706325000
C	-5.423665000	1.085297000	1.212311000
C	-4.552750000	-0.149324000	-1.386110000
H	-5.016959000	0.560489000	-2.083234000
H	-4.023299000	-0.895661000	-1.987915000
C	-4.328179000	1.679591000	0.301631000
H	-3.635040000	2.254369000	0.925165000
H	-4.788246000	2.381974000	-0.405304000
C	-5.658923000	-0.866101000	-0.584000000
C	2.139384000	2.222857000	-2.321930000
H	1.887304000	3.140145000	-1.788418000
H	2.156450000	2.482969000	-3.389192000
C	-0.018917000	-2.706971000	-0.919103000
H	-0.045495000	-3.670402000	-1.444580000
H	-1.017301000	-2.265296000	-0.996593000
C	0.369252000	-1.124580000	-2.727477000
H	-0.686358000	-0.935900000	-2.529587000
H	0.405550000	-1.805273000	-3.588867000
C	-4.821121000	0.437749000	2.478201000
H	-5.611224000	-0.064622000	3.043474000
H	-4.375931000	1.211215000	3.113106000
H	-4.044235000	-0.296398000	2.246380000
C	-6.391223000	2.206215000	1.628086000
H	-6.887976000	2.635475000	0.751638000
H	-5.831763000	3.000480000	2.133101000
H	-7.154532000	1.825848000	2.309618000
C	4.023033000	-2.015463000	1.375889000
H	5.047360000	-2.409928000	1.370391000
H	3.369650000	-2.808694000	1.751836000
C	-6.806920000	-1.237464000	-1.537516000
H	-6.418796000	-1.864279000	-2.346960000

H	-7.251727000	-0.338841000	-1.977686000
H	-7.586807000	-1.788294000	-1.008418000
C	4.891028000	0.519892000	-0.310876000
H	5.200725000	0.577920000	0.732920000
H	5.725958000	0.918062000	-0.903165000
C	4.667538000	-0.933266000	-0.722684000
H	4.432385000	-0.982843000	-1.786530000
H	5.613166000	-1.478097000	-0.591473000
C	-5.128228000	-2.145213000	0.098620000
H	-4.870353000	-2.890561000	-0.661343000
H	-5.904375000	-2.562834000	0.746170000
H	-4.236493000	-1.961003000	0.705268000
C	3.131641000	-2.832776000	-0.738013000
H	2.632601000	-3.510382000	-0.043625000
H	3.998844000	-3.380282000	-1.131769000
C	3.532907000	1.740696000	-1.927687000
H	3.805021000	0.868195000	-2.523116000
H	4.257262000	2.526135000	-2.185479000
C	3.878070000	-0.863619000	2.355609000
C	2.210679000	-2.496639000	-1.907538000
H	2.741638000	-1.878116000	-2.631930000
H	1.957932000	-3.430797000	-2.428724000
C	1.075543000	0.171783000	-3.114099000
H	2.112451000	-0.034900000	-3.383231000
H	0.597343000	0.567153000	-4.021394000
O	3.020471000	0.029246000	2.149092000
O	0.245487000	0.428797000	2.423083000
H	-0.535984000	0.984216000	2.256537000
H	-0.107973000	-0.435432000	2.701038000
N	4.646935000	-0.862427000	3.436932000
H	5.348802000	-1.572723000	3.599738000
H	4.520989000	-0.146369000	4.143162000

95°

Y	1.516353000	0.066656000	0.337694000
O	-0.761645000	0.353977000	-0.167528000
O	0.800666000	-2.005128000	1.226490000
O	-7.304265000	-0.345745000	1.027885000
O	1.409764000	2.374432000	0.754262000
N	-6.222874000	0.052366000	0.457815000
N	1.074540000	1.220532000	-2.040339000
N	3.671749000	1.378345000	-0.477891000
N	-2.514782000	1.229832000	-1.309795000
H	-2.803278000	1.828445000	-2.076873000
N	0.967268000	-1.768236000	-1.525982000
N	3.578647000	-1.617163000	0.017147000
N	2.303842000	4.432315000	1.008871000
H	1.415525000	4.812279000	1.315416000
H	3.096640000	5.058821000	0.958317000
N	-0.190542000	-4.031202000	1.113603000
H	-0.104778000	-4.161305000	2.115287000

H	-0.630356000	-4.766346000	0.575046000
C	-0.247271000	1.883853000	-1.949513000
H	-0.670052000	2.092859000	-2.940689000
H	-0.122792000	2.842961000	-1.437738000
C	-3.570972000	0.613390000	-0.491432000
H	-3.050794000	-0.067679000	0.183210000
C	-1.213826000	1.085665000	-1.089037000
C	0.240246000	-2.908788000	0.555386000
C	3.774673000	2.588539000	0.370601000
H	4.415635000	3.354517000	-0.083888000
H	4.227210000	2.309919000	1.327313000
C	2.402340000	3.142984000	0.713908000
C	-5.430320000	1.084713000	1.209726000
C	-4.549291000	-0.153910000	-1.383435000
H	-5.013944000	0.552703000	-2.083464000
H	-4.016053000	-0.900114000	-1.982039000
C	-4.334488000	1.680059000	0.300210000
H	-3.644614000	2.258582000	0.923885000
H	-4.794916000	2.379174000	-0.409711000
C	-5.655119000	-0.872167000	-0.582159000
C	2.137416000	2.232686000	-2.314439000
H	1.883142000	3.148672000	-1.779878000
H	2.156203000	2.494752000	-3.381171000
C	-0.011610000	-2.704765000	-0.928538000
H	-0.043058000	-3.662341000	-1.464138000
H	-1.009675000	-2.260450000	-0.995059000
C	0.371806000	-1.115252000	-2.730627000
H	-0.683925000	-0.928931000	-2.530663000
H	0.407952000	-1.793743000	-3.593730000
C	-4.828682000	0.442867000	2.478930000
H	-5.618315000	-0.061083000	3.043441000
H	-4.388178000	1.219757000	3.112924000
H	-4.048310000	-0.288886000	2.251105000
C	-6.402728000	2.203609000	1.619592000
H	-6.898133000	2.628953000	0.740465000
H	-5.847458000	3.001030000	2.124256000
H	-7.166928000	1.822491000	2.299685000
C	4.027188000	-2.010809000	1.370861000
H	5.054652000	-2.396943000	1.366784000
H	3.378889000	-2.811190000	1.740194000
C	-6.799822000	-1.249213000	-1.537406000
H	-6.408084000	-1.876950000	-2.344403000
H	-7.246195000	-0.352968000	-1.980814000
H	-7.579316000	-1.800959000	-1.008681000
C	4.890961000	0.531713000	-0.302839000
H	5.196467000	0.585324000	0.742571000
H	5.726683000	0.935937000	-0.889912000
C	4.673087000	-0.919768000	-0.722437000
H	4.440168000	-0.965241000	-1.786976000
H	5.619750000	-1.462847000	-0.591642000
C	-5.122081000	-2.148054000	0.104653000
H	-4.860656000	-2.894567000	-0.652941000

H	-5.898259000	-2.566233000	0.751791000
H	-4.232052000	-1.959746000	0.712530000
C	3.141626000	-2.822594000	-0.748673000
H	2.646893000	-3.506341000	-0.057466000
H	4.010884000	-3.363774000	-1.146548000
C	3.531027000	1.751667000	-1.918806000
H	3.805025000	0.880747000	-2.515617000
H	4.254598000	2.538606000	-2.174152000
C	3.869930000	-0.866924000	2.358163000
C	2.217946000	-2.484893000	-1.915936000
H	2.746611000	-1.862483000	-2.638724000
H	1.967264000	-3.418001000	-2.439922000
C	1.075205000	0.183467000	-3.114415000
H	2.112185000	-0.020150000	-3.385672000
H	0.594952000	0.580778000	-4.019744000
O	3.003737000	0.019665000	2.157549000
O	0.226981000	0.403670000	2.417431000
H	-0.632483000	0.802711000	2.193420000
H	0.012179000	-0.481950000	2.762395000
N	4.636693000	-0.866278000	3.440630000
H	5.345406000	-1.570763000	3.599166000
H	4.502797000	-0.156598000	4.151867000

105°

Y	1.516187000	0.065722000	0.338313000
O	-0.762647000	0.361513000	-0.158751000
O	0.817631000	-2.017634000	1.219435000
O	-7.307301000	-0.349073000	1.025406000
O	1.407682000	2.376235000	0.751700000
N	-6.225046000	0.049945000	0.457644000
N	1.072165000	1.226448000	-2.037218000
N	3.670627000	1.382985000	-0.473374000
N	-2.516160000	1.231313000	-1.305188000
H	-2.804986000	1.828441000	-2.073327000
N	0.968921000	-1.762240000	-1.529526000
N	3.582314000	-1.612066000	0.011960000
N	2.299230000	4.434395000	1.014321000
H	1.409632000	4.813097000	1.318614000
H	3.091751000	5.061521000	0.967729000
N	-0.163746000	-4.048601000	1.097542000
H	-0.069659000	-4.187354000	2.097291000
H	-0.603397000	-4.781251000	0.555471000
C	-0.249356000	1.889895000	-1.942710000
H	-0.673492000	2.101626000	-2.932705000
H	-0.123760000	2.847455000	-1.428362000
C	-3.572555000	0.612232000	-0.488911000
H	-3.052948000	-0.072654000	0.182224000
C	-1.215477000	1.090845000	-1.082530000
C	0.256330000	-2.918377000	0.546151000
C	3.772669000	2.592507000	0.376078000
H	4.414200000	3.358786000	-0.077137000

H	4.224192000	2.313414000	1.333175000
C	2.399355000	3.145579000	0.716717000
C	-5.431438000	1.077960000	1.214405000
C	-4.551616000	-0.150162000	-1.384178000
H	-5.016072000	0.559984000	-2.080777000
H	-4.019178000	-0.894105000	-1.986288000
C	-4.334715000	1.676135000	0.307712000
H	-3.644060000	2.250817000	0.934051000
H	-4.794132000	2.379022000	-0.399088000
C	-5.657678000	-0.871080000	-0.585656000
C	2.135311000	2.238964000	-2.309440000
H	1.880798000	3.154471000	-1.774337000
H	2.154728000	2.502040000	-3.375893000
C	-0.007511000	-2.702405000	-0.933839000
H	-0.044403000	-3.654972000	-1.477763000
H	-1.005171000	-2.255586000	-0.989567000
C	0.370065000	-1.107661000	-2.731494000
H	-0.685394000	-0.922827000	-2.528343000
H	0.404561000	-1.784560000	-3.595906000
C	-4.830777000	0.430003000	2.480949000
H	-5.621147000	-0.075024000	3.043480000
H	-4.389101000	1.203671000	3.118057000
H	-4.051516000	-0.302049000	2.250272000
C	-6.402565000	2.196240000	1.628983000
H	-6.897950000	2.625413000	0.751718000
H	-5.846244000	2.991159000	2.136413000
H	-7.166834000	1.813375000	2.308033000
C	4.029821000	-2.008980000	1.365172000
H	5.059585000	-2.388924000	1.361988000
H	3.385381000	-2.814809000	1.729235000
C	-6.802443000	-1.244011000	-1.542435000
H	-6.410890000	-1.868954000	-2.351675000
H	-7.248380000	-0.345947000	-1.982590000
H	-7.582265000	-1.797336000	-1.015849000
C	4.891283000	0.538546000	-0.299243000
H	5.194052000	0.588726000	0.747258000
H	5.727531000	0.946815000	-0.882797000
C	4.676713000	-0.911520000	-0.724302000
H	4.445158000	-0.954083000	-1.789280000
H	5.623940000	-1.453727000	-0.594023000
C	-5.125404000	-2.149852000	0.096383000
H	-4.863913000	-2.893488000	-0.664005000
H	-5.902123000	-2.570223000	0.741465000
H	-4.235624000	-1.964451000	0.705525000
C	3.147454000	-2.815435000	-0.758647000
H	2.656540000	-3.504283000	-0.069999000
H	4.017740000	-3.351683000	-1.160895000
C	3.528920000	1.757612000	-1.913988000
H	3.802686000	0.887187000	-2.511584000
H	4.252424000	2.544770000	-2.168889000
C	3.863723000	-0.872000000	2.359244000
C	2.220708000	-2.475560000	-1.923156000

H	2.747158000	-1.849865000	-2.644789000
H	1.970861000	-3.407464000	-2.449656000
C	1.071081000	0.192577000	-3.114234000
H	2.107520000	-0.009042000	-3.389047000
H	0.587820000	0.591694000	-4.017133000
O	2.991411000	0.010484000	2.164401000
O	0.214328000	0.400604000	2.408621000
H	-0.689500000	0.652172000	2.146666000
H	0.119495000	-0.460210000	2.854194000
N	4.628980000	-0.873522000	3.442490000
H	5.342502000	-1.574104000	3.596843000
H	4.489383000	-0.169793000	4.158562000

- XYZ coordinates for $[Y(L_2)]^{3+}$ as a function of the dihedral angle O(amide)-Y-O(water)-H(water):

-65°

Y	-1.531873000	0.209481000	-0.479159000
O	0.720138000	0.379132000	0.023893000
O	-0.903268000	-1.893333000	-1.311480000
O	7.327202000	-0.703992000	-0.807612000
O	-1.262662000	2.468281000	-1.050110000
N	6.232347000	-0.235499000	-0.323729000
N	-1.095923000	1.443581000	1.804221000
N	-3.620418000	1.708032000	0.157868000
N	2.500383000	1.199819000	1.173313000
H	2.799409000	1.816886000	1.921994000
N	-1.133066000	-1.556409000	1.409263000
N	-3.710710000	-1.304480000	-0.208834000
N	-1.996998000	4.558675000	-1.481390000
H	-1.074325000	4.848820000	-1.785493000
H	-2.741937000	5.243389000	-1.506064000
N	-0.021961000	-3.963685000	-1.111294000
H	-0.095998000	-4.124033000	-2.109666000
H	0.363796000	-4.703473000	-0.538454000
C	0.270304000	2.012916000	1.731278000
H	0.677854000	2.220975000	2.728328000
H	0.226380000	2.963246000	1.190790000
C	3.552745000	0.489635000	0.429955000
H	3.029246000	-0.179120000	-0.254420000
C	1.201070000	1.122940000	0.923732000
C	-0.403520000	-2.803286000	-0.600051000
C	-3.615107000	2.878688000	-0.750951000
H	-4.199976000	3.714169000	-0.345831000
H	-4.078505000	2.590882000	-1.700702000
C	-2.198837000	3.308046000	-1.095526000
C	5.543166000	0.807486000	-1.157413000
C	4.430094000	-0.301774000	1.403710000
H	4.880047000	0.401848000	2.116162000
H	3.820746000	-1.003120000	1.983752000

C	4.424024000	1.486648000	-0.340745000
H	3.809121000	2.081881000	-1.024372000
H	4.874491000	2.181926000	0.379221000
C	5.551523000	-1.096005000	0.702585000
C	-2.092694000	2.542126000	2.000428000
H	-1.757984000	3.409603000	1.430491000
H	-2.117398000	2.854418000	3.052813000
C	-0.174523000	-2.555041000	0.879666000
H	-0.196316000	-3.488260000	1.455542000
H	0.837623000	-2.146067000	0.954045000
C	-0.557976000	-0.894631000	2.621593000
H	0.516058000	-0.778637000	2.471045000
H	-0.677935000	-1.538124000	3.502964000
C	4.991043000	0.151880000	-2.441665000
H	5.785402000	-0.418088000	-2.931751000
H	4.640894000	0.926868000	-3.131795000
H	4.154271000	-0.524348000	-2.242745000
C	6.595563000	1.863391000	-1.535021000
H	7.053003000	2.293036000	-0.637547000
H	6.116538000	2.669930000	-2.099711000
H	7.382936000	1.423125000	-2.149796000
C	-4.185140000	-1.731815000	-1.566846000
C	6.609637000	-1.491122000	1.746327000
H	6.136357000	-2.074829000	2.542679000
H	7.064864000	-0.600873000	2.192967000
H	7.397910000	-2.092948000	1.290084000
C	-4.878981000	0.919398000	-0.027528000
H	-5.113751000	0.910919000	-1.094070000
H	-5.719887000	1.412293000	0.478112000
C	-4.763535000	-0.509787000	0.491277000
H	-4.540179000	-0.512425000	1.559084000
H	-5.739225000	-1.001104000	0.380349000
C	5.004311000	-2.368510000	0.020570000
H	4.662634000	-3.078365000	0.781324000
H	5.798897000	-2.840388000	-0.564209000
H	4.162962000	-2.159507000	-0.646809000
C	-3.347098000	-2.514198000	0.587566000
H	-2.878336000	-3.229420000	-0.090829000
H	-4.249736000	-3.004446000	0.974556000
C	-3.505143000	2.144369000	1.583491000
H	-3.863092000	1.328357000	2.212243000
H	-4.176005000	2.994158000	1.770285000
C	-2.431525000	-2.212880000	1.770994000
H	-2.945995000	-1.559644000	2.477159000
H	-2.234335000	-3.151195000	2.306269000
C	-1.204180000	0.455433000	2.920679000
H	-2.262874000	0.321343000	3.145936000
H	-0.744576000	0.866593000	3.830068000
O	-0.689871000	0.391034000	-2.719801000
H	-0.253069000	1.219284000	-2.982828000
H	-0.152620000	-0.346285000	-3.057705000
C	-5.364572000	-2.605076000	-1.554963000

