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**C-H Bond Activation by High-valent Iron/Cobalt-Oxo Complexes: A Quantum  
Chemical Modeling Approach**

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**Table S1** Energy computed using DLPNO-CCSD(T) method for species **1** and **2**.

<b>Spin States</b>	<b>Relative energy (kJ/mol)</b>
<sup>5</sup> <b>1</b> <sub>hs</sub>	25.6
<sup>3</sup> <b>1</b> <sub>is</sub>	0.0
<sup>1</sup> <b>1</b> <sub>is</sub>	128.6
<sup>6</sup> <b>2</b> <sub>hs</sub>	134.4
<sup>4</sup> <b>2</b> <sub>is</sub>	34.3
<sup>2</sup> <b>2</b> <sub>is</sub>	0.0

**Table S2** Computed salient bond parameters of all the studied species. *Given bond length in Å and angle in °.*

Fe-oxo										
Species	Fe-O	O-H	H-C <sub>DHA</sub>	Fe-O-H	O-H-C <sub>DHA</sub>	Fe-C <sub>NHC</sub>	Fe-N1	Fe-N2	Fe-N3	Fe-N4
<sup>5</sup> 1 <sub>HS</sub>	1.661	-	-	-	-	2.208	2.052	2.072	2.051	2.072
<sup>3</sup> 1 <sub>IS</sub>	1.671	-	-	-	-	2.180	1.983	1.988	1.984	1.988
<sup>1</sup> 1 <sub>LS</sub>	1.671	-	-	-	-	2.178	1.987	1.981	1.987	1.982
<sup>5</sup> TS1 <sub>HS</sub>	1.755	1.263	1.295	119.7	158.6	2.145	2.040	2.084	2.043	2.070
<sup>3</sup> TS1 <sub>IS</sub>	1.768	1.267	1.296	116.7	160.7	2.130	1.978	1.988	1.983	1.977
<sup>1</sup> TS1 <sub>LS</sub>	1.752	1.332	1.220	115.3	159.6	2.110	1.973	2.012	2.000	1.952
<sup>6</sup> Int1 <sub>HS</sub>	1.881	0.976	-	122.5	-	2.475	2.082	2.077	2.055	2.084
<sup>4</sup> Int1 <sub>IS</sub>	1.917	0.979	-	117.8	-	2.487	2.011	2.007	1.996	2.013
<sup>2</sup> Int1 <sub>LS</sub>	1.839	0.982	-	108.9	-	2.107	1.986	1.984	1.979	1.984
<sup>7</sup> TS2 <sub>HS</sub>	2.017	1.272	1.340	126.3	170.9	2.315	2.039	2.069	2.076	2.053
<sup>5</sup> TS2 <sub>HS</sub>	1.953	1.385	1.249	135.3	169.9	2.175	2.042	2.091	2.053	2.094
<sup>5</sup> TS2 <sub>IS</sub>	2.029	1.338	1.284	127.7	173.4	2.366	1.977	2.000	2.000	1.986
<sup>3</sup> TS2 <sub>IS</sub>	1.934	1.228	1.400	144.4	167.2	2.146	1.986	1.991	1.992	1.984
<sup>3</sup> TS2 <sub>LS</sub>	1.904	1.267	1.342	132.6	171.5	2.068	1.973	1.978	1.981	1.970
<sup>5</sup> Int2 <sub>HS</sub>	2.129	0.979	-	-	-	1.982	2.08394	2.092	2.145	2.116
<sup>3</sup> Int2 <sub>IS</sub>	1.763	0.971	-	-	-	2.213	1.99651	1.984	1.996	1.984
<sup>1</sup> Int2 <sub>LS</sub>	2.142	0.978	-	-	-	1.984	1.98250	1.980	1.998	1.992
Co-oxyl										
Species	Co-O	O-H	H-C <sub>DHA</sub>	Co-O-H	O-H-C <sub>DHA</sub>	Co-C <sub>NHC</sub>	Co-N1	Co-N2	Co-N3	Co-N4
<sup>6</sup> 2 <sub>HS</sub>	1.924	-	-	-	-	2.277	2.068	2.097	2.033	2.066
<sup>4</sup> 2 <sub>IS</sub>	1.698	-	-	-	-	2.115	2.103	1.992	2.103	1.992
<sup>2</sup> 2 <sub>LS</sub>	1.854	-	-	-	-	2.058	1.954	1.960	1.954	1.960
<sup>6</sup> TS1 <sub>HS</sub>	1.893	1.396	1.213	110.9	156.3	2.327	2.064	2.053	2.042	2.069
<sup>4</sup> TS1 <sub>IS</sub>	1.768	1.315	1.258	117.3	156.3	2.124	1.984	2.101	1.976	2.099
<sup>2</sup> TS1 <sub>LS</sub>	1.873	1.309	1.254	113.6	159.1	2.054	1.954	1.960	1.954	1.952
<sup>5</sup> Int1 <sub>HS</sub>	1.865	0.980	-	116.7	-	2.373	2.032	2.073	2.079	2.068
<sup>3</sup> Int1 <sub>IS</sub>	1.830	0.982	-	109.1	-	2.138	1.974	2.103	1.961	2.109
<sup>1</sup> Int1 <sub>LS</sub>	1.893	0.981	-	105.8	-	2.050	1.958	1.958	1.951	1.959
<sup>6</sup> TS2 <sub>HS</sub>	2.096	1.332	1.272	117.1	165.7	2.272	2.045	2.088	2.104	2.060