C	-6.335140000	-3.324537000	-1.544061000
H	-3.347794000	-2.236622000	-2.058707000
H	-4.395832000	-0.834563000	-2.157306000
H	-7.191686000	-3.962793000	-1.539757000

-75°

Y	-1.530036000	0.209371000	-0.480460000
O	0.721299000	0.368041000	0.031646000
O	-0.899926000	-1.893370000	-1.310137000
O	7.328656000	-0.699707000	-0.810088000
O	-1.268378000	2.468859000	-1.056468000
N	6.233672000	-0.232729000	-0.325022000
N	-1.096407000	1.442062000	1.803737000
N	-3.622208000	1.707421000	0.158847000
N	2.501069000	1.198119000	1.174879000
H	2.799886000	1.819150000	1.920363000
N	-1.133830000	-1.558040000	1.410366000
N	-3.709972000	-1.304552000	-0.209524000
N	-2.001887000	4.562980000	-1.471196000
H	-1.079658000	4.854556000	-1.775348000
H	-2.746380000	5.248406000	-1.489525000
N	-0.019596000	-3.963996000	-1.109725000
H	-0.092291000	-4.123689000	-2.108279000
H	0.364751000	-4.704361000	-0.536728000
C	0.270216000	2.010231000	1.731017000
H	0.676866000	2.220440000	2.728037000
H	0.227514000	2.959374000	1.188273000
C	3.553894000	0.489161000	0.431010000
H	3.030677000	-0.179236000	-0.253903000
C	1.201585000	1.117473000	0.927043000
C	-0.401600000	-2.803559000	-0.598392000
C	-3.619308000	2.878685000	-0.748943000
H	-4.205573000	3.712812000	-0.343125000
H	-4.082322000	2.590823000	-1.698870000
C	-2.203923000	3.309913000	-1.093586000
C	5.543422000	0.810999000	-1.156863000
C	4.432299000	-0.302809000	1.403312000
H	4.882074000	0.400113000	2.116552000
H	3.823781000	-1.005453000	1.982659000
C	4.423939000	1.487921000	-0.338851000
H	3.808131000	2.083407000	-1.021444000
H	4.874034000	2.182768000	0.381779000
C	5.553940000	-1.095220000	0.700387000
C	-2.092619000	2.541051000	1.999900000
H	-1.758096000	3.408113000	1.429189000
H	-2.116435000	2.854015000	3.052114000
C	-0.174626000	-2.556457000	0.881787000
H	-0.197465000	-3.490032000	1.457075000
H	0.837404000	-2.147590000	0.957766000
C	-0.560267000	-0.896276000	2.623238000
H	0.514120000	-0.781389000	2.474685000
H	-0.682452000	-1.539077000	3.504826000

C	4.991442000	0.157096000	-2.442048000
H	5.786079000	-0.411445000	-2.933337000
H	4.640505000	0.932990000	-3.130769000
H	4.155205000	-0.520048000	-2.244010000
C	6.594832000	1.868413000	-1.533053000
H	7.052205000	2.296941000	-0.635007000
H	6.114932000	2.675503000	-2.096215000
H	7.382367000	1.429859000	-2.148838000
C	-4.183809000	-1.730388000	-1.568250000
C	6.612922000	-1.491195000	1.742911000
H	6.140502000	-2.076432000	2.538649000
H	7.067798000	-0.601310000	2.190630000
H	7.401341000	-2.091781000	1.285286000
C	-4.880141000	0.917999000	-0.026091000
H	-5.115616000	0.910076000	-1.092488000
H	-5.721149000	1.409838000	0.480458000
C	-4.763304000	-0.511422000	0.491386000
H	-4.539781000	-0.514740000	1.559160000
H	-5.738600000	-1.003502000	0.380217000
C	5.007331000	-2.367076000	0.016666000
H	4.666520000	-3.078376000	0.776453000
H	5.802008000	-2.837455000	-0.569201000
H	4.165545000	-2.157686000	-0.650038000
C	-3.346584000	-2.515147000	0.585618000
H	-2.876683000	-3.229239000	-0.093168000
H	-4.249445000	-3.006288000	0.970966000
C	-3.505564000	2.143171000	1.584403000
H	-3.862617000	1.326866000	2.213286000
H	-4.176361000	2.992738000	1.772479000
C	-2.432526000	-2.214571000	1.770318000
H	-2.947810000	-1.561682000	2.476220000
H	-2.236120000	-3.153231000	2.305323000
C	-1.205890000	0.454396000	2.920569000
H	-2.264825000	0.320835000	3.144926000
H	-0.746979000	0.866128000	3.830068000
O	-0.688685000	0.386475000	-2.714146000
H	-0.376207000	1.243484000	-3.050106000
H	-0.116497000	-0.309099000	-3.080131000
C	-5.362919000	-2.604078000	-1.558012000
C	-6.333230000	-3.323910000	-1.548537000
H	-3.346017000	-2.234228000	-2.060380000
H	-4.394586000	-0.832480000	-2.157674000
H	-7.189554000	-3.962470000	-1.545518000

-85°

Y	-1.526755000	0.210365000	-0.480877000
O	0.722838000	0.363198000	0.039863000
O	-0.899966000	-1.896862000	-1.305363000
O	7.327112000	-0.698765000	-0.815112000
O	-1.267131000	2.467107000	-1.059142000
N	6.232984000	-0.231789000	-0.328089000
N	-1.095921000	1.444142000	1.804393000

N	-3.620959000	1.708895000	0.157232000
N	2.502764000	1.199344000	1.177944000
H	2.802104000	1.823292000	1.920755000
N	-1.135095000	-1.556782000	1.414141000
N	-3.708717000	-1.302814000	-0.208716000
N	-1.998429000	4.561909000	-1.474229000
H	-1.075870000	4.852523000	-1.778261000
H	-2.742205000	5.248094000	-1.492474000
N	-0.019619000	-3.967080000	-1.101185000
H	-0.091686000	-4.128380000	-2.099511000
H	0.364426000	-4.706480000	-0.526773000
C	0.271156000	2.011395000	1.733052000
H	0.676418000	2.222993000	2.730372000
H	0.229890000	2.959708000	1.188698000
C	3.554720000	0.490291000	0.433002000
H	3.030495000	-0.178157000	-0.251073000
C	1.202927000	1.116429000	0.931888000
C	-0.401919000	-2.805714000	-0.591946000
C	-3.617469000	2.879348000	-0.751464000
H	-4.202971000	3.714284000	-0.346163000
H	-4.080923000	2.591120000	-1.701052000
C	-2.201689000	3.308997000	-1.096345000
C	5.541457000	0.812213000	-1.158501000
C	4.434777000	-0.301875000	1.403616000
H	4.886073000	0.400762000	2.116170000
H	3.827217000	-1.004543000	1.983955000
C	4.423414000	1.489039000	-0.338423000
H	3.806331000	2.084456000	-1.019924000
H	4.874781000	2.183927000	0.381383000
C	5.554880000	-1.094419000	0.698316000
C	-2.091783000	2.543716000	1.998319000
H	-1.756584000	3.409854000	1.426560000
H	-2.116248000	2.858235000	3.050075000
C	-0.175859000	-2.556286000	0.887959000
H	-0.199431000	-3.488962000	1.464735000
H	0.836224000	-2.147578000	0.963968000
C	-0.562665000	-0.894030000	2.626927000
H	0.512012000	-0.780337000	2.479818000
H	-0.686778000	-1.535612000	3.509156000
C	4.987230000	0.158787000	-2.442981000
H	5.781040000	-0.409420000	-2.935995000
H	4.634929000	0.934974000	-3.130680000
H	4.151454000	-0.518556000	-2.243754000
C	6.592321000	1.869607000	-1.536264000
H	7.051297000	2.297914000	-0.638932000
H	6.111508000	2.676853000	-2.098429000
H	7.378742000	1.431126000	-2.153530000
C	-4.180948000	-1.728954000	-1.567855000
C	6.615730000	-1.491116000	1.738648000
H	6.144653000	-2.076522000	2.535058000
H	7.071743000	-0.601549000	2.185836000
H	7.403093000	-2.091758000	1.279274000

C	-4.879037000	0.919775000	-0.027501000
H	-5.114298000	0.911293000	-1.093945000
H	-5.720059000	1.412088000	0.478593000
C	-4.762580000	-0.509291000	0.490769000
H	-4.539869000	-0.511937000	1.558712000
H	-5.737805000	-1.001454000	0.379192000
C	5.006717000	-2.365899000	0.015128000
H	4.667035000	-3.077351000	0.775280000
H	5.800264000	-2.836292000	-0.572266000
H	4.163859000	-2.156124000	-0.650092000
C	-3.347139000	-2.513097000	0.587529000
H	-2.876747000	-3.227946000	-0.090082000
H	-4.250825000	-3.003422000	0.972009000
C	-3.504619000	2.145661000	1.582481000
H	-3.861957000	1.329820000	2.211785000
H	-4.175419000	2.995425000	1.769707000
C	-2.434490000	-2.211956000	1.773137000
H	-2.950270000	-1.557946000	2.477633000
H	-2.239534000	-3.150199000	2.309452000
C	-1.207477000	0.457564000	2.921908000
H	-2.266773000	0.325016000	3.145133000
H	-0.749369000	0.869775000	3.831614000
O	-0.691035000	0.365090000	-2.708026000
H	-0.489766000	1.198085000	-3.165395000
H	-0.201924000	-0.353778000	-3.141722000
C	-5.360660000	-2.601914000	-1.558798000
C	-6.331492000	-3.321057000	-1.550050000
H	-3.342781000	-2.233546000	-2.058533000
H	-4.390426000	-0.831196000	-2.157984000
H	-7.188261000	-3.959022000	-1.547657000

-95°

Y	-1.523628000	0.210522000	-0.479707000
O	0.723679000	0.369953000	0.041349000
O	-0.904571000	-1.902807000	-1.298920000
O	7.323661000	-0.703655000	-0.818397000
O	-1.259152000	2.463547000	-1.060240000
N	6.230803000	-0.234392000	-0.330702000
N	-1.094074000	1.449751000	1.805124000
N	-3.616828000	1.711577000	0.153610000
N	2.504642000	1.204454000	1.178349000
H	2.805268000	1.828154000	1.920831000
N	-1.135220000	-1.552812000	1.418988000
N	-3.707254000	-1.300235000	-0.205983000
N	-1.987143000	4.557794000	-1.483563000
H	-1.063770000	4.846120000	-1.787254000
H	-2.729986000	5.244865000	-1.505151000
N	-0.022662000	-3.971913000	-1.089384000
H	-0.095867000	-4.136598000	-2.087070000
H	0.362959000	-4.709011000	-0.513082000
C	0.273036000	2.016990000	1.735045000
H	0.677922000	2.227743000	2.732700000

H	0.232274000	2.965708000	1.191378000
C	3.554768000	0.493148000	0.432904000
H	3.028625000	-0.175125000	-0.249875000
C	1.204534000	1.122371000	0.933430000
C	-0.404792000	-2.809086000	-0.583476000
C	-3.609703000	2.880020000	-0.757629000
H	-4.193941000	3.717065000	-0.354799000
H	-4.072722000	2.590649000	-1.707080000
C	-2.192520000	3.306290000	-1.101728000
C	5.539905000	0.809691000	-1.161573000
C	4.434624000	-0.299481000	1.403322000
H	4.887963000	0.403080000	2.114662000
H	3.826491000	-1.000518000	1.985042000
C	4.424080000	1.489485000	-0.340846000
H	3.807064000	2.084968000	-1.022353000
H	4.877569000	2.184551000	0.377448000
C	5.552569000	-1.094697000	0.697567000
C	-2.090208000	2.549422000	1.995791000
H	-1.754140000	3.414702000	1.423230000
H	-2.116546000	2.865691000	3.047002000
C	-0.176882000	-2.554468000	0.895329000
H	-0.200317000	-3.485194000	1.475288000
H	0.835492000	-2.145996000	0.969074000
C	-0.562456000	-0.887734000	2.630398000
H	0.512166000	-0.774193000	2.482598000
H	-0.686205000	-1.527837000	3.513762000
C	4.983000000	0.155477000	-2.444503000
H	5.775398000	-0.414361000	-2.937917000
H	4.630762000	0.931303000	-3.132632000
H	4.146642000	-0.520566000	-2.243396000
C	6.592040000	1.864786000	-1.542169000
H	7.052942000	2.293562000	-0.646055000
H	6.111832000	2.672045000	-2.104834000
H	7.376902000	1.424123000	-2.159878000
C	-4.177623000	-1.729373000	-1.564875000
C	6.614053000	-1.491866000	1.737069000
H	6.142988000	-2.075540000	2.534758000
H	7.072071000	-0.602510000	2.182621000
H	7.399873000	-2.094360000	1.277474000
C	-4.875779000	0.923867000	-0.031369000
H	-5.109638000	0.913623000	-1.098111000
H	-5.716803000	1.418285000	0.472658000
C	-4.761666000	-0.504318000	0.489956000
H	-4.540642000	-0.504932000	1.558254000
H	-5.737134000	-0.995834000	0.377804000
C	5.001510000	-2.366168000	0.016672000
H	4.661566000	-3.076038000	0.778195000
H	5.793586000	-2.838650000	-0.571034000
H	4.158208000	-2.155923000	-0.647825000
C	-3.348063000	-2.508822000	0.593960000
H	-2.878530000	-3.226461000	-0.081227000
H	-4.252727000	-2.996530000	0.979454000

C	-3.502254000	2.150654000	1.578295000
H	-3.860530000	1.335807000	2.208316000
H	-4.173361000	3.000746000	1.763032000
C	-2.435470000	-2.205567000	1.779100000
H	-2.950840000	-1.549159000	2.481642000
H	-2.241786000	-3.142587000	2.318031000
C	-1.207123000	0.464492000	2.923395000
H	-2.266663000	0.332617000	3.145854000
H	-0.749669000	0.877210000	3.833214000
O	-0.693306000	0.338139000	-2.707342000
H	-0.600854000	1.124356000	-3.269744000
H	-0.420903000	-0.443842000	-3.215570000
C	-5.358601000	-2.600608000	-1.555452000
C	-6.330557000	-3.318224000	-1.545992000
H	-3.339254000	-2.236475000	-2.052502000
H	-4.384803000	-0.832853000	-2.157737000
H	-7.188280000	-3.954902000	-1.542988000

-105°

Y	-1.523158000	0.209715000	-0.479016000
O	0.723591000	0.374319000	0.037881000
O	-0.908217000	-1.905706000	-1.296594000
O	7.324130000	-0.705847000	-0.817199000
O	-1.257050000	2.462456000	-1.060203000
N	6.231157000	-0.235527000	-0.330780000
N	-1.092541000	1.452016000	1.804454000
N	-3.615436000	1.712010000	0.153592000
N	2.505268000	1.206923000	1.175160000
H	2.806312000	1.830019000	1.917983000
N	-1.133327000	-1.551279000	1.420268000
N	-3.706676000	-1.299754000	-0.203474000
N	-1.983820000	4.557296000	-1.482890000
H	-1.060216000	4.845251000	-1.786249000
H	-2.726324000	5.244735000	-1.504423000
N	-0.023878000	-3.973750000	-1.086251000
H	-0.098555000	-4.139727000	-2.083611000
H	0.363736000	-4.709631000	-0.509728000
C	0.274217000	2.019829000	1.733262000
H	0.680010000	2.230442000	2.730575000
H	0.232701000	2.968661000	1.189879000
C	3.555016000	0.494234000	0.430464000
H	3.028599000	-0.174524000	-0.251645000
C	1.205118000	1.125702000	0.930528000
C	-0.405995000	-2.810596000	-0.581160000
C	-3.607476000	2.879873000	-0.758424000
H	-4.192085000	3.717172000	-0.356686000
H	-4.069685000	2.589797000	-1.708063000
C	-2.189938000	3.305716000	-1.101663000
C	5.541050000	0.807653000	-1.163478000
C	4.434072000	-0.297557000	1.402301000
H	4.887340000	0.405766000	2.112945000
H	3.825313000	-0.997539000	1.984640000

C	4.425096000	1.489102000	-0.344275000
H	3.808643000	2.083841000	-1.026934000
H	4.878526000	2.184976000	0.373271000
C	5.552069000	-1.094172000	0.698280000
C	-2.089030000	2.551263000	1.995214000
H	-1.753461000	3.416663000	1.422545000
H	-2.115327000	2.867661000	3.046388000
C	-0.175723000	-2.553789000	0.896940000
H	-0.198532000	-3.483652000	1.478302000
H	0.836811000	-2.145349000	0.968787000
C	-0.559530000	-0.884936000	2.630519000
H	0.514892000	-0.771056000	2.481348000
H	-0.681970000	-1.524402000	3.514526000
C	4.984564000	0.151772000	-2.445737000
H	5.777027000	-0.419087000	-2.937867000
H	4.632977000	0.926695000	-3.135206000
H	4.147841000	-0.523655000	-2.244109000
C	6.593805000	1.861779000	-1.545034000
H	7.054423000	2.291633000	-0.649289000
H	6.114221000	2.668434000	-2.109093000
H	7.378806000	1.419908000	-2.161703000
C	-4.176571000	-1.730396000	-1.562129000
C	6.612798000	-1.490276000	1.738979000
H	6.141038000	-2.072667000	2.537198000
H	7.070855000	-0.600461000	2.183580000
H	7.398691000	-2.093691000	1.280721000
C	-4.874754000	0.924762000	-0.031004000
H	-5.108553000	0.913817000	-1.097764000
H	-5.715613000	1.419899000	0.472571000
C	-4.761165000	-0.503084000	0.491452000
H	-4.540369000	-0.502862000	1.559807000
H	-5.736710000	-0.994461000	0.379435000
C	5.000841000	-2.366370000	0.018893000
H	4.660366000	-3.075081000	0.781263000
H	5.792981000	-2.839923000	-0.567861000
H	4.157840000	-2.156732000	-0.646185000
C	-3.347473000	-2.507443000	0.597945000
H	-2.878996000	-3.226351000	-0.076569000
H	-4.252083000	-2.993997000	0.985004000
C	-3.500940000	2.151820000	1.578024000
H	-3.858945000	1.337169000	2.208455000
H	-4.172315000	3.001801000	1.762297000
C	-2.433697000	-2.203096000	1.781976000
H	-2.948302000	-1.545694000	2.484145000
H	-2.239982000	-3.139579000	2.321821000
C	-1.204543000	0.467216000	2.923215000
H	-2.263905000	0.335022000	3.146357000
H	-0.746751000	0.880491000	3.832612000
O	-0.689198000	0.333802000	-2.713122000
H	-0.731661000	1.103501000	-3.304345000
H	-0.584782000	-0.465068000	-3.256864000
C	-5.357722000	-2.601322000	-1.552110000

C	-6.329772000	-3.318796000	-1.542007000
H	-3.338036000	-2.238285000	-2.048604000
H	-4.383252000	-0.834472000	-2.156083000
H	-7.187579000	-3.955359000	-1.538441000

-115°

Y	-1.523387000	0.210219000	-0.477974000
O	0.723265000	0.374843000	0.036341000
O	-0.906343000	-1.905401000	-1.295478000
O	7.324873000	-0.706093000	-0.815562000
O	-1.259942000	2.462475000	-1.060148000
N	6.231733000	-0.234906000	-0.330364000
N	-1.092303000	1.453387000	1.803248000
N	-3.616713000	1.710960000	0.153968000
N	2.505191000	1.209877000	1.171586000
H	2.806201000	1.833872000	1.913675000
N	-1.131194000	-1.550316000	1.421106000
N	-3.705351000	-1.300785000	-0.201771000
N	-1.987907000	4.556532000	-1.484646000
H	-1.064494000	4.844658000	-1.788426000
H	-2.730769000	5.243563000	-1.506673000
N	-0.020844000	-3.972943000	-1.084839000
H	-0.095482000	-4.139138000	-2.082177000
H	0.367241000	-4.708523000	-0.508225000
C	0.274120000	2.021902000	1.730648000
H	0.680556000	2.233331000	2.727515000
H	0.231687000	2.970352000	1.186681000
C	3.555080000	0.496080000	0.428136000
H	3.028869000	-0.173434000	-0.253376000
C	1.204985000	1.127580000	0.927900000
C	-0.403356000	-2.809990000	-0.579927000
C	-3.610329000	2.878545000	-0.758418000
H	-4.195373000	3.715495000	-0.356585000
H	-4.072866000	2.587845000	-1.707702000
C	-2.193285000	3.305172000	-1.102361000
C	5.542174000	0.807131000	-1.164956000
C	4.433459000	-0.294542000	1.401564000
H	4.886203000	0.409685000	2.111649000
H	3.824236000	-0.993744000	1.984354000
C	4.425705000	1.489793000	-0.347441000
H	3.809731000	2.083603000	-1.031337000
H	4.878717000	2.186635000	0.369426000
C	5.551978000	-1.092088000	0.699449000
C	-2.089466000	2.552085000	1.994161000
H	-1.754884000	3.417461000	1.420906000
H	-2.115239000	2.868887000	3.045218000
C	-0.173197000	-2.552572000	0.898043000
H	-0.195549000	-3.482261000	1.479692000
H	0.839187000	-2.143722000	0.969648000
C	-0.557362000	-0.882769000	2.630714000
H	0.516937000	-0.768390000	2.481041000

H	-0.679109000	-1.521661000	3.515221000
C	4.986589000	0.149444000	-2.446686000
H	5.779430000	-0.422069000	-2.937453000
H	4.635451000	0.923368000	-3.137495000
H	4.149761000	-0.525743000	-2.244729000
C	6.595222000	1.860677000	-1.547274000
H	7.055277000	2.291737000	-0.651820000
H	6.116046000	2.666573000	-2.112762000
H	7.380601000	1.417907000	-2.162815000
C	-4.174667000	-1.732064000	-1.560469000
C	6.611982000	-1.486586000	1.741503000
H	6.139663000	-2.067813000	2.540239000
H	7.069653000	-0.596082000	2.185126000
H	7.398251000	-2.090637000	1.284732000
C	-4.875528000	0.922673000	-0.029627000
H	-5.109932000	0.911271000	-1.096260000
H	-5.716481000	1.417296000	0.474285000
C	-4.760548000	-0.504971000	0.493076000
H	-4.539630000	-0.504325000	1.561415000
H	-5.735646000	-0.997266000	0.381232000
C	5.001278000	-2.365321000	0.021569000
H	4.660363000	-3.072937000	0.784764000
H	5.793822000	-2.839683000	-0.563986000
H	4.158677000	-2.156711000	-0.644341000
C	-3.345052000	-2.508011000	0.599941000
H	-2.876317000	-3.226851000	-0.074469000
H	-4.249197000	-2.995044000	0.987457000
C	-3.501452000	2.151440000	1.578182000
H	-3.858452000	1.336801000	2.209199000
H	-4.173269000	3.001025000	1.762612000
C	-2.431086000	-2.202657000	1.783601000
H	-2.945833000	-1.545202000	2.485616000
H	-2.236709000	-3.138792000	2.323808000
C	-1.203112000	0.469187000	2.922714000
H	-2.262291000	0.336472000	3.146411000
H	-0.745223000	0.883423000	3.831614000
O	-0.682955000	0.330162000	-2.719160000
H	-0.863011000	1.064388000	-3.330010000
H	-0.644540000	-0.489847000	-3.240813000
C	-5.354972000	-2.604088000	-1.550454000
C	-6.326264000	-3.322578000	-1.540162000
H	-3.335513000	-2.239239000	-2.046633000
H	-4.382071000	-0.836410000	-2.154578000
H	-7.183418000	-3.960023000	-1.536428000

-125°

Y	-1.523100000	0.211616000	-0.478433000
O	0.722647000	0.368777000	0.041339000
O	-0.902919000	-1.906575000	-1.294522000
O	7.324714000	-0.700731000	-0.816697000
O	-1.266523000	2.463193000	-1.060525000

N	6.231252000	-0.231133000	-0.330687000
N	-1.094538000	1.452368000	1.803178000
N	-3.620321000	1.710421000	0.154099000
N	2.503892000	1.208957000	1.173810000
H	2.804480000	1.835163000	1.914220000
N	-1.132552000	-1.551406000	1.421723000
N	-3.704701000	-1.300426000	-0.202700000
N	-1.996319000	4.555131000	-1.491789000
H	-1.073369000	4.842796000	-1.797347000
H	-2.739638000	5.241593000	-1.515366000
N	-0.017913000	-3.974149000	-1.082209000
H	-0.091036000	-4.140452000	-2.079661000
H	0.369193000	-4.709768000	-0.504954000
C	0.272074000	2.020524000	1.730839000
H	0.677574000	2.233849000	2.727696000
H	0.230129000	2.967909000	1.184931000
C	3.554372000	0.496362000	0.429994000
H	3.028636000	-0.173645000	-0.251378000
C	1.203756000	1.124584000	0.930723000
C	-0.401102000	-2.811342000	-0.577942000
C	-3.616568000	2.878548000	-0.757514000
H	-4.199954000	3.715499000	-0.353207000
H	-4.082290000	2.588930000	-1.705546000
C	-2.200413000	3.304948000	-1.104823000
C	5.540003000	0.810506000	-1.164360000
C	4.434308000	-0.293510000	1.402580000
H	4.886840000	0.410962000	2.112547000
H	3.826334000	-0.993605000	1.985600000
C	4.423260000	1.491441000	-0.345806000
H	3.806070000	2.084744000	-1.029044000
H	4.875919000	2.188570000	0.371008000
C	5.553094000	-1.089576000	0.699176000
C	-2.091673000	2.551323000	1.993424000
H	-1.757187000	3.416155000	1.419300000
H	-2.116989000	2.868871000	3.044262000
C	-0.173455000	-2.553372000	0.900190000
H	-0.196129000	-3.482949000	1.482016000
H	0.838659000	-2.144080000	0.972973000
C	-0.560437000	-0.883711000	2.632004000
H	0.514100000	-0.769647000	2.484034000
H	-0.683732000	-1.522300000	3.516518000
C	4.984338000	0.152875000	-2.446080000
H	5.777511000	-0.417432000	-2.937711000
H	4.631820000	0.926781000	-3.136207000
H	4.148429000	-0.523386000	-2.243921000
C	6.591587000	1.865477000	-1.546806000
H	7.051674000	2.296671000	-0.651433000
H	6.111119000	2.671068000	-2.111632000
H	7.377114000	1.423931000	-2.163038000
C	-4.171855000	-1.729129000	-1.562810000
C	6.614293000	-1.483644000	1.740165000
H	6.143178000	-2.065782000	2.538947000

H	7.071459000	-0.592949000	2.183926000
H	7.400786000	-2.086664000	1.282417000
C	-4.878250000	0.920837000	-0.028953000
H	-5.113249000	0.909670000	-1.095465000
H	-5.719561000	1.414124000	0.475709000
C	-4.761323000	-0.506908000	0.492568000
H	-4.540737000	-0.506921000	1.560966000
H	-5.735598000	-1.000650000	0.379902000
C	5.003147000	-2.362920000	0.020901000
H	4.663537000	-3.071389000	0.783886000
H	5.795733000	-2.836087000	-0.565564000
H	4.159828000	-2.154747000	-0.644245000
C	-3.344846000	-2.508811000	0.597380000
H	-2.874904000	-3.226396000	-0.077523000
H	-4.249282000	-2.996877000	0.982899000
C	-3.503929000	2.150377000	1.578376000
H	-3.860206000	1.335443000	2.209423000
H	-4.175810000	2.999695000	1.763825000
C	-2.432516000	-2.204328000	1.782457000
H	-2.948205000	-1.547510000	2.484372000
H	-2.238568000	-3.140816000	2.322215000
C	-1.206169000	0.468505000	2.922868000
H	-2.265484000	0.336050000	3.146033000
H	-0.748736000	0.883028000	3.831869000
O	-0.640572000	0.326702000	-2.712955000
H	-0.927662000	0.992463000	-3.360623000
H	-0.583951000	-0.526539000	-3.177545000
C	-5.351812000	-2.601667000	-1.556369000
C	-6.322767000	-3.320642000	-1.548916000
H	-3.331739000	-2.235167000	-2.048565000
H	-4.378650000	-0.832493000	-2.155661000
H	-7.179638000	-3.958476000	-1.547657000

-135°

Y	-1.523717000	0.212447000	-0.479324000
O	0.721535000	0.363967000	0.043005000
O	-0.898698000	-1.908880000	-1.292833000
O	7.325496000	-0.697280000	-0.815885000
O	-1.267988000	2.465239000	-1.056918000
N	6.231512000	-0.228465000	-0.330291000
N	-1.096386000	1.452251000	1.801811000
N	-3.622151000	1.710920000	0.152666000
N	2.502504000	1.208564000	1.172821000
H	2.802658000	1.836637000	1.911836000
N	-1.134508000	-1.551656000	1.422738000
N	-3.705337000	-1.299253000	-0.203568000
N	-1.998640000	4.555846000	-1.493346000
H	-1.075354000	4.843726000	-1.797630000
H	-2.742497000	5.241613000	-1.519420000
N	-0.016558000	-3.977330000	-1.076728000
H	-0.087695000	-4.144436000	-2.074207000

H	0.368490000	-4.712924000	-0.498035000
C	0.270571000	2.019553000	1.729304000
H	0.675871000	2.233607000	2.726080000
H	0.229219000	2.966386000	1.182410000
C	3.553709000	0.496228000	0.429825000
H	3.028767000	-0.175536000	-0.250415000
C	1.202387000	1.122358000	0.930502000
C	-0.399493000	-2.813888000	-0.574243000
C	-3.618685000	2.878858000	-0.759218000
H	-4.203057000	3.715452000	-0.355566000
H	-4.083411000	2.588689000	-1.707556000
C	-2.202357000	3.306033000	-1.104693000
C	5.538659000	0.811010000	-1.165319000
C	4.434971000	-0.290908000	1.403405000
H	4.886624000	0.415295000	2.112214000
H	3.828167000	-0.991015000	1.987628000
C	4.421041000	1.491445000	-0.347569000
H	3.802868000	2.082902000	-1.031517000
H	4.872773000	2.190204000	0.368234000
C	5.554750000	-1.086373000	0.700926000
C	-2.093039000	2.551840000	1.991755000
H	-1.758118000	3.416462000	1.417645000
H	-2.118197000	2.869355000	3.042592000
C	-0.174877000	-2.554430000	0.903900000
H	-0.198662000	-3.483306000	1.486802000
H	0.837218000	-2.145264000	0.977757000
C	-0.563614000	-0.883235000	2.633194000
H	0.511139000	-0.769745000	2.486406000
H	-0.688280000	-1.521061000	3.518064000
C	4.983731000	0.150832000	-2.446055000
H	5.777624000	-0.419021000	-2.937050000
H	4.630001000	0.923294000	-3.137173000
H	4.148812000	-0.526318000	-2.242811000
C	6.588655000	1.866981000	-1.549382000
H	7.048244000	2.300084000	-0.654675000
H	6.106946000	2.671092000	-2.115261000
H	7.374731000	1.425718000	-2.165115000
C	-4.171573000	-1.727071000	-1.564360000
C	6.616680000	-1.477419000	1.742318000
H	6.146520000	-2.059073000	2.542013000
H	7.072614000	-0.585417000	2.184729000
H	7.403989000	-2.079947000	1.285331000
C	-4.880056000	0.921316000	-0.029892000
H	-5.115626000	0.910196000	-1.096283000
H	-5.721207000	1.414405000	0.475212000
C	-4.762559000	-0.506400000	0.491508000
H	-4.542283000	-0.506387000	1.559973000
H	-5.736514000	-1.000686000	0.378481000
C	5.006491000	-2.361440000	0.024536000
H	4.668054000	-3.069361000	0.788552000
H	5.799655000	-2.834247000	-0.561440000
H	4.162727000	-2.155390000	-0.640726000