<sup>4</sup> TS2 <sub>HS</sub>	1.926	1.479	1.202	132.4	170.9	2.177	2.014	2.093	2.019	2.086
<sup>4</sup> TS2 <sub>IS</sub>	1.926	1.478	1.202	132.4	170.8	2.177	2.014	2.093	2.018	2.086
<sup>2</sup> TS2 <sub>LS</sub>	1.942	1.276	1.352	123.7	166.2	1.994	1.945	1.953	1.958	1.949
<sup>4</sup> Int2 <sub>HS</sub>	2.195	0.977	-	-	-	2.294	2.084	2.085	2.066	2.061
<sup>2</sup> Int2 <sub>LS</sub>	2.069	0.977	-	-	-	1.937	1.959	1.955	1.950	1.944

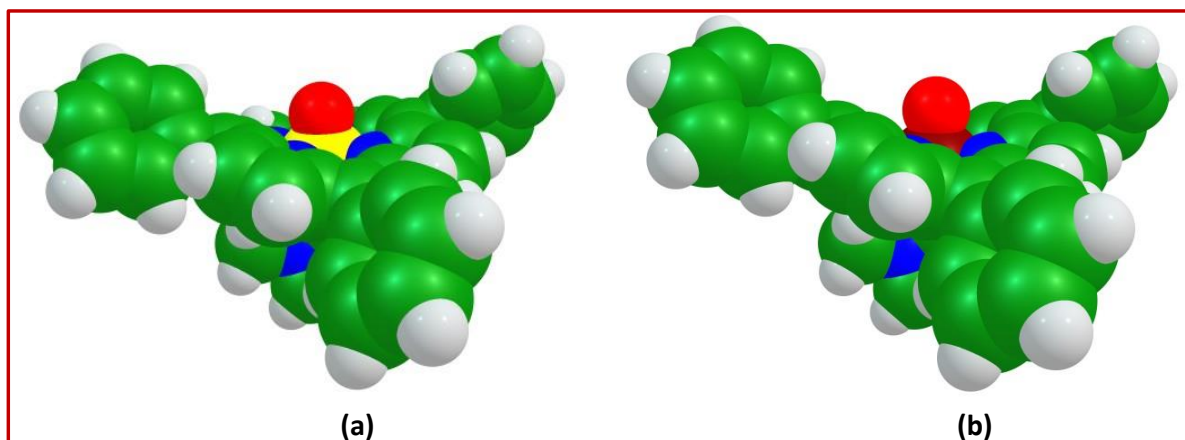


Fig. S1 van der Waal's images for oxidants a) species 1 and b) 2.