C	-3.346029000	-2.508111000	0.596046000
H	-2.875143000	-3.225122000	-0.078808000
H	-4.250767000	-2.996630000	0.980257000
C	-3.505509000	2.151353000	1.576802000
H	-3.862138000	1.336781000	2.208129000
H	-4.177036000	3.000996000	1.761984000
C	-2.435088000	-2.203922000	1.782215000
H	-2.951304000	-1.546740000	2.483395000
H	-2.242205000	-3.140392000	2.322370000
C	-1.209068000	0.469357000	2.922255000
H	-2.268587000	0.337450000	3.144731000
H	-0.752211000	0.884652000	3.831191000
O	-0.612495000	0.322114000	-2.714478000
H	-0.999572000	0.897633000	-3.396130000
H	-0.510248000	-0.560245000	-3.113987000
C	-5.351067000	-2.600183000	-1.559181000
C	-6.321499000	-3.319864000	-1.552547000
H	-3.330939000	-2.232414000	-2.050012000
H	-4.378390000	-0.830072000	-2.156634000
H	-7.177942000	-3.958277000	-1.551985000

-145°

Y	-1.525220000	0.213670000	-0.479501000
O	0.720015000	0.359675000	0.042456000
O	-0.894607000	-1.910672000	-1.290853000
O	7.327207000	-0.693698000	-0.814504000
O	-1.266836000	2.467643000	-1.049966000
N	6.232330000	-0.226190000	-0.329674000
N	-1.097956000	1.451948000	1.800980000
N	-3.622958000	1.712127000	0.151000000
N	2.500906000	1.206584000	1.171026000
H	2.800661000	1.835556000	1.909459000
N	-1.136677000	-1.551496000	1.423959000
N	-3.706117000	-1.297907000	-0.204767000
N	-1.997664000	4.556398000	-1.495029000
H	-1.073656000	4.844220000	-1.797099000
H	-2.742053000	5.241384000	-1.525357000
N	-0.015132000	-3.979938000	-1.071199000
H	-0.084101000	-4.147670000	-2.068746000
H	0.367987000	-4.715508000	-0.491164000
C	0.269511000	2.017768000	1.727402000
H	0.675359000	2.232194000	2.723879000
H	0.228670000	2.964190000	1.179802000
C	3.553024000	0.494941000	0.428641000
H	3.029111000	-0.177873000	-0.251343000
C	1.200894000	1.119521000	0.929034000
C	-0.398009000	-2.815967000	-0.570366000
C	-3.618547000	2.879936000	-0.761183000
H	-4.203894000	3.716376000	-0.358600000
H	-4.081606000	2.589392000	-1.710196000
C	-2.201485000	3.307383000	-1.103530000

C	5.538391000	0.811802000	-1.165635000
C	4.434957000	-0.290356000	1.403088000
H	4.885214000	0.416967000	2.111672000
H	3.828907000	-0.990981000	1.987468000
C	4.419313000	1.490979000	-0.348873000
H	3.800644000	2.081198000	-1.033435000
H	4.869628000	2.190746000	0.366835000
C	5.556266000	-1.084542000	0.701643000
C	-2.093818000	2.552438000	1.990665000
H	-1.757965000	3.417039000	1.417200000
H	-2.119224000	2.869398000	3.041645000
C	-0.176592000	-2.555201000	0.907790000
H	-0.201677000	-3.483425000	1.491653000
H	0.835534000	-2.146322000	0.982880000
C	-0.566807000	-0.882803000	2.634745000
H	0.508170000	-0.769987000	2.489041000
H	-0.692787000	-1.520109000	3.519794000
C	4.985132000	0.150123000	-2.446314000
H	5.780104000	-0.418878000	-2.936548000
H	4.630686000	0.921682000	-3.138067000
H	4.151058000	-0.528087000	-2.243127000
C	6.587023000	1.869165000	-1.549619000
H	7.045394000	2.303443000	-0.654855000
H	6.104449000	2.672244000	-2.116223000
H	7.374143000	1.428759000	-2.164625000
C	-4.171596000	-1.725545000	-1.565947000
C	6.618173000	-1.473451000	1.743871000
H	6.148407000	-2.055347000	2.543621000
H	7.072516000	-0.580522000	2.186061000
H	7.406648000	-2.075050000	1.287682000
C	-4.880967000	0.922816000	-0.031761000
H	-5.116358000	0.911755000	-1.098192000
H	-5.722159000	1.416009000	0.473163000
C	-4.763774000	-0.504966000	0.489693000
H	-4.544154000	-0.504931000	1.558289000
H	-5.737643000	-0.999282000	0.376088000
C	5.010199000	-2.360712000	0.025593000
H	4.672504000	-3.068825000	0.789761000
H	5.804320000	-2.832563000	-0.559855000
H	4.166383000	-2.156184000	-0.640093000
C	-3.347536000	-2.507006000	0.594912000
H	-2.875851000	-3.223722000	-0.079720000
H	-4.252699000	-2.995689000	0.977878000
C	-3.506483000	2.152964000	1.575073000
H	-3.864001000	1.338842000	2.206481000
H	-4.177451000	3.003155000	1.759723000
C	-2.437954000	-2.203099000	1.782148000
H	-2.954644000	-1.545576000	2.482652000
H	-2.246137000	-3.139576000	2.322651000
C	-1.211598000	0.470282000	2.922297000
H	-2.271288000	0.339227000	3.144444000
H	-0.754896000	0.886244000	3.831003000

O	-0.596054000	0.318853000	-2.719534000
H	-1.076755000	0.786643000	-3.424470000
H	-0.441823000	-0.585807000	-3.048137000
C	-5.350544000	-2.599314000	-1.561465000
C	-6.320430000	-3.319729000	-1.555349000
H	-3.330430000	-2.230303000	-2.051364000
H	-4.378631000	-0.828486000	-2.158025000
H	-7.176419000	-3.958754000	-1.555240000

-155°

Y	-1.526666000	0.214444000	-0.482425000
O	0.716813000	0.352242000	0.052528000
O	-0.875518000	-1.910294000	-1.290124000
O	7.320907000	-0.690337000	-0.817717000
O	-1.261948000	2.472958000	-1.038421000
N	6.226760000	-0.223543000	-0.330541000
N	-1.105026000	1.450099000	1.801762000
N	-3.624521000	1.711593000	0.143790000
N	2.496525000	1.205521000	1.177453000
H	2.796032000	1.836799000	1.913991000
N	-1.143992000	-1.552992000	1.425186000
N	-3.707156000	-1.297327000	-0.212456000
N	-1.995890000	4.558328000	-1.494248000
H	-1.070483000	4.848355000	-1.789783000
H	-2.742266000	5.240732000	-1.532305000
N	-0.008982000	-3.983939000	-1.061021000
H	-0.070322000	-4.152108000	-2.058995000
H	0.364559000	-4.721367000	-0.477124000
C	0.263643000	2.013928000	1.733257000
H	0.666699000	2.226254000	2.731326000
H	0.225878000	2.961215000	1.186983000
C	3.548665000	0.494699000	0.434314000
H	3.024624000	-0.180613000	-0.243060000
C	1.196355000	1.115368000	0.936707000
C	-0.390803000	-2.817931000	-0.564250000
C	-3.617330000	2.878366000	-0.769809000
H	-4.207844000	3.713563000	-0.372219000
H	-4.073009000	2.585176000	-1.721560000
C	-2.198784000	3.309252000	-1.101920000
C	5.528845000	0.811899000	-1.166350000
C	4.434650000	-0.287102000	1.407821000
H	4.885950000	0.422303000	2.113661000
H	3.831512000	-0.987570000	1.995401000
C	4.411064000	1.490766000	-0.347500000
H	3.789426000	2.078730000	-1.031323000
H	4.862312000	2.192524000	0.365653000
C	5.554999000	-1.080957000	0.704408000
C	-2.100005000	2.551979000	1.988215000
H	-1.761052000	3.416404000	1.416497000
H	-2.128792000	2.868328000	3.039289000
C	-0.180773000	-2.556988000	0.915303000

H	-0.209728000	-3.484883000	1.499512000
H	0.830853000	-2.148105000	0.996795000
C	-0.579555000	-0.884247000	2.638610000
H	0.496106000	-0.771887000	2.497927000
H	-0.710094000	-1.521450000	3.523055000
C	4.972878000	0.147155000	-2.444297000
H	5.767430000	-0.420920000	-2.936282000
H	4.614588000	0.916962000	-3.136017000
H	4.140939000	-0.532517000	-2.237412000
C	6.574709000	1.870133000	-1.555416000
H	7.034992000	2.306915000	-0.662864000
H	6.089248000	2.671308000	-2.122254000
H	7.360717000	1.429714000	-2.171842000
C	-4.171492000	-1.722807000	-1.574771000
C	6.620646000	-1.466498000	1.744044000
H	6.154157000	-2.047630000	2.546259000
H	7.075066000	-0.572134000	2.183243000
H	7.408588000	-2.067773000	1.286498000
C	-4.882687000	0.922961000	-0.040417000
H	-5.117490000	0.912339000	-1.106965000
H	-5.724069000	1.416294000	0.464007000
C	-4.765955000	-0.504853000	0.481108000
H	-4.547828000	-0.504975000	1.549984000
H	-5.739424000	-0.999594000	0.366085000
C	5.008781000	-2.359097000	0.032209000
H	4.674271000	-3.066348000	0.798577000
H	5.801895000	-2.830833000	-0.554699000
H	4.162777000	-2.156956000	-0.631443000
C	-3.350421000	-2.507753000	0.585997000
H	-2.874556000	-3.222111000	-0.088329000
H	-4.256636000	-2.998599000	0.963624000
C	-3.511702000	2.154144000	1.567865000
H	-3.872510000	1.341180000	2.198883000
H	-4.182177000	3.005409000	1.749195000
C	-2.446519000	-2.204866000	1.777580000
H	-2.966233000	-1.547824000	2.476278000
H	-2.257121000	-3.141701000	2.318287000
C	-1.224579000	0.469119000	2.922848000
H	-2.285347000	0.338997000	3.140340000
H	-0.771616000	0.885122000	3.833403000
O	-0.507685000	0.327803000	-2.707668000
H	-1.044389000	0.675094000	-3.441933000
H	-0.279256000	-0.586221000	-2.959400000
C	-5.349936000	-2.597213000	-1.572504000
C	-6.319342000	-3.318270000	-1.567701000
H	-3.329727000	-2.226489000	-2.060498000
H	-4.378412000	-0.824936000	-2.165587000
H	-7.174982000	-3.957768000	-1.568661000

-165°

Y	-1.527774000	0.215282000	-0.485154000
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O	0.715300000	0.346883000	0.051246000
O	-0.862719000	-1.910716000	-1.288602000
O	7.323372000	-0.682459000	-0.817520000
O	-1.263736000	2.476600000	-1.031198000
N	6.227911000	-0.219073000	-0.330053000
N	-1.107845000	1.446719000	1.801584000
N	-3.626832000	1.711809000	0.143597000
N	2.494098000	1.198940000	1.178873000
H	2.792687000	1.829361000	1.916541000
N	-1.147041000	-1.555437000	1.425471000
N	-3.709121000	-1.295851000	-0.216305000
N	-1.998747000	4.561342000	-1.488557000
H	-1.072812000	4.852820000	-1.780943000
H	-2.745959000	5.242701000	-1.528551000
N	-0.004888000	-3.987476000	-1.055459000
H	-0.061320000	-4.155018000	-2.053822000
H	0.363691000	-4.726091000	-0.469931000
C	0.261869000	2.008026000	1.733737000
H	0.664998000	2.218930000	2.732070000
H	0.225771000	2.955794000	1.188195000
C	3.547750000	0.491242000	0.434927000
H	3.025382000	-0.184541000	-0.243278000
C	1.194244000	1.109240000	0.936782000
C	-0.385398000	-2.820244000	-0.560381000
C	-3.620010000	2.878483000	-0.770099000
H	-4.213314000	3.712485000	-0.374159000
H	-4.072483000	2.584146000	-1.723019000
C	-2.201189000	3.311631000	-1.097644000
C	5.527683000	0.815734000	-1.164695000
C	4.435471000	-0.289451000	1.407698000
H	4.884778000	0.420348000	2.114418000
H	3.834047000	-0.992141000	1.994381000
C	4.407854000	1.490543000	-0.345369000
H	3.784893000	2.077835000	-1.028558000
H	4.857007000	2.192497000	0.368918000
C	5.558008000	-1.079536000	0.703581000
C	-2.101106000	2.550269000	1.988142000
H	-1.760704000	3.414508000	1.417143000
H	-2.129631000	2.865852000	3.039443000
C	-0.182093000	-2.559860000	0.919844000
H	-0.213803000	-3.487565000	1.504220000
H	0.829356000	-2.151353000	1.005383000
C	-0.585740000	-0.887177000	2.640466000
H	0.490386000	-0.775388000	2.502662000
H	-0.718961000	-1.524321000	3.524564000
C	4.973788000	0.151434000	-2.443761000
H	5.769839000	-0.414080000	-2.936267000
H	4.613919000	0.921357000	-3.134538000
H	4.143337000	-0.530425000	-2.238046000
C	6.570950000	1.877266000	-1.551804000
H	7.029710000	2.313960000	-0.658418000
H	6.083627000	2.678006000	-2.117658000

H	7.358358000	1.439816000	-2.168547000
C	-4.175765000	-1.717587000	-1.579181000
C	6.624339000	-1.463711000	1.743020000
H	6.159111000	-2.047012000	2.544390000
H	7.076383000	-0.568748000	2.183457000
H	7.413915000	-2.062407000	1.284918000
C	-4.885235000	0.923609000	-0.039587000
H	-5.122160000	0.914493000	-1.105666000
H	-5.725784000	1.416163000	0.466982000
C	-4.767246000	-0.504725000	0.479973000
H	-4.547726000	-0.506107000	1.548533000
H	-5.740582000	-0.999897000	0.365598000
C	5.015220000	-2.358112000	0.029460000
H	4.682303000	-3.067319000	0.794708000
H	5.809707000	-2.826983000	-0.557885000
H	4.168882000	-2.157169000	-0.634143000
C	-3.351821000	-2.508075000	0.579116000
H	-2.873544000	-3.219563000	-0.096602000
H	-4.258000000	-3.001406000	0.953587000
C	-3.513370000	2.154560000	1.567524000
H	-3.875395000	1.342218000	2.198666000
H	-4.182643000	3.006781000	1.748752000
C	-2.450726000	-2.207275000	1.773441000
H	-2.971917000	-1.551174000	2.471918000
H	-2.263184000	-3.145080000	2.313099000
C	-1.230226000	0.466472000	2.922905000
H	-2.291499000	0.337215000	3.138405000
H	-0.778675000	0.882720000	3.834057000
O	-0.484349000	0.335735000	-2.711141000
H	-1.075364000	0.546362000	-3.456046000
H	-0.163270000	-0.567054000	-2.894852000
C	-5.352921000	-2.593636000	-1.577600000
C	-6.321131000	-3.316292000	-1.573670000
H	-3.334293000	-2.218519000	-2.068419000
H	-4.384949000	-0.818042000	-2.166538000
H	-7.175808000	-3.957079000	-1.575386000

-175°

Y	-1.527870000	0.215235000	-0.487905000
O	0.714563000	0.348747000	0.045124000
O	-0.858030000	-1.912406000	-1.285410000
O	7.325136000	-0.680423000	-0.815330000
O	-1.263551000	2.479525000	-1.023428000
N	6.228791000	-0.218256000	-0.328714000
N	-1.108865000	1.445642000	1.800893000
N	-3.627960000	1.712134000	0.142601000
N	2.492705000	1.196036000	1.177550000
H	2.790699000	1.824006000	1.917571000
N	-1.148537000	-1.555443000	1.426913000
N	-3.710563000	-1.294348000	-0.217699000
N	-1.998653000	4.563860000	-1.483060000
H	-1.071953000	4.856454000	-1.771829000