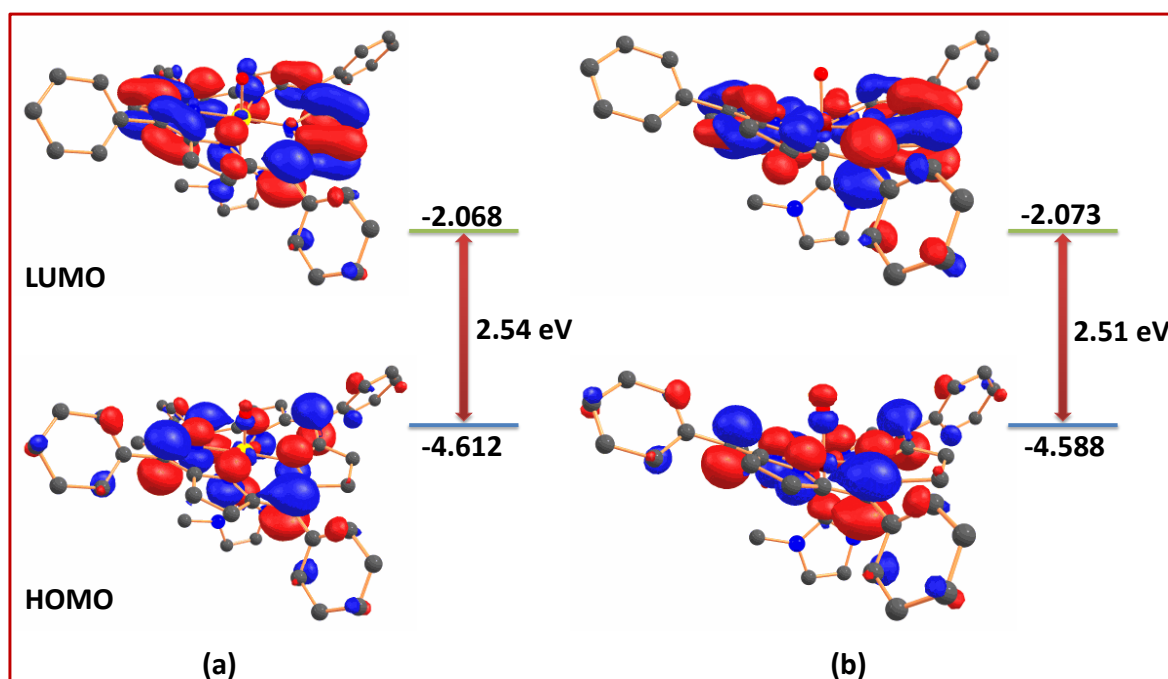


Fig. S2 Computed frontier molecular orbitals (FMOs) of (a) species 