H	-2.746447000	5.244420000	-1.525457000
N	-0.007634000	-3.991837000	-1.048984000
H	-0.063093000	-4.160117000	-2.047258000
H	0.357662000	-4.731034000	-0.462179000
C	0.261211000	2.006012000	1.732425000
H	0.665263000	2.215583000	2.730644000
H	0.225248000	2.954357000	1.187921000
C	3.547289000	0.489665000	0.433613000
H	3.025962000	-0.185432000	-0.246089000
C	1.193220000	1.108278000	0.933693000
C	-0.385321000	-2.822727000	-0.555666000
C	-3.620674000	2.878805000	-0.770990000
H	-4.216444000	3.711855000	-0.376715000
H	-4.069873000	2.583721000	-1.725222000
C	-2.201267000	3.313644000	-1.093466000
C	5.529086000	0.817219000	-1.162961000
C	4.434122000	-0.291806000	1.406573000
H	4.882066000	0.417421000	2.114728000
H	3.832297000	-0.995530000	1.991603000
C	4.407912000	1.490450000	-0.344219000
H	3.785570000	2.078393000	-1.027403000
H	4.855817000	2.191644000	0.371597000
C	5.558065000	-1.080356000	0.703005000
C	-2.101640000	2.549719000	1.987446000
H	-1.760710000	3.414205000	1.417292000
H	-2.130386000	2.864548000	3.038964000
C	-0.183773000	-2.561479000	0.924412000
H	-0.217553000	-3.488378000	1.509987000
H	0.828028000	-2.154082000	1.011205000
C	-0.588030000	-0.887044000	2.641980000
H	0.488237000	-0.775440000	2.504611000
H	-0.721758000	-1.523839000	3.526276000
C	4.977073000	0.154200000	-2.443485000
H	5.773899000	-0.410638000	-2.935507000
H	4.617994000	0.924793000	-3.133931000
H	4.146445000	-0.528010000	-2.239591000
C	6.572311000	1.879767000	-1.547394000
H	7.029687000	2.315559000	-0.652855000
H	6.085303000	2.680982000	-2.112843000
H	7.360740000	1.443506000	-2.163668000
C	-4.177550000	-1.715376000	-1.580821000
C	6.623267000	-1.465072000	1.743402000
H	6.157373000	-2.049620000	2.543475000
H	7.074149000	-0.570333000	2.185482000
H	7.413830000	-2.062712000	1.285627000
C	-4.886782000	0.924841000	-0.040332000
H	-5.124356000	0.916349000	-1.106277000
H	-5.726893000	1.417512000	0.466867000
C	-4.768939000	-0.503669000	0.478669000
H	-4.549711000	-0.505323000	1.547273000
H	-5.742160000	-0.998974000	0.363878000
C	5.016917000	-2.358446000	0.026668000

H	4.683552000	-3.068814000	0.790637000
H	5.812394000	-2.826086000	-0.560313000
H	4.171235000	-2.157193000	-0.637676000
C	-3.353103000	-2.506647000	0.577523000
H	-2.873697000	-3.217535000	-0.098031000
H	-4.259338000	-3.000686000	0.950928000
C	-3.514051000	2.154723000	1.566477000
H	-3.876477000	1.342528000	2.197576000
H	-4.182890000	3.007271000	1.747855000
C	-2.453457000	-2.205741000	1.773030000
H	-2.975160000	-1.548917000	2.470415000
H	-2.267643000	-3.143461000	2.313443000
C	-1.232034000	0.466781000	2.923164000
H	-2.293431000	0.338138000	3.138412000
H	-0.780652000	0.883784000	3.834056000
O	-0.479101000	0.343126000	-2.721848000
H	-1.111118000	0.403356000	-3.461197000
H	-0.042399000	-0.519775000	-2.849147000
C	-5.353437000	-2.593070000	-1.579637000
C	-6.320594000	-3.317132000	-1.576352000
H	-3.335585000	-2.214425000	-2.071209000
H	-4.388420000	-0.815414000	-2.166896000
H	-7.174398000	-3.959081000	-1.578639000

175°

Y	-1.527352000	0.215362000	-0.491578000
O	0.714760000	0.351996000	0.036149000
O	-0.871292000	-1.917260000	-1.281973000
O	7.327283000	-0.682784000	-0.811069000
O	-1.262223000	2.484684000	-1.016137000
N	6.230131000	-0.220601000	-0.326314000
N	-1.108597000	1.445695000	1.798741000
N	-3.628310000	1.712856000	0.139872000
N	2.491995000	1.193851000	1.174148000
H	2.789356000	1.819500000	1.916411000
N	-1.150679000	-1.553292000	1.428372000
N	-3.712305000	-1.292828000	-0.217370000
N	-1.997764000	4.569571000	-1.473513000
H	-1.070298000	4.864266000	-1.757583000
H	-2.746368000	5.249134000	-1.517199000
N	-0.025317000	-3.998476000	-1.044151000
H	-0.085818000	-4.169412000	-2.041642000
H	0.341242000	-4.736652000	-0.456924000
C	0.261312000	2.006198000	1.727432000
H	0.666930000	2.216634000	2.724804000
H	0.224197000	2.953957000	1.182039000
C	3.547397000	0.487551000	0.431294000
H	3.026960000	-0.187074000	-0.249597000
C	1.192972000	1.108690000	0.927861000
C	-0.397730000	-2.826572000	-0.552438000
C	-3.620285000	2.879975000	-0.773022000

H	-4.219943000	3.711276000	-0.380966000
H	-4.064536000	2.584056000	-1.729303000
C	-2.200291000	3.317739000	-1.088381000
C	5.532029000	0.815187000	-1.161535000
C	4.432317000	-0.294372000	1.405646000
H	4.878994000	0.414687000	2.114768000
H	3.829318000	-0.998138000	1.989409000
C	4.409656000	1.488488000	-0.344543000
H	3.788735000	2.076966000	-1.028553000
H	4.856516000	2.189209000	0.372380000
C	5.557500000	-1.082835000	0.704043000
C	-2.101771000	2.549478000	1.985595000
H	-1.760871000	3.414773000	1.416833000
H	-2.131081000	2.863049000	3.037460000
C	-0.189110000	-2.562261000	0.926079000
H	-0.222830000	-3.487528000	1.514311000
H	0.823661000	-2.156387000	1.008657000
C	-0.587374000	-0.885283000	2.641937000
H	0.488757000	-0.774454000	2.502292000
H	-0.719714000	-1.521581000	3.526840000
C	4.981932000	0.152485000	-2.443031000
H	5.779306000	-0.412857000	-2.933576000
H	4.624580000	0.923260000	-3.134166000
H	4.150498000	-0.529206000	-2.240591000
C	6.576105000	1.877620000	-1.543980000
H	7.032112000	2.313040000	-0.648560000
H	6.090215000	2.679121000	-2.109982000
H	7.365446000	1.441353000	-2.159072000
C	-4.175732000	-1.716934000	-1.580697000
C	6.620744000	-1.467686000	1.746394000
H	6.153349000	-2.052279000	2.545559000
H	7.070854000	-0.573006000	2.189386000
H	7.412110000	-2.065329000	1.290024000
C	-4.887726000	0.926999000	-0.044421000
H	-5.123622000	0.918320000	-1.110767000
H	-5.728070000	1.420856000	0.461288000
C	-4.772247000	-0.501304000	0.475345000
H	-4.555894000	-0.502390000	1.544546000
H	-5.745429000	-0.996138000	0.358214000
C	5.017459000	-2.360794000	0.026575000
H	4.682543000	-3.071183000	0.789840000
H	5.813964000	-2.828501000	-0.558947000
H	4.173052000	-2.159300000	-0.639317000
C	-3.356840000	-2.503282000	0.581474000
H	-2.878691000	-3.217194000	-0.091647000
H	-4.263919000	-2.994605000	0.956419000
C	-3.514155000	2.154450000	1.563949000
H	-3.876472000	1.341837000	2.194566000
H	-4.183000000	3.006889000	1.746003000
C	-2.456791000	-2.200103000	1.776136000
H	-2.977602000	-1.540538000	2.471555000
H	-2.272564000	-3.136567000	2.319335000

C	-1.230022000	0.468976000	2.922921000
H	-2.291078000	0.341207000	3.140380000
H	-0.776696000	0.887277000	3.832230000
O	-0.463721000	0.355493000	-2.723074000
H	-1.094594000	0.261624000	-3.460210000
H	0.112149000	-0.426975000	-2.804686000
C	-5.351358000	-2.595023000	-1.580693000
C	-6.318286000	-3.319408000	-1.578563000
H	-3.332205000	-2.216593000	-2.067713000
H	-4.385712000	-0.818205000	-2.169067000
H	-7.171857000	-3.961656000	-1.581860000

-55°

symmetry c1

Y	-1.533127000	0.210315000	-0.477872000
O	0.719198000	0.387524000	0.017802000
O	-0.909216000	-1.896862000	-1.310028000
O	7.326485000	-0.707597000	-0.805325000
O	-1.255771000	2.467391000	-1.044464000
N	6.231599000	-0.238033000	-0.322562000
N	-1.095408000	1.446272000	1.803862000
N	-3.618251000	1.710403000	0.155203000
N	2.500018000	1.200902000	1.171701000
H	2.799303000	1.815090000	1.922653000
N	-1.134079000	-1.554014000	1.409786000
N	-3.711931000	-1.302455000	-0.208005000
N	-1.989298000	4.554393000	-1.492926000
H	-1.065783000	4.842672000	-1.796129000
H	-2.734265000	5.238757000	-1.524254000
N	-0.026098000	-3.966373000	-1.107650000
H	-0.101730000	-4.128729000	-2.105595000
H	0.361355000	-4.704748000	-0.534102000
C	0.270879000	2.015544000	1.730959000
H	0.679118000	2.221666000	2.728083000
H	0.226727000	2.966752000	1.192115000
C	3.551995000	0.489833000	0.428626000
H	3.028247000	-0.178369000	-0.256119000
C	1.200862000	1.127141000	0.920880000
C	-0.407528000	-2.805472000	-0.597927000
C	-3.609588000	2.879646000	-0.755562000
H	-4.193135000	3.716982000	-0.352282000
H	-4.072717000	2.591248000	-1.705246000
C	-2.191900000	3.306218000	-1.099025000
C	5.544083000	0.805422000	-1.157053000
C	4.427767000	-0.302328000	1.403219000
H	4.877733000	0.401019000	2.115941000
H	3.817227000	-1.002984000	1.982834000
C	4.424927000	1.485876000	-0.341456000
H	3.811243000	2.081665000	-1.025691000
H	4.875489000	2.180768000	0.378813000
C	5.549109000	-1.097706000	0.703314000

C	-2.092062000	2.545159000	1.999141000
H	-1.756366000	3.412563000	1.429737000
H	-2.117840000	2.857219000	3.051558000
C	-0.176390000	-2.553902000	0.880860000
H	-0.197373000	-3.485847000	1.458808000
H	0.835941000	-2.144878000	0.952954000
C	-0.557876000	-0.891621000	2.621392000
H	0.516008000	-0.775460000	2.469583000
H	-0.676772000	-1.534914000	3.503040000
C	4.992486000	0.150002000	-2.441624000
H	5.786768000	-0.420842000	-2.930815000
H	4.643692000	0.925114000	-3.132294000
H	4.154918000	-0.525419000	-2.243300000
C	6.597814000	1.860224000	-1.533986000
H	7.054898000	2.289618000	-0.636211000
H	6.120059000	2.667100000	-2.099267000
H	7.385291000	1.419049000	-2.147974000
C	-4.186311000	-1.731415000	-1.565557000
C	6.605905000	-1.493479000	1.748156000
H	6.131378000	-2.076593000	2.544202000
H	7.061469000	-0.603513000	2.195016000
H	7.394091000	-2.096093000	1.292806000
C	-4.877783000	0.923132000	-0.030338000
H	-5.111800000	0.913759000	-1.097028000
H	-5.718390000	1.417718000	0.474106000
C	-4.764450000	-0.505644000	0.490378000
H	-4.541770000	-0.507253000	1.558323000
H	-5.740594000	-0.996000000	0.379346000
C	5.001320000	-2.369893000	0.021177000
H	4.658431000	-3.079240000	0.781860000
H	5.795924000	-2.842627000	-0.562879000
H	4.160656000	-2.160274000	-0.646871000
C	-3.349609000	-2.511289000	0.590364000
H	-2.882239000	-3.228353000	-0.087013000
H	-4.252696000	-2.999611000	0.978717000
C	-3.504188000	2.148128000	1.580587000
H	-3.863606000	1.332979000	2.209621000
H	-4.174623000	2.998649000	1.765549000
C	-2.432962000	-2.209274000	1.772871000
H	-2.946571000	-1.554905000	2.478605000
H	-2.236010000	-3.147082000	2.309084000
C	-1.203925000	0.458518000	2.920562000
H	-2.262643000	0.324780000	3.145944000
H	-0.744122000	0.869564000	3.829888000
O	-0.686414000	0.382230000	-2.723343000
H	-0.124917000	1.146826000	-2.938776000
H	-0.225070000	-0.413236000	-3.043064000
C	-5.366658000	-2.603401000	-1.552624000
C	-6.338016000	-3.321779000	-1.540794000
H	-3.349359000	-2.237911000	-2.056304000
H	-4.395885000	-0.834835000	-2.157443000
H	-7.195242000	-3.959115000	-1.535737000

-45°

symmetry c1

Y	-1.533509000	0.211234000	-0.476935000
O	0.718655000	0.398047000	0.011064000
O	-0.913559000	-1.902157000	-1.306067000
O	7.324330000	-0.711394000	-0.803350000
O	-1.252648000	2.466547000	-1.041441000
N	6.229769000	-0.240084000	-0.321558000
N	-1.095691000	1.450093000	1.802474000
N	-3.617809000	1.711725000	0.151477000
N	2.499264000	1.204545000	1.169947000
H	2.798705000	1.815706000	1.923311000
N	-1.133388000	-1.550364000	1.411431000
N	-3.711976000	-1.301192000	-0.207077000
N	-1.985850000	4.550498000	-1.504309000
H	-1.061712000	4.837463000	-1.806750000
H	-2.731078000	5.234242000	-1.541430000
N	-0.026744000	-3.969872000	-1.099737000
H	-0.104223000	-4.135355000	-2.097044000
H	0.363123000	-4.705947000	-0.524845000
C	0.270477000	2.019962000	1.729752000
H	0.679032000	2.224595000	2.727022000
H	0.225710000	2.972044000	1.192548000
C	3.550849000	0.492214000	0.427387000
H	3.026694000	-0.175240000	-0.257790000
C	1.200347000	1.133600000	0.917606000
C	-0.408872000	-2.808298000	-0.592615000
C	-3.607426000	2.879418000	-0.761366000
H	-4.190517000	3.717975000	-0.359917000
H	-4.070099000	2.589816000	-1.710875000
C	-2.188811000	3.304298000	-1.103801000
C	5.544374000	0.804144000	-1.156856000
C	4.424583000	-0.301124000	1.402872000
H	4.875027000	0.401705000	2.115804000
H	3.812441000	-1.000706000	1.982086000
C	4.425925000	1.486789000	-0.342085000
H	3.813772000	2.083565000	-1.026821000
H	4.877241000	2.180951000	0.378408000
C	5.545312000	-1.098384000	0.704140000
C	-2.092980000	2.548807000	1.995990000
H	-1.756977000	3.415945000	1.426461000
H	-2.119911000	2.861376000	3.048223000
C	-0.175602000	-2.551368000	0.884797000
H	-0.194981000	-3.481233000	1.466127000
H	0.836537000	-2.141251000	0.953997000
C	-0.557292000	-0.886309000	2.622313000
H	0.516466000	-0.769315000	2.469763000
H	-0.675191000	-1.528992000	3.504510000
C	4.992389000	0.148975000	-2.441373000
H	5.786019000	-0.423421000	-2.929808000