1, and (b) 2.

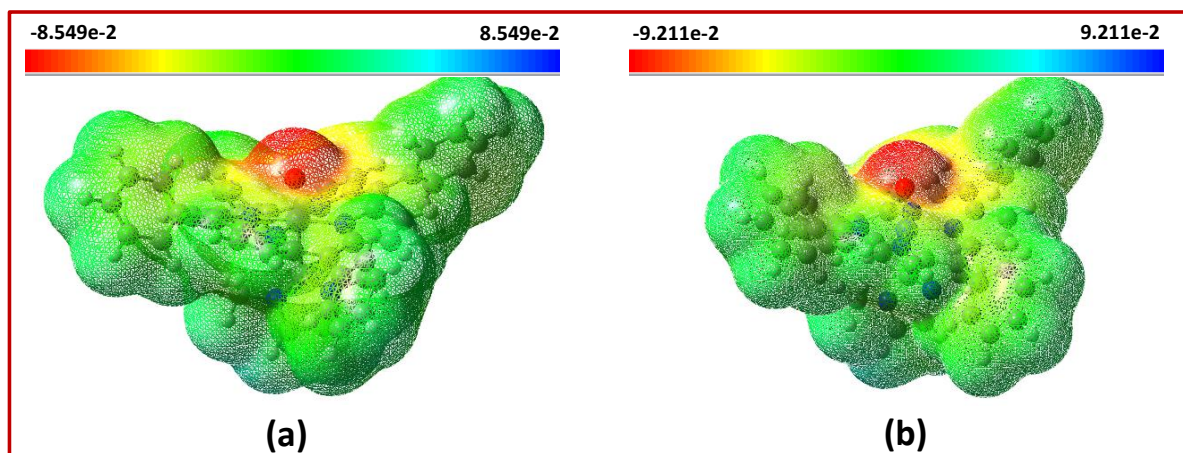
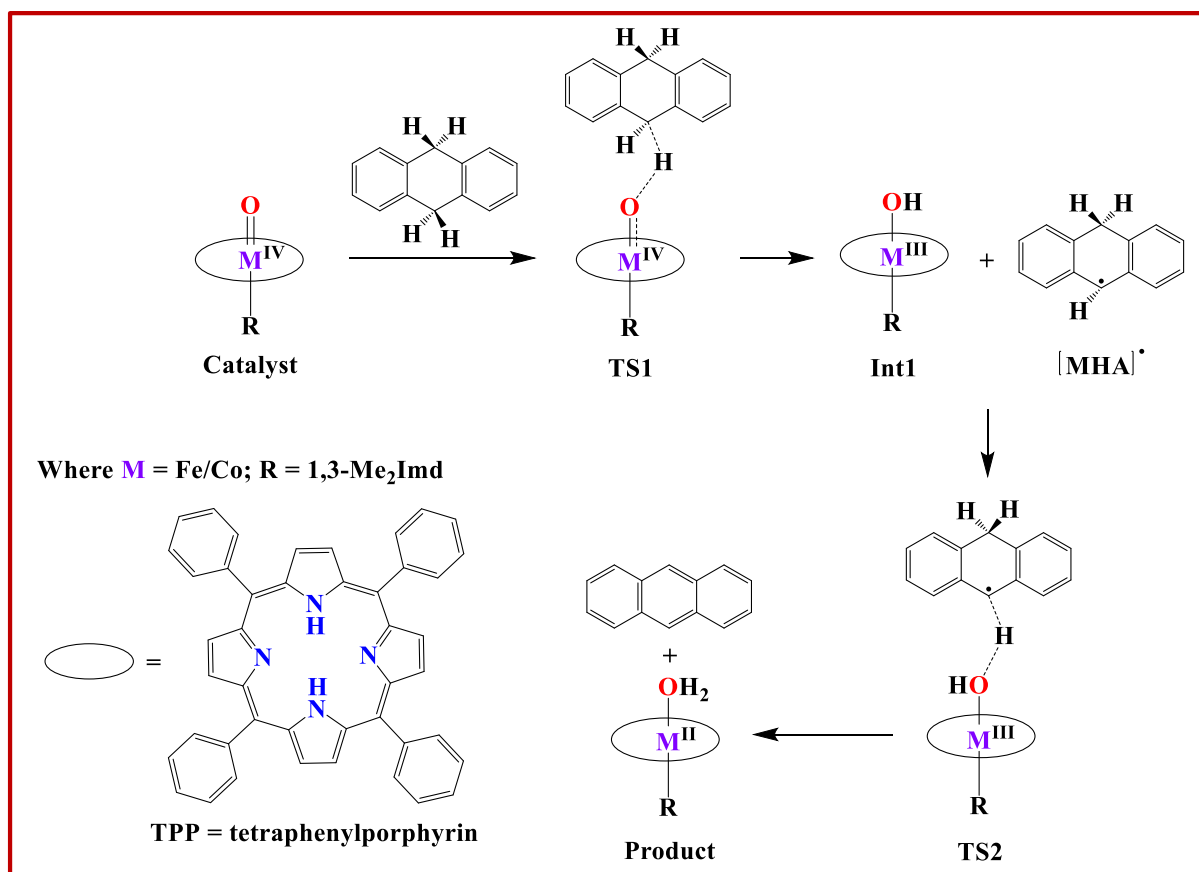


Fig. S3 Computed molecular electrostatic potential (MEP) maps of (a) species 1, and (b) 2.



Scheme S1 Plausible mechanism adopted for the C–H bond activation reaction by species 1 and 2.

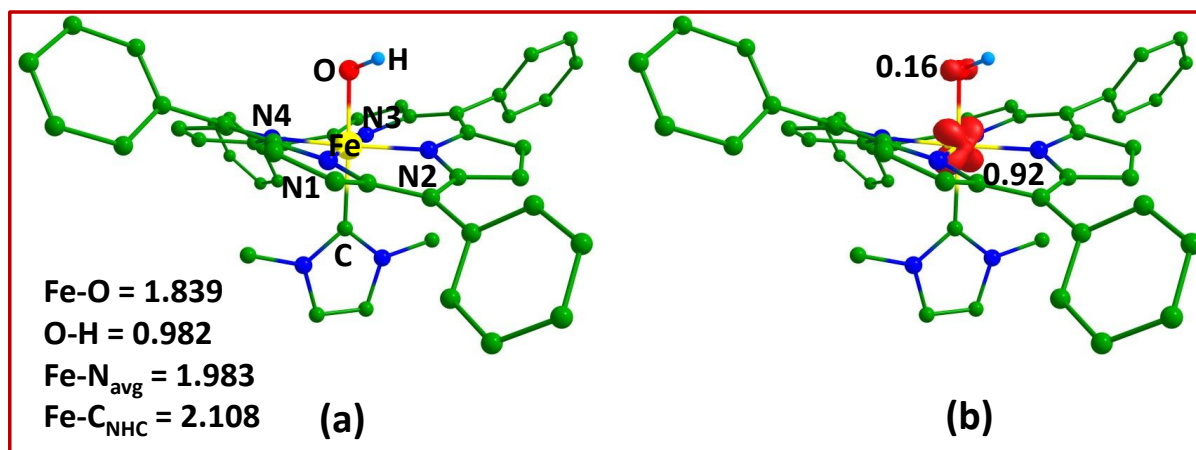
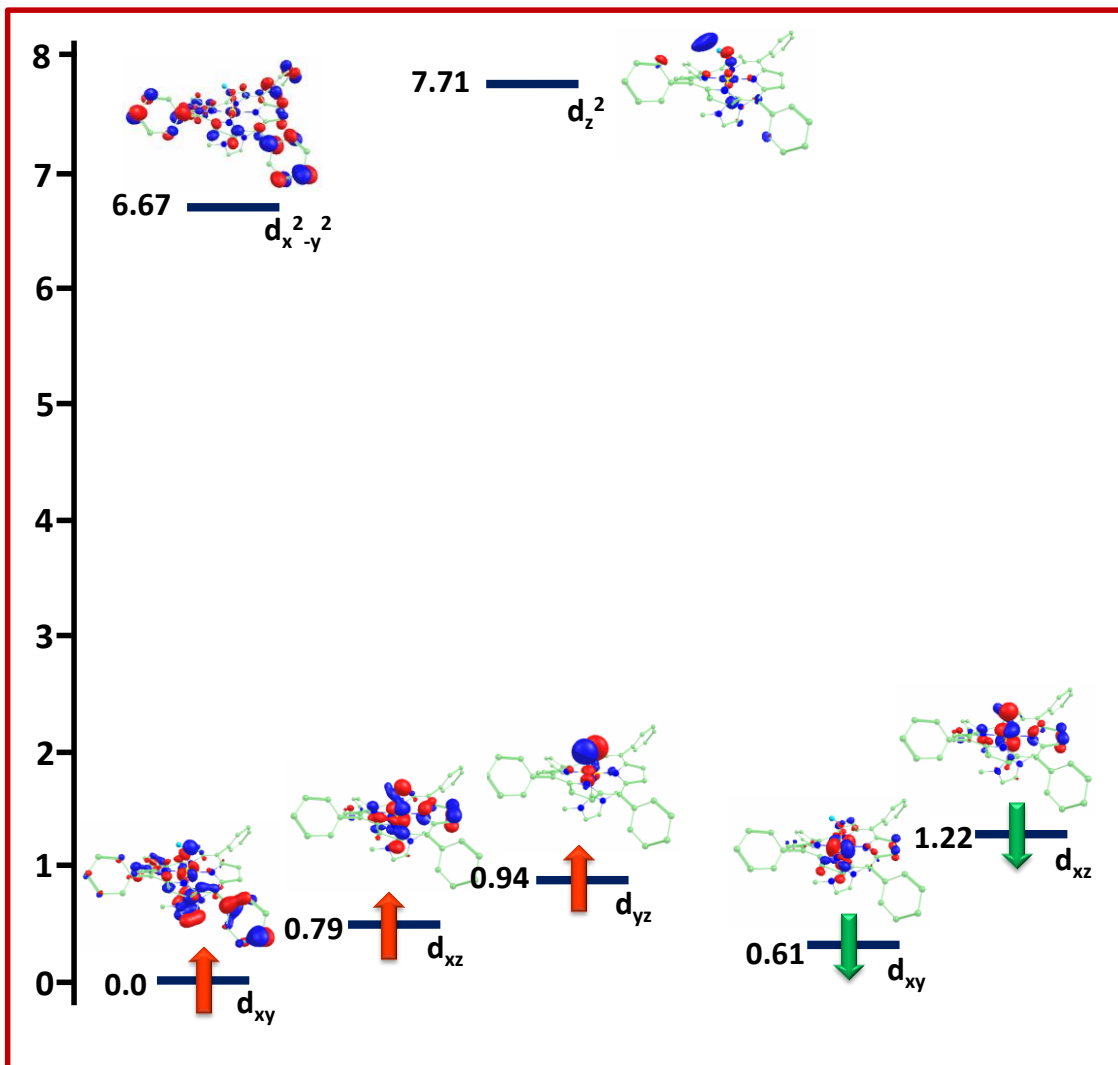
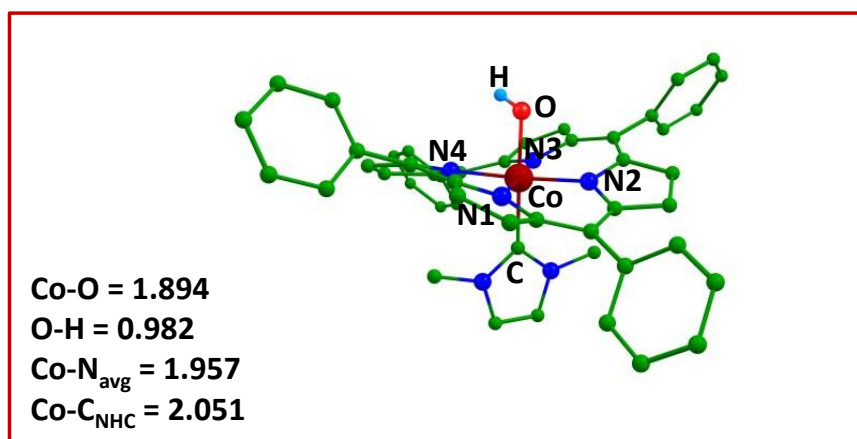