H	4.645229000	0.924275000	-3.132651000
H	4.153624000	-0.525007000	-2.243172000
C	6.600040000	1.857028000	-1.533711000
H	7.057355000	2.286070000	-0.635886000
H	6.123934000	2.664428000	-2.099628000
H	7.387116000	1.414243000	-2.147057000
C	-4.185565000	-1.732401000	-1.564263000
C	6.600732000	-1.495236000	1.749973000
H	6.124757000	-2.077348000	2.545887000
H	7.057231000	-0.605746000	2.196820000
H	7.388390000	-2.099181000	1.295475000
C	-4.877561000	0.924704000	-0.033697000
H	-5.110913000	0.913775000	-1.100520000
H	-5.718275000	1.420428000	0.469432000
C	-4.764978000	-0.503313000	0.489334000
H	-4.543089000	-0.503368000	1.557470000
H	-5.741118000	-0.993663000	0.378299000
C	4.996151000	-2.370088000	0.022204000
H	4.651652000	-3.078540000	0.782995000
H	5.790466000	-2.844305000	-0.561036000
H	4.156281000	-2.159535000	-0.646544000
C	-3.349863000	-2.508624000	0.593614000
H	-2.883320000	-3.227369000	-0.082470000
H	-4.253014000	-2.995623000	0.983477000
C	-3.504639000	2.151223000	1.576417000
H	-3.864734000	1.336860000	2.206100000
H	-4.175184000	3.002014000	1.759758000
C	-2.432639000	-2.204962000	1.775353000
H	-2.945975000	-1.549543000	2.480292000
H	-2.235682000	-3.142039000	2.312803000
C	-1.204445000	0.463561000	2.920143000
H	-2.263240000	0.329383000	3.144873000
H	-0.745537000	0.875736000	3.829380000
O	-0.675976000	0.365688000	-2.727053000
H	-0.000179000	1.043589000	-2.901549000
H	-0.302569000	-0.483018000	-3.026268000
C	-5.366311000	-2.603792000	-1.550537000
C	-6.338091000	-3.321588000	-1.538054000
H	-3.348494000	-2.240098000	-2.053509000
H	-4.394379000	-0.836727000	-2.157810000
H	-7.195675000	-3.958438000	-1.532439000

-35°

symmetry c1

Y	-1.533751000	0.211198000	-0.481586000
O	0.716545000	0.399900000	0.020591000
O	-0.904201000	-1.908745000	-1.302939000
O	7.310567000	-0.715488000	-0.808294000
O	-1.249682000	2.470449000	-1.034235000
N	6.219094000	-0.240456000	-0.323149000
N	-1.103913000	1.454287000	1.800273000

N	-3.620903000	1.710819000	0.139195000
N	2.494529000	1.212232000	1.177657000
H	2.794177000	1.826041000	1.928741000
N	-1.138829000	-1.546865000	1.413222000
N	-3.711446000	-1.301324000	-0.213692000
N	-1.986599000	4.548634000	-1.516727000
H	-1.061222000	4.836881000	-1.813977000
H	-2.734038000	5.229247000	-1.564336000
N	-0.023740000	-3.977895000	-1.082375000
H	-0.097335000	-4.148441000	-2.079112000
H	0.361690000	-4.711978000	-0.502013000
C	0.262225000	2.025304000	1.733074000
H	0.666460000	2.231146000	2.731864000
H	0.218860000	2.976716000	1.194597000
C	3.544832000	0.497309000	0.435496000
H	3.018845000	-0.174345000	-0.244105000
C	1.195628000	1.138796000	0.925543000
C	-0.405435000	-2.812905000	-0.582818000
C	-3.608151000	2.876484000	-0.776052000
H	-4.195434000	3.714600000	-0.379706000
H	-4.064784000	2.583759000	-1.727499000
C	-2.188112000	3.303951000	-1.109952000
C	5.529957000	0.799565000	-1.160619000
C	4.422955000	-0.290529000	1.411355000
H	4.877449000	0.416025000	2.118006000
H	3.813530000	-0.986620000	1.997585000
C	4.416379000	1.487564000	-0.343460000
H	3.801080000	2.081114000	-1.028185000
H	4.871938000	2.185109000	0.371014000
C	5.539537000	-1.092431000	0.711102000
C	-2.102715000	2.552486000	1.988252000
H	-1.765076000	3.419244000	1.419277000
H	-2.134284000	2.866102000	3.040057000
C	-0.177832000	-2.548762000	0.894101000
H	-0.197458000	-3.475714000	1.480081000
H	0.833322000	-2.136373000	0.964337000
C	-0.567976000	-0.880233000	2.625351000
H	0.506262000	-0.762671000	2.476865000
H	-0.689023000	-1.521738000	3.507959000
C	4.970666000	0.137637000	-2.438579000
H	5.761519000	-0.437240000	-2.928601000
H	4.619493000	0.909317000	-3.131857000
H	4.133279000	-0.535512000	-2.232184000
C	6.584309000	1.849334000	-1.549465000
H	7.046919000	2.283383000	-0.656806000
H	6.105738000	2.653649000	-2.117701000
H	7.367619000	1.402181000	-2.164485000
C	-4.180786000	-1.734440000	-1.571805000
C	6.600283000	-1.484116000	1.753460000
H	6.128182000	-2.061479000	2.555115000
H	7.059720000	-0.592449000	2.192887000
H	7.385134000	-2.091090000	1.298132000

C	-4.879893000	0.923255000	-0.047793000
H	-5.110681000	0.910293000	-1.115150000
H	-5.722057000	1.419545000	0.452344000
C	-4.767695000	-0.503657000	0.478198000
H	-4.549263000	-0.501607000	1.547045000
H	-5.742811000	-0.995439000	0.364898000
C	4.986068000	-2.367662000	0.039284000
H	4.645005000	-3.071510000	0.805891000
H	5.777114000	-2.845681000	-0.545296000
H	4.142943000	-2.160482000	-0.626433000
C	-3.351623000	-2.507642000	0.589682000
H	-2.882159000	-3.226990000	-0.083715000
H	-4.255918000	-2.994552000	0.976956000
C	-3.512317000	2.153026000	1.563766000
H	-3.874096000	1.339531000	2.193544000
H	-4.184143000	3.003666000	1.743150000
C	-2.438879000	-2.201350000	1.774005000
H	-2.954927000	-1.544708000	2.475771000
H	-2.243349000	-3.137182000	2.314122000
C	-1.217049000	0.469569000	2.918634000
H	-2.276667000	0.335345000	3.139402000
H	-0.762004000	0.883020000	3.829248000
O	-0.541564000	0.357707000	-2.696682000
H	0.241235000	0.931213000	-2.770869000
H	-0.250138000	-0.531270000	-2.970561000
C	-5.361638000	-2.605726000	-1.559768000
C	-6.333434000	-3.323496000	-1.547108000
H	-3.342292000	-2.243373000	-2.057381000
H	-4.387468000	-0.839703000	-2.167493000
H	-7.191069000	-3.960284000	-1.541233000

-25°

symmetry c1

Y	-1.533693000	0.211000000	-0.484399000
O	0.716389000	0.408808000	0.015665000
O	-0.909798000	-1.917100000	-1.297784000
O	7.307265000	-0.717885000	-0.807532000
O	-1.249508000	2.471222000	-1.036516000
N	6.216458000	-0.241845000	-0.321894000
N	-1.105548000	1.457223000	1.798035000
N	-3.621839000	1.712570000	0.134607000
N	2.493093000	1.213649000	1.179566000
H	2.792521000	1.824582000	1.933109000
N	-1.140832000	-1.544052000	1.414708000
N	-3.712958000	-1.299196000	-0.214631000
N	-1.985773000	4.548849000	-1.522354000
H	-1.060078000	4.836727000	-1.818893000
H	-2.733080000	5.229486000	-1.571200000
N	-0.028756000	-3.985532000	-1.071483000
H	-0.104062000	-4.159812000	-2.067446000
H	0.358162000	-4.717240000	-0.489143000

C	0.260493000	2.028815000	1.732251000
H	0.663838000	2.234282000	2.731442000
H	0.217199000	2.980440000	1.194135000
C	3.543295000	0.498736000	0.437028000
H	3.017055000	-0.171397000	-0.243876000
C	1.194762000	1.143681000	0.924626000
C	-0.409617000	-2.818715000	-0.575628000
C	-3.608134000	2.877863000	-0.781044000
H	-4.195040000	3.716438000	-0.385057000
H	-4.064707000	2.585144000	-1.732500000
C	-2.187629000	3.304467000	-1.114207000
C	5.529107000	0.800464000	-1.157989000
C	4.419847000	-0.291663000	1.412191000
H	4.875224000	0.413196000	2.119943000
H	3.809193000	-0.987697000	1.997200000
C	4.416486000	1.489051000	-0.340001000
H	3.802322000	2.084642000	-1.023955000
H	4.872974000	2.184736000	0.375684000
C	5.535402000	-1.094266000	0.711015000
C	-2.104777000	2.555417000	1.983983000
H	-1.766928000	3.421617000	1.414346000
H	-2.137107000	2.870052000	3.035459000
C	-0.180083000	-2.548294000	0.899647000
H	-0.199340000	-3.472532000	1.489941000
H	0.831166000	-2.135597000	0.967296000
C	-0.570535000	-0.875948000	2.626255000
H	0.503771000	-0.758400000	2.477835000
H	-0.691698000	-1.516534000	3.509512000
C	4.968962000	0.141249000	-2.436973000
H	5.758999000	-0.434127000	-2.927721000
H	4.619044000	0.914468000	-3.129176000
H	4.130540000	-0.530955000	-2.231660000
C	6.585164000	1.849132000	-1.545164000
H	7.048332000	2.281155000	-0.651814000
H	6.107935000	2.655012000	-2.112304000
H	7.367851000	1.401625000	-2.160721000
C	-4.180802000	-1.733942000	-1.572940000
C	6.595340000	-1.489034000	1.753021000
H	6.122234000	-2.066879000	2.553736000
H	7.056044000	-0.598705000	2.193816000
H	7.379339000	-2.096527000	1.296919000
C	-4.881109000	0.925662000	-0.052726000
H	-5.110877000	0.911683000	-1.120293000
H	-5.723467000	1.422954000	0.446106000
C	-4.770120000	-0.500681000	0.474878000
H	-4.553286000	-0.497566000	1.544048000
H	-5.745138000	-0.992397000	0.360621000
C	4.980204000	-2.367768000	0.037318000
H	4.637765000	-3.072080000	0.802878000
H	5.770732000	-2.846245000	-0.547583000
H	4.137690000	-2.158450000	-0.628486000
C	-3.354544000	-2.504389000	0.591088000

H	-2.885649000	-3.225543000	-0.080659000
H	-4.259464000	-2.989553000	0.979086000
C	-3.513908000	2.155179000	1.559001000
H	-3.875749000	1.341887000	2.188976000
H	-4.186050000	3.005716000	1.737815000
C	-2.442079000	-2.196566000	1.775343000
H	-2.958043000	-1.538202000	2.475517000
H	-2.247815000	-3.131542000	2.317371000
C	-1.219798000	0.474050000	2.917534000
H	-2.279577000	0.340196000	3.137661000
H	-0.765480000	0.888539000	3.828018000
O	-0.482369000	0.345216000	-2.690494000
H	0.378785000	0.798935000	-2.680569000
H	-0.288498000	-0.567796000	-2.973298000
C	-5.362208000	-2.604398000	-1.561376000
C	-6.334629000	-3.321326000	-1.549263000
H	-3.341869000	-2.244006000	-2.056531000
H	-4.386162000	-0.839772000	-2.169960000
H	-7.192819000	-3.957367000	-1.543862000

-15°

symmetry c1

Y	-1.531340000	0.210675000	-0.489794000
O	0.718682000	0.406177000	0.016484000
O	-0.933867000	-1.934678000	-1.287254000
O	7.310641000	-0.712950000	-0.810500000
O	-1.249490000	2.466656000	-1.054539000
N	6.219436000	-0.241232000	-0.321562000
N	-1.104776000	1.457628000	1.795851000
N	-3.620926000	1.722687000	0.129861000
N	2.494726000	1.202599000	1.187435000
H	2.793840000	1.810897000	1.943304000
N	-1.153366000	-1.544127000	1.418860000
N	-3.720731000	-1.287994000	-0.216254000
N	-1.973630000	4.551963000	-1.525418000
H	-1.047371000	4.835359000	-1.824474000
H	-2.716588000	5.237836000	-1.566878000
N	-0.053904000	-4.003041000	-1.055165000
H	-0.133520000	-4.181998000	-2.049956000
H	0.335171000	-4.732088000	-0.470993000
C	0.263357000	2.024260000	1.734572000
H	0.664378000	2.228009000	2.735038000
H	0.225233000	2.976452000	1.196889000
C	3.545653000	0.493111000	0.440612000
H	3.020077000	-0.169737000	-0.247924000
C	1.197089000	1.137215000	0.928965000
C	-0.431450000	-2.833313000	-0.563441000
C	-3.603611000	2.888209000	-0.784937000
H	-4.184359000	3.729918000	-0.386442000
H	-4.064995000	2.598857000	-1.735089000
C	-2.182002000	3.306723000	-1.122835000

C	5.534676000	0.810817000	-1.147441000
C	4.419726000	-0.308302000	1.408953000
H	4.874604000	0.388488000	2.124905000
H	3.807446000	-1.010047000	1.985409000
C	4.420929000	1.491095000	-0.324284000
H	3.808331000	2.094284000	-1.002928000
H	4.876438000	2.178986000	0.399564000
C	5.535739000	-1.104302000	0.700787000
C	-2.100327000	2.559866000	1.978069000
H	-1.759259000	3.422984000	1.405597000
H	-2.131502000	2.877772000	3.028603000
C	-0.196763000	-2.554869000	0.909241000
H	-0.218321000	-3.475355000	1.505426000
H	0.816032000	-2.145100000	0.972447000
C	-0.582248000	-0.876502000	2.629810000
H	0.492922000	-0.764166000	2.482996000
H	-0.707840000	-1.514649000	3.514256000
C	4.976407000	0.166523000	-2.434760000
H	5.766751000	-0.404286000	-2.930315000
H	4.628727000	0.947845000	-3.118994000
H	4.136689000	-0.506853000	-2.238494000
C	6.592217000	1.863157000	-1.520540000
H	7.053850000	2.284620000	-0.621346000
H	6.116568000	2.675830000	-2.079247000
H	7.375853000	1.422303000	-2.139659000
C	-4.185082000	-1.719485000	-1.576793000
C	6.593661000	-1.511670000	1.739943000
H	6.118836000	-2.097931000	2.533488000
H	7.054648000	-0.626781000	2.191225000
H	7.377653000	-2.114867000	1.278158000
C	-4.882809000	0.940409000	-0.057437000
H	-5.112573000	0.927088000	-1.125016000
H	-5.723602000	1.440551000	0.441278000
C	-4.776795000	-0.485957000	0.470369000
H	-4.562204000	-0.483208000	1.539985000
H	-5.753076000	-0.974841000	0.354303000
C	4.980691000	-2.369813000	0.012039000
H	4.635790000	-3.082084000	0.769041000
H	5.772044000	-2.842728000	-0.576263000
H	4.140028000	-2.152403000	-0.653445000
C	-3.370806000	-2.494177000	0.591215000
H	-2.905016000	-3.219173000	-0.078315000
H	-4.279279000	-2.973356000	0.978421000
C	-3.510826000	2.163730000	1.554130000
H	-3.874578000	1.351333000	2.184113000
H	-4.180147000	3.016286000	1.734214000
C	-2.459190000	-2.188843000	1.776926000
H	-2.973451000	-1.526544000	2.474578000
H	-2.271212000	-3.123835000	2.321173000
C	-1.226104000	0.476811000	2.916746000
H	-2.286977000	0.347705000	3.134077000
H	-0.772641000	0.891179000	3.827689000

O	-0.395090000	0.303403000	-2.663548000
H	0.522851000	0.614187000	-2.566204000
H	-0.314917000	-0.617485000	-2.974888000
C	-5.370793000	-2.584071000	-1.571762000
C	-6.347166000	-3.295691000	-1.566443000
H	-3.346354000	-2.232716000	-2.057294000
H	-4.383789000	-0.823599000	-2.173631000
H	-7.208777000	-3.927099000	-1.567020000

-5°

symmetry c1

Y	-1.531678000	0.210177000	-0.492801000
O	0.719319000	0.408860000	0.006683000
O	-0.947026000	-1.940820000	-1.283633000
O	7.316292000	-0.712352000	-0.804989000
O	-1.251694000	2.468774000	-1.050822000
N	6.223526000	-0.241276000	-0.318949000
N	-1.102983000	1.457698000	1.792795000
N	-3.622500000	1.725094000	0.130055000
N	2.495201000	1.200925000	1.181601000
H	2.793454000	1.807510000	1.939226000
N	-1.154723000	-1.543104000	1.419522000
N	-3.724355000	-1.284489000	-0.214178000
N	-1.974082000	4.554446000	-1.523209000
H	-1.047444000	4.837293000	-1.821532000
H	-2.716826000	5.240448000	-1.565926000
N	-0.066717000	-4.009221000	-1.051898000
H	-0.150621000	-4.190139000	-2.045949000
H	0.324413000	-4.737230000	-0.467857000
C	0.264968000	2.024457000	1.728050000
H	0.667857000	2.229350000	2.727496000
H	0.225525000	2.975939000	1.189251000
C	3.547433000	0.491384000	0.436680000
H	3.023497000	-0.172381000	-0.252267000
C	1.198046000	1.137503000	0.921486000
C	-0.441898000	-2.838151000	-0.560877000
C	-3.605271000	2.891337000	-0.783559000
H	-4.185745000	3.732902000	-0.384241000
H	-4.066878000	2.602930000	-1.733893000
C	-2.183385000	3.309224000	-1.120554000
C	5.539736000	0.809617000	-1.147133000
C	4.420093000	-0.308541000	1.407536000
H	4.872845000	0.389335000	2.123788000
H	3.807151000	-1.010234000	1.983345000
C	4.423556000	1.489521000	-0.327050000
H	3.811982000	2.091739000	-1.007471000
H	4.876843000	2.178273000	0.397367000
C	5.538284000	-1.104160000	0.702502000
C	-2.098301000	2.560097000	1.976402000
H	-1.757882000	3.423451000	1.404029000
H	-2.128005000	2.877452000	3.027135000

C	-0.201765000	-2.557391000	0.910461000
H	-0.224749000	-3.476583000	1.508658000
H	0.812364000	-2.150497000	0.970868000
C	-0.580240000	-0.875377000	2.628524000
H	0.494713000	-0.764112000	2.478879000
H	-0.704174000	-1.512699000	3.513833000
C	4.984880000	0.163923000	-2.435200000
H	5.776663000	-0.407031000	-2.928284000
H	4.638526000	0.944435000	-3.121018000
H	4.144946000	-0.509603000	-2.240280000
C	6.597221000	1.862650000	-1.518445000
H	7.056381000	2.285055000	-0.618423000
H	6.122192000	2.674585000	-2.078748000
H	7.382688000	1.422089000	-2.135441000
C	-4.187443000	-1.716995000	-1.574846000
C	6.594125000	-1.509860000	1.744451000
H	6.117953000	-2.095926000	2.537333000
H	7.053295000	-0.624235000	2.196159000
H	7.379711000	-2.112729000	1.284965000
C	-4.885324000	0.944569000	-0.056654000
H	-5.115435000	0.931598000	-1.124191000
H	-5.725437000	1.445616000	0.442380000
C	-4.780739000	-0.481868000	0.470978000
H	-4.567199000	-0.479115000	1.540811000
H	-5.757168000	-0.970235000	0.353929000
C	4.985644000	-2.370560000	0.013483000
H	4.639702000	-3.082589000	0.770239000
H	5.778575000	-2.843259000	-0.572854000
H	4.146172000	-2.154175000	-0.653850000
C	-3.375610000	-2.489681000	0.595297000
H	-2.912131000	-3.217137000	-0.073042000
H	-4.284518000	-2.966211000	0.984758000
C	-3.509599000	2.164437000	1.554402000
H	-3.872357000	1.351554000	2.184323000
H	-4.178322000	3.017034000	1.736788000
C	-2.462148000	-2.183466000	1.779562000
H	-2.974435000	-1.518426000	2.476024000
H	-2.276198000	-3.117672000	2.325900000
C	-1.222123000	0.478711000	2.915493000
H	-2.282544000	0.350828000	3.135728000
H	-0.766013000	0.894042000	3.824660000
O	-0.372522000	0.301846000	-2.658505000
H	0.576929000	0.460910000	-2.507214000
H	-0.410350000	-0.593206000	-3.043712000
C	-5.372816000	-2.582045000	-1.570342000
C	-6.348795000	-3.294216000	-1.565552000
H	-3.348022000	-2.230045000	-2.054253000
H	-4.386127000	-0.821391000	-2.172164000
H	-7.210056000	-3.926097000	-1.566634000

5°

symmetry c1

Y	-1.531219000	0.209570000	-0.497503000
O	0.719617000	0.404474000	0.000653000
O	-0.955109000	-1.943879000	-1.281435000
O	7.322698000	-0.709912000	-0.799856000
O	-1.256113000	2.473954000	-1.042599000
N	6.228250000	-0.239873000	-0.316625000
N	-1.101800000	1.455235000	1.791024000
N	-3.625198000	1.725458000	0.132553000
N	2.495298000	1.198622000	1.175144000
H	2.792507000	1.806022000	1.932545000
N	-1.155560000	-1.543405000	1.420040000
N	-3.726816000	-1.282533000	-0.212862000
N	-1.979414000	4.559829000	-1.513231000
H	-1.052717000	4.843872000	-1.810139000
H	-2.723019000	5.244795000	-1.557017000
N	-0.077893000	-4.013740000	-1.050735000
H	-0.164836000	-4.195341000	-2.044349000
H	0.313253000	-4.741917000	-0.466985000
C	0.265794000	2.022115000	1.721463000
H	0.671109000	2.229425000	2.719442000
H	0.224633000	2.972257000	1.180475000
C	3.549304000	0.489307000	0.432598000
H	3.027454000	-0.176450000	-0.256000000
C	1.198314000	1.134282000	0.914892000
C	-0.449803000	-2.841134000	-0.559760000
C	-3.609753000	2.893565000	-0.778454000
H	-4.191708000	3.733444000	-0.377636000
H	-4.070434000	2.606359000	-1.729609000
C	-2.188088000	3.313506000	-1.112871000
C	5.544041000	0.808186000	-1.148055000
C	4.421631000	-0.307371000	1.406447000
H	4.871654000	0.392744000	2.122246000
H	3.808897000	-1.009082000	1.982459000
C	4.425079000	1.487569000	-0.331373000
H	3.813697000	2.087480000	-1.014003000
H	4.875766000	2.178401000	0.392678000
C	5.542716000	-1.102127000	0.705137000
C	-2.097005000	2.557424000	1.977048000
H	-1.757756000	3.421550000	1.405297000
H	-2.125002000	2.873540000	3.028202000
C	-0.205739000	-2.560408000	0.910864000
H	-0.230594000	-3.479159000	1.509747000
H	0.809539000	-2.156255000	0.969890000
C	-0.578041000	-0.876745000	2.627738000
H	0.496738000	-0.766605000	2.475777000
H	-0.700717000	-1.513861000	3.513421000
C	4.992784000	0.158968000	-2.435878000
H	5.786414000	-0.411845000	-2.926152000
H	4.646638000	0.937479000	-3.124058000
H	4.153445000	-0.515377000	-2.241176000
C	6.600319000	1.862452000	-1.519306000

H	7.056984000	2.287337000	-0.619177000
H	6.124894000	2.672499000	-2.081994000
H	7.387769000	1.422186000	-2.133976000
C	-4.188585000	-1.715412000	-1.573906000
C	6.597290000	-1.503619000	1.750001000
H	6.120694000	-2.089056000	2.543091000
H	7.053738000	-0.616162000	2.200891000
H	7.385037000	-2.105798000	1.293326000
C	-4.888394000	0.946024000	-0.054008000
H	-5.119112000	0.934258000	-1.121469000
H	-5.728130000	1.446788000	0.446049000
C	-4.783985000	-0.480875000	0.471896000
H	-4.571276000	-0.478943000	1.541890000
H	-5.760172000	-0.969450000	0.353654000
C	4.993872000	-2.370924000	0.017501000
H	4.647882000	-3.082200000	0.774945000
H	5.788843000	-2.843192000	-0.566416000
H	4.155221000	-2.157420000	-0.651807000
C	-3.378430000	-2.487226000	0.597569000
H	-2.916061000	-3.215972000	-0.070047000
H	-4.287547000	-2.962452000	0.988145000
C	-3.509176000	2.161981000	1.557254000
H	-3.870276000	1.347941000	2.186626000
H	-4.177629000	3.014148000	1.742930000
C	-2.464187000	-2.180316000	1.781141000
H	-2.975303000	-1.513289000	2.476537000
H	-2.280067000	-3.113975000	2.329122000
C	-1.217761000	0.477961000	2.915435000
H	-2.277564000	0.351085000	3.139264000
H	-0.758435000	0.894281000	3.822530000
O	-0.357072000	0.317391000	-2.656848000
H	0.602113000	0.314584000	-2.484186000
H	-0.515905000	-0.504908000	-3.155076000
C	-5.372806000	-2.582047000	-1.570461000
C	-6.347614000	-3.295834000	-1.566532000
H	-3.348044000	-2.227221000	-2.052657000
H	-4.388120000	-0.819862000	-2.171068000
H	-7.207853000	-3.929100000	-1.568349000

15°

symmetry c1

Y	-1.529252000	0.209582000	-0.502997000
O	0.719971000	0.392931000	0.000838000
O	-0.960786000	-1.946248000	-1.280560000
O	7.329058000	-0.704948000	-0.797158000
O	-1.260244000	2.480281000	-1.033287000
N	6.232810000	-0.237302000	-0.315690000
N	-1.101055000	1.450633000	1.790600000
N	-3.627490000	1.726580000	0.135212000
N	2.495530000	1.193682000	1.171524000
H	2.791881000	1.803925000	1.926979000

N	-1.159202000	-1.546452000	1.420371000
N	-3.729594000	-1.279786000	-0.213494000
N	-1.983521000	4.567260000	-1.499664000
H	-1.056439000	4.852798000	-1.793837000
H	-2.727445000	5.251920000	-1.542369000
N	-0.092420000	-4.019933000	-1.050932000
H	-0.179790000	-4.200635000	-2.044631000
H	0.296579000	-4.749495000	-0.467520000
C	0.266478000	2.016730000	1.717280000
H	0.673487000	2.226829000	2.714026000
H	0.224724000	2.965187000	1.173410000
C	3.551174000	0.485479000	0.430396000
H	3.031160000	-0.182773000	-0.257170000
C	1.198513000	1.126550000	0.912289000
C	-0.459232000	-2.845494000	-0.559541000
C	-3.613629000	2.897579000	-0.771772000
H	-4.196852000	3.735438000	-0.368465000
H	-4.073466000	2.612922000	-1.724097000
C	-2.192084000	3.319521000	-1.102976000
C	5.546148000	0.807247000	-1.149533000
C	4.425231000	-0.306905000	1.406173000
H	4.872726000	0.395966000	2.120876000
H	3.814212000	-1.009228000	1.983263000
C	4.424586000	1.484785000	-0.334956000
H	3.811860000	2.081615000	-1.019089000
H	4.872709000	2.178277000	0.388144000
C	5.549066000	-1.099672000	0.707145000
C	-2.095657000	2.552933000	1.979370000
H	-1.756844000	3.418124000	1.409105000
H	-2.122403000	2.867009000	3.031169000
C	-0.213690000	-2.567099000	0.911248000
H	-0.243022000	-3.486245000	1.509417000
H	0.803381000	-2.167675000	0.971085000
C	-0.578568000	-0.881631000	2.627030000
H	0.496176000	-0.773543000	2.473313000
H	-0.700954000	-1.518563000	3.512975000
C	4.997674000	0.154116000	-2.436560000
H	5.793125000	-0.415753000	-2.924977000
H	4.650284000	0.930400000	-3.126617000
H	4.159741000	-0.521800000	-2.241225000
C	6.599606000	1.863968000	-1.521865000
H	7.054334000	2.291768000	-0.622133000
H	6.122235000	2.671641000	-2.086318000
H	7.388813000	1.424955000	-2.135168000
C	-4.189442000	-1.711804000	-1.575497000
C	6.604063000	-1.496136000	1.753515000
H	6.128609000	-2.081520000	2.547327000
H	7.057507000	-0.606489000	2.203147000
H	7.393978000	-2.096775000	1.298564000
C	-4.890970000	0.948581000	-0.052717000
H	-5.121254000	0.938661000	-1.120335000
H	-5.730748000	1.448907000	0.447847000

C	-4.787666000	-0.479068000	0.470617000
H	-4.576602000	-0.478725000	1.540928000
H	-5.763729000	-0.967383000	0.350165000
C	5.004318000	-2.371197000	0.021341000
H	4.660080000	-3.082288000	0.779761000
H	5.800970000	-2.842033000	-0.561444000
H	4.165314000	-2.161199000	-0.648663000
C	-3.383400000	-2.484800000	0.597255000
H	-2.921465000	-3.214506000	-0.069570000
H	-4.293521000	-2.958662000	0.987154000
C	-3.508747000	2.158753000	1.560718000
H	-3.868795000	1.343126000	2.188629000
H	-4.176573000	3.010616000	1.750347000
C	-2.469889000	-2.178140000	1.781373000
H	-2.979973000	-1.508325000	2.474807000
H	-2.289462000	-3.111289000	2.331583000
C	-1.214997000	0.474142000	2.915857000
H	-2.274372000	0.348990000	3.142724000
H	-0.752470000	0.890412000	3.821357000
O	-0.331918000	0.339050000	-2.648151000
H	0.612899000	0.171121000	-2.478167000
H	-0.598931000	-0.365748000	-3.265102000
C	-5.372730000	-2.579734000	-1.574363000
C	-6.346497000	-3.294959000	-1.572187000
H	-3.347736000	-2.222193000	-2.053732000
H	-4.389284000	-0.815785000	-2.171875000
H	-7.205829000	-3.929448000	-1.575527000

25°

symmetry c1

Y	-1.526822000	0.210452000	-0.505689000
O	0.719483000	0.380450000	0.006323000
O	-0.954816000	-1.945411000	-1.279623000
O	7.331443000	-0.699871000	-0.797536000
O	-1.264923000	2.485829000	-1.026471000
N	6.234295000	-0.233932000	-0.316458000
N	-1.101997000	1.447591000	1.791278000
N	-3.629506000	1.724463000	0.136948000
N	2.494842000	1.191811000	1.169911000
H	2.790785000	1.806131000	1.922193000
N	-1.159737000	-1.548229000	1.421931000
N	-3.727928000	-1.280921000	-0.214649000
N	-1.990611000	4.573694000	-1.485719000
H	-1.063492000	4.862089000	-1.776943000
H	-2.735698000	5.257169000	-1.526936000
N	-0.092593000	-4.021439000	-1.048663000
H	-0.178231000	-4.201523000	-2.042595000
H	0.292600000	-4.752395000	-0.464516000
C	0.265447000	2.013293000	1.715416000
H	0.673226000	2.226348000	2.711268000
H	0.223352000	2.960035000	1.168605000

C	3.551206000	0.484102000	0.429537000
H	3.031871000	-0.186097000	-0.256639000
C	1.197476000	1.120196000	0.912948000
C	-0.457676000	-2.845999000	-0.557656000
C	-3.618576000	2.897624000	-0.767237000
H	-4.205051000	3.732613000	-0.362715000
H	-4.076186000	2.613741000	-1.720857000
C	-2.197689000	3.323850000	-1.094486000
C	5.545064000	0.807786000	-1.151709000
C	4.427394000	-0.304952000	1.406092000
H	4.873557000	0.399970000	2.119620000
H	3.818158000	-1.007750000	1.984498000
C	4.422173000	1.483970000	-0.337895000
H	3.807801000	2.078258000	-1.022781000
H	4.868946000	2.179695000	0.383903000
C	5.552738000	-1.096257000	0.707903000
C	-2.096943000	2.549348000	1.981337000
H	-1.758928000	3.415424000	1.412032000
H	-2.123434000	2.862255000	3.033491000
C	-0.214535000	-2.569428000	0.913770000
H	-0.246018000	-3.489068000	1.511128000
H	0.802823000	-2.171174000	0.975713000
C	-0.579443000	-0.884206000	2.628896000
H	0.495455000	-0.776986000	2.475902000
H	-0.702947000	-1.521049000	3.514786000
C	4.997720000	0.151529000	-2.437642000
H	5.794283000	-0.417345000	-2.925409000
H	4.648495000	0.926026000	-3.128771000
H	4.161279000	-0.525864000	-2.241082000
C	6.596015000	1.866349000	-1.525883000
H	7.050026000	2.296511000	-0.626912000
H	6.116654000	2.672118000	-2.091377000
H	7.386041000	1.428242000	-2.138775000
C	-4.185602000	-1.712411000	-1.577449000
C	6.608902000	-1.488849000	1.754566000
H	6.134936000	-2.074000000	2.549443000
H	7.060533000	-0.597511000	2.202689000
H	7.400014000	-2.088466000	1.300355000
C	-4.892110000	0.945665000	-0.052307000
H	-5.121720000	0.936788000	-1.120113000
H	-5.732681000	1.444556000	0.448406000
C	-4.787679000	-0.482383000	0.469155000
H	-4.577844000	-0.482963000	1.539693000
H	-5.763018000	-0.971790000	0.347098000
C	5.010510000	-2.369920000	0.024099000
H	4.668199000	-3.080757000	0.783637000
H	5.807949000	-2.839768000	-0.558408000
H	4.170698000	-2.162673000	-0.645773000
C	-3.381909000	-2.486170000	0.595718000
H	-2.918003000	-3.214985000	-0.070729000
H	-4.292299000	-2.961225000	0.983542000
C	-3.510134000	2.154346000	1.563102000