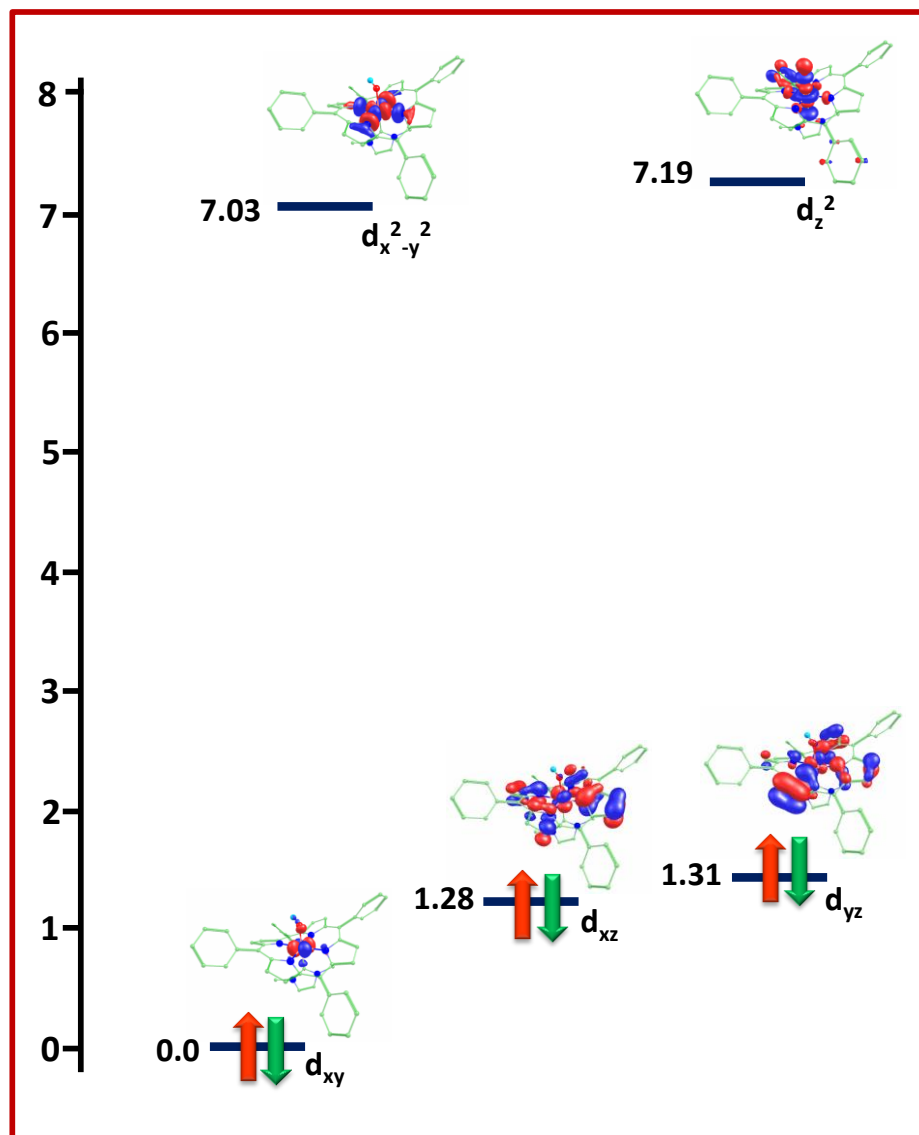
Fig. S4 (a) Optimized structure and key geometric parameters, and (b) spin density plot of ground spin state of Int1 of species 1.



**Fig. S5** DFT computed frontier d-based qualitative molecular orbital diagram of ground spin state of **Int1** of species **1**. (Given energy in eV)

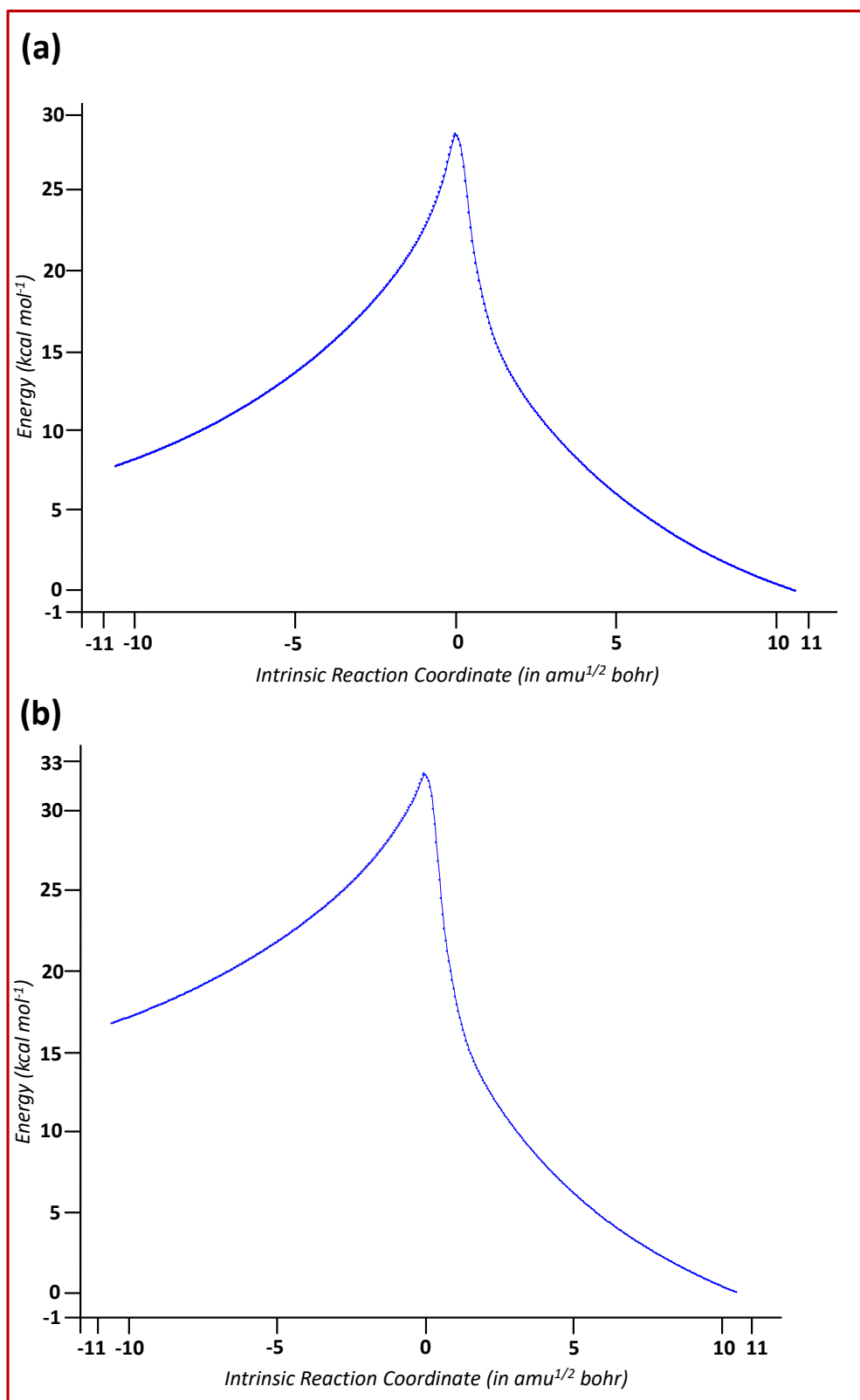


**Fig. S6** Optimized structure and key geometric parameters of ground spin state of **Int1'** of species **2**.



**Fig. S7** DFT computed frontier d-based qualitative molecular orbital diagram of ground spin state of Int1' of species 2. (Given energy in eV)





**Fig. S8** Potential Energy ( $E$ , in kcal mol<sup>-1</sup>) vs. Intrinsic Reaction Coordinate (in amu<sup>1/2</sup> bohr) for first H-abstraction from DHA by (a) species **1** and (b) **2**.

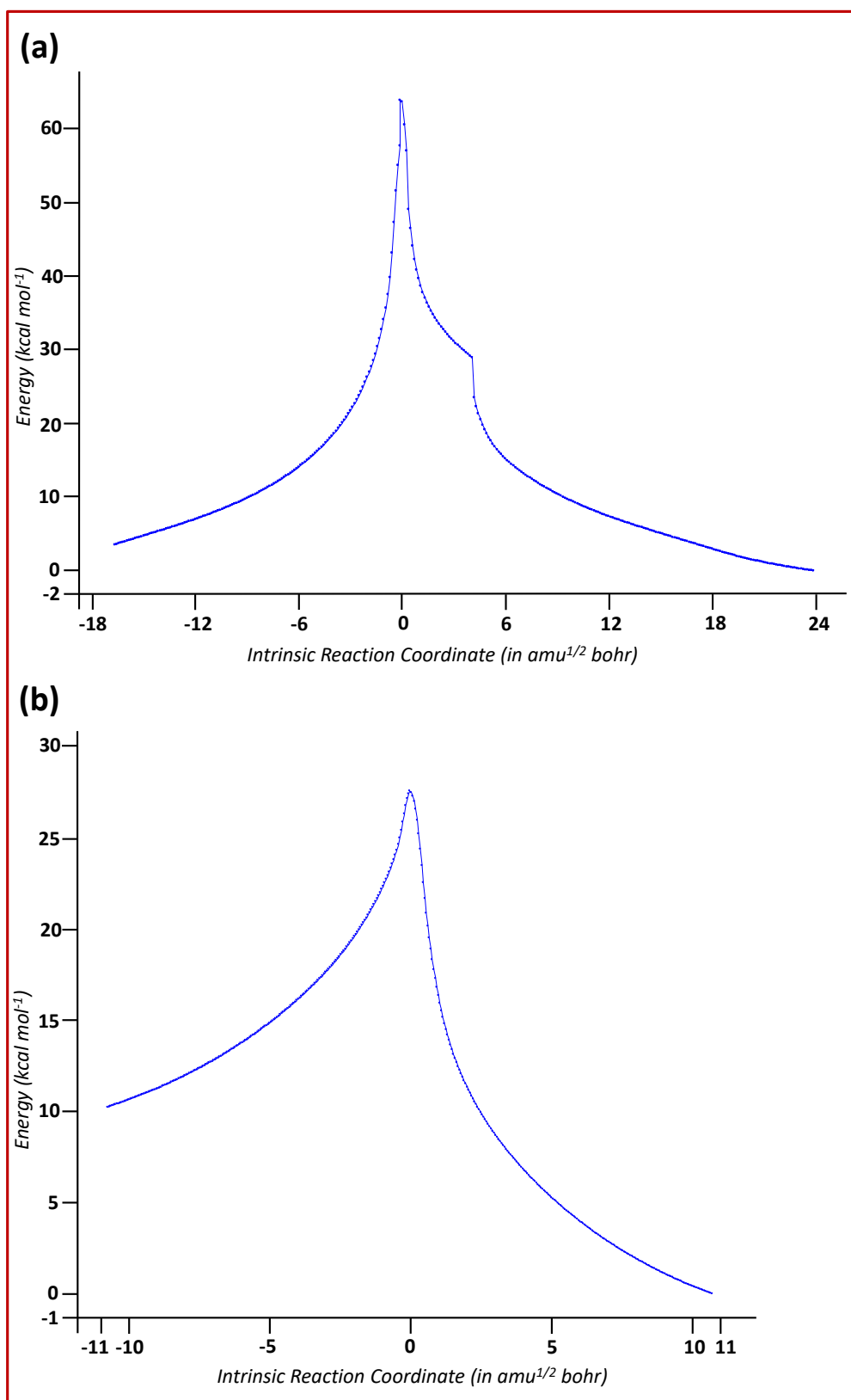
**Table S3** Possible interactions of Fe<sup>III</sup>-OH(Int1) and Co<sup>III</sup>-OH(Int1') with MHA molecule in second transition state.

Species	Valence Electrons	CH' <sub>(MHA)</sub>	Possible Interaction
<sup>7</sup> TS2-Fe <sub>HS</sub>	↑↑↑↑↑	↑	Ferromagnetic
<sup>5</sup> TS2-Fe <sub>HS</sub>	↑↑↑↑↑	↓	Anti-Ferromagnetic
<sup>5</sup> TS2-Fe <sub>IS</sub>	↑↓↑↑↑	↑	Ferromagnetic
<sup>3</sup> TS2-Fe <sub>IS</sub>	↑↓↑↑↑	↓	Anti-Ferromagnetic
<sup>3</sup> TS2-Fe <sub>LS</sub>	↑↓↑↓↑	↑	Ferromagnetic
<sup>1</sup> TS2-Fe <sub>LS</sub>	↑↓↑↓↑	↓	Anti-Ferromagnetic
<sup>6</sup> TS2-Co <sub>HS</sub>	↑↓↑↑↑↑	↑	Ferromagnetic
<sup>4</sup> TS2-Co <sub>HS</sub>	↑↓↑↑↑↑	↓	Anti-Ferromagnetic
<sup>4</sup> TS2-Co <sub>IS</sub>	↑↓↑↓↑↑	↑	Ferromagnetic
<sup>2</sup> TS2-Co <sub>IS</sub>	↑↓↑↓↑↑	↓	Anti-Ferromagnetic
<sup>2</sup> TS2-Co <sub>LS</sub>	↑↓↑↓↑↓	↑	Ferromagnetic