H	-3.868707000	1.337307000	2.190006000
H	-4.178723000	3.005161000	1.754764000
C	-2.470778000	-2.179163000	1.781446000
H	-2.981937000	-1.508970000	2.473708000
H	-2.291667000	-3.112166000	2.332424000
C	-1.214786000	0.471989000	2.917324000
H	-2.273955000	0.347509000	3.145615000
H	-0.751024000	0.888917000	3.821915000
O	-0.330246000	0.356936000	-2.649888000
H	0.581328000	0.033879000	-2.534325000
H	-0.703358000	-0.197416000	-3.358190000
C	-5.367107000	-2.582828000	-1.578485000
C	-6.339164000	-3.300382000	-1.577933000
H	-3.342242000	-2.220644000	-2.055158000
H	-4.386712000	-0.816237000	-2.173160000
H	-7.197013000	-3.936866000	-1.582663000

35°

symmetry c1

Y	-1.524605000	0.211735000	-0.505378000
O	0.718839000	0.369432000	0.015767000
O	-0.932216000	-1.941208000	-1.277527000
O	7.330450000	-0.694417000	-0.801791000
O	-1.266378000	2.488865000	-1.022608000
N	6.233308000	-0.230167000	-0.319039000
N	-1.104365000	1.446199000	1.792713000
N	-3.630290000	1.721333000	0.136638000
N	2.493924000	1.190729000	1.172292000
H	2.789923000	1.808581000	1.921638000
N	-1.159261000	-1.550280000	1.425294000
N	-3.723905000	-1.283449000	-0.216921000
N	-1.994641000	4.578115000	-1.471998000
H	-1.067297000	4.869882000	-1.759198000
H	-2.740988000	5.260325000	-1.511730000
N	-0.080789000	-4.020959000	-1.041706000
H	-0.159839000	-4.199672000	-2.036428000
H	0.297375000	-4.753999000	-0.455597000
C	0.263827000	2.010161000	1.718143000
H	0.670700000	2.223427000	2.714357000
H	0.223441000	2.956570000	1.170619000
C	3.550286000	0.484469000	0.430658000
H	3.030755000	-0.185214000	-0.255847000
C	1.196150000	1.114878000	0.917806000
C	-0.444664000	-2.844433000	-0.552246000
C	-3.621006000	2.893904000	-0.768367000
H	-4.213544000	3.726235000	-0.367372000
H	-4.072568000	2.606907000	-1.723945000
C	-2.200512000	3.325610000	-1.088887000
C	5.542447000	0.812155000	-1.152152000
C	4.428135000	-0.305221000	1.405196000
H	4.874457000	0.398962000	2.119345000

H	3.820050000	-1.009378000	1.983170000
C	4.419575000	1.486068000	-0.336444000
H	3.803890000	2.080484000	-1.020039000
H	4.866290000	2.181455000	0.385737000
C	5.553374000	-1.094611000	0.704636000
C	-2.098990000	2.548309000	1.981830000
H	-1.760282000	3.414533000	1.413234000
H	-2.126589000	2.860983000	3.034036000
C	-0.210666000	-2.569978000	0.920831000
H	-0.244341000	-3.490351000	1.516952000
H	0.805949000	-2.170843000	0.988399000
C	-0.583743000	-0.885081000	2.633797000
H	0.491689000	-0.777893000	2.484921000
H	-0.710674000	-1.521031000	3.519866000
C	4.994643000	0.157361000	-2.438629000
H	5.791335000	-0.409924000	-2.928031000
H	4.643989000	0.932621000	-3.128190000
H	4.159036000	-0.521128000	-2.242367000
C	6.592115000	1.872257000	-1.525622000
H	7.046420000	2.301562000	-0.626389000
H	6.111516000	2.678381000	-2.089560000
H	7.382076000	1.435821000	-2.139792000
C	-4.181039000	-1.713179000	-1.580479000
C	6.610939000	-1.488113000	1.749521000
H	6.138239000	-2.074848000	2.543982000
H	7.062424000	-0.597162000	2.198561000
H	7.401990000	-2.086443000	1.293501000
C	-4.891845000	0.940936000	-0.052302000
H	-5.122453000	0.932710000	-1.119892000
H	-5.732711000	1.438181000	0.449528000
C	-4.784857000	-0.487395000	0.467930000
H	-4.574818000	-0.488466000	1.538416000
H	-5.759339000	-0.978442000	0.345595000
C	5.011469000	-2.367565000	0.019246000
H	4.670444000	-3.079935000	0.777923000
H	5.808714000	-2.835825000	-0.564812000
H	4.170863000	-2.159876000	-0.649496000
C	-3.376600000	-2.489852000	0.591174000
H	-2.907978000	-3.215061000	-0.076038000
H	-4.286769000	-2.969020000	0.974423000
C	-3.511955000	2.153020000	1.562491000
H	-3.871008000	1.336508000	2.189821000
H	-4.180858000	3.003877000	1.752702000
C	-2.470119000	-2.183307000	1.780416000
H	-2.984291000	-1.514621000	2.471919000
H	-2.291665000	-3.116833000	2.330751000
C	-1.220044000	0.471180000	2.918920000
H	-2.279810000	0.346559000	3.144297000
H	-0.758982000	0.889000000	3.824514000
O	-0.352769000	0.361625000	-2.663941000
H	0.501682000	-0.102693000	-2.621215000
H	-0.819920000	-0.037704000	-3.419245000

C	-5.360673000	-2.586071000	-1.583223000
C	-6.331204000	-3.305675000	-1.584144000
H	-3.336560000	-2.218654000	-2.059397000
H	-4.384091000	-0.816322000	-2.174436000
H	-7.187772000	-3.943877000	-1.590142000

45°

symmetry c1

Y	-1.524205000	0.212613000	-0.501861000
O	0.716889000	0.363269000	0.020193000
O	-0.905202000	-1.931801000	-1.276993000
O	7.329240000	-0.691521000	-0.804705000
O	-1.260410000	2.493887000	-1.005777000
N	6.231877000	-0.227121000	-0.322584000
N	-1.105772000	1.444954000	1.796374000
N	-3.628043000	1.714965000	0.137860000
N	2.492596000	1.193549000	1.168952000
H	2.789119000	1.814288000	1.915662000
N	-1.152895000	-1.550987000	1.428172000
N	-3.716771000	-1.289596000	-0.216942000
N	-1.995735000	4.580940000	-1.455002000
H	-1.067644000	4.878245000	-1.734068000
H	-2.745119000	5.259616000	-1.498159000
N	-0.056699000	-4.012474000	-1.039975000
H	-0.128668000	-4.188541000	-2.035710000
H	0.316522000	-4.747400000	-0.453032000
C	0.262459000	2.008587000	1.720088000
H	0.670910000	2.221169000	2.715839000
H	0.221373000	2.955266000	1.173199000
C	3.548548000	0.485926000	0.428156000
H	3.028670000	-0.187940000	-0.253966000
C	1.194205000	1.113308000	0.918336000
C	-0.423494000	-2.837130000	-0.550062000
C	-3.619001000	2.885692000	-0.769931000
H	-4.221417000	3.714437000	-0.376575000
H	-4.059413000	2.592885000	-1.728948000
C	-2.198242000	3.326214000	-1.077582000
C	5.537314000	0.809328000	-1.159966000
C	4.429796000	-0.297061000	1.405024000
H	4.875757000	0.411720000	2.114881000
H	3.824194000	-0.999546000	1.987629000
C	4.414453000	1.485181000	-0.345759000
H	3.796326000	2.074779000	-1.031337000
H	4.861047000	2.185157000	0.372039000
C	5.555571000	-1.087609000	0.706784000
C	-2.101014000	2.546330000	1.985801000
H	-1.761924000	3.414090000	1.419948000
H	-2.131026000	2.856852000	3.038573000
C	-0.199308000	-2.566779000	0.925170000
H	-0.233502000	-3.488953000	1.518409000
H	0.815909000	-2.165294000	0.998898000

C	-0.581842000	-0.884718000	2.638335000
H	0.493675000	-0.775097000	2.492079000
H	-0.709500000	-1.521193000	3.523908000
C	4.988751000	0.146565000	-2.442076000
H	5.786040000	-0.421032000	-2.930150000
H	4.634730000	0.917392000	-3.134859000
H	4.155372000	-0.533151000	-2.240882000
C	6.584095000	1.869594000	-1.540956000
H	7.039025000	2.304760000	-0.644867000
H	6.100861000	2.671606000	-2.108499000
H	7.373933000	1.431461000	-2.154083000
C	-4.175215000	-1.719879000	-1.579971000
C	6.615693000	-1.473163000	1.752071000
H	6.145521000	-2.056585000	2.550464000
H	7.065887000	-0.578784000	2.195582000
H	7.407390000	-2.072197000	1.298108000
C	-4.888499000	0.932465000	-0.050966000
H	-5.119705000	0.924077000	-1.118417000
H	-5.729857000	1.428424000	0.451194000
C	-4.778694000	-0.495788000	0.469343000
H	-4.567649000	-0.496515000	1.539615000
H	-5.752310000	-0.988704000	0.347810000
C	5.015259000	-2.365312000	0.029067000
H	4.677468000	-3.074567000	0.792118000
H	5.812413000	-2.834695000	-0.554218000
H	4.172715000	-2.163004000	-0.638927000
C	-3.365221000	-2.496225000	0.589291000
H	-2.891925000	-3.217385000	-0.079197000
H	-4.273865000	-2.980553000	0.969588000
C	-3.512946000	2.150141000	1.563333000
H	-3.873154000	1.334468000	2.191124000
H	-4.182868000	3.000910000	1.749949000
C	-2.461895000	-2.189020000	1.780636000
H	-2.979189000	-1.523227000	2.472642000
H	-2.281352000	-3.123029000	2.329452000
C	-1.221245000	0.470141000	2.922482000
H	-2.281110000	0.343687000	3.146570000
H	-0.762082000	0.888962000	3.828621000
O	-0.442569000	0.378687000	-2.707034000
H	0.334390000	-0.202959000	-2.777986000
H	-0.996273000	0.163686000	-3.478160000
C	-5.351390000	-2.597381000	-1.580480000
C	-6.318769000	-3.321203000	-1.578838000
H	-3.329896000	-2.221917000	-2.061188000
H	-4.382906000	-0.823539000	-2.172973000
H	-7.172630000	-3.963050000	-1.582557000

55°

symmetry c1

Y	-1.523406000	0.213314000	-0.500898000
O	0.716959000	0.346443000	0.036947000

O	-0.879319000	-1.920110000	-1.282770000
O	7.326777000	-0.685535000	-0.812758000
O	-1.263050000	2.496421000	-1.001111000
N	6.230263000	-0.221956000	-0.327888000
N	-1.108135000	1.440885000	1.799358000
N	-3.629054000	1.708689000	0.140236000
N	2.492502000	1.194159000	1.172653000
H	2.789260000	1.821806000	1.913426000
N	-1.150250000	-1.555567000	1.426831000
N	-3.712061000	-1.295657000	-0.220290000
N	-2.004276000	4.583429000	-1.441317000
H	-1.076543000	4.885142000	-1.716924000
H	-2.755647000	5.260081000	-1.481993000
N	-0.035262000	-4.002572000	-1.047574000
H	-0.099290000	-4.173945000	-2.044677000
H	0.331411000	-4.741034000	-0.460901000
C	0.260351000	2.003977000	1.724838000
H	0.667071000	2.218364000	2.720994000
H	0.220432000	2.949682000	1.176133000
C	3.548186000	0.486507000	0.431590000
H	3.027938000	-0.192593000	-0.244979000
C	1.193379000	1.106127000	0.926958000
C	-0.404987000	-2.829284000	-0.555187000
C	-3.623095000	2.878755000	-0.768526000
H	-4.232074000	3.704268000	-0.378717000
H	-4.057575000	2.582321000	-1.729151000
C	-2.203511000	3.326318000	-1.070657000
C	5.528844000	0.808332000	-1.167162000
C	4.436235000	-0.288736000	1.408382000
H	4.883251000	0.424882000	2.112734000
H	3.835551000	-0.990239000	1.997228000
C	4.407498000	1.484597000	-0.351132000
H	3.784398000	2.068879000	-1.036782000
H	4.855080000	2.189411000	0.361280000
C	5.561152000	-1.079350000	0.708811000
C	-2.103411000	2.541968000	1.989332000
H	-1.764028000	3.410466000	1.424773000
H	-2.134451000	2.851445000	3.042403000
C	-0.191874000	-2.566434000	0.923058000
H	-0.227125000	-3.491990000	1.510896000
H	0.821949000	-2.163089000	1.004500000
C	-0.584050000	-0.889916000	2.639752000
H	0.491826000	-0.779455000	2.497854000
H	-0.714712000	-1.527280000	3.524240000
C	4.976650000	0.137853000	-2.443751000
H	5.773712000	-0.428816000	-2.933273000
H	4.616344000	0.904317000	-3.138120000
H	4.146925000	-0.544171000	-2.235625000
C	6.570659000	1.869863000	-1.558082000
H	7.028201000	2.310994000	-0.666261000
H	6.082475000	2.667465000	-2.127609000
H	7.359108000	1.431007000	-2.172490000

C	-4.173368000	-1.722816000	-1.583306000
C	6.627191000	-1.456702000	1.751068000
H	6.162355000	-2.037542000	2.554446000
H	7.076755000	-0.558838000	2.188146000
H	7.418597000	-2.055619000	1.296440000
C	-4.887960000	0.923455000	-0.047681000
H	-5.121225000	0.916137000	-1.114673000
H	-5.729531000	1.416761000	0.456682000
C	-4.773790000	-0.505278000	0.470359000
H	-4.559984000	-0.507173000	1.540063000
H	-5.746640000	-1.000148000	0.350612000
C	5.021619000	-2.361865000	0.039647000
H	4.689354000	-3.068507000	0.807553000
H	5.817602000	-2.831594000	-0.544969000
H	4.175467000	-2.165311000	-0.625540000
C	-3.356983000	-2.504435000	0.581182000
H	-2.878970000	-3.220208000	-0.089959000
H	-4.264340000	-2.994551000	0.957107000
C	-3.515050000	2.145577000	1.565549000
H	-3.875684000	1.330231000	2.193550000
H	-4.185410000	2.996253000	1.750737000
C	-2.457238000	-2.199001000	1.775421000
H	-2.977647000	-1.537109000	2.468887000
H	-2.274903000	-3.134429000	2.321250000
C	-1.225242000	0.464203000	2.923634000
H	-2.285529000	0.336470000	3.145088000
H	-0.768537000	0.882248000	3.831435000
O	-0.479262000	0.395855000	-2.700447000
H	0.199243000	-0.276030000	-2.885137000
H	-1.011192000	0.478912000	-3.510298000
C	-5.348050000	-2.602389000	-1.582656000
C	-6.313875000	-3.328273000	-1.579011000
H	-3.328819000	-2.222604000	-2.068334000
H	-4.383784000	-0.825412000	-2.173603000
H	-7.166417000	-3.971891000	-1.580924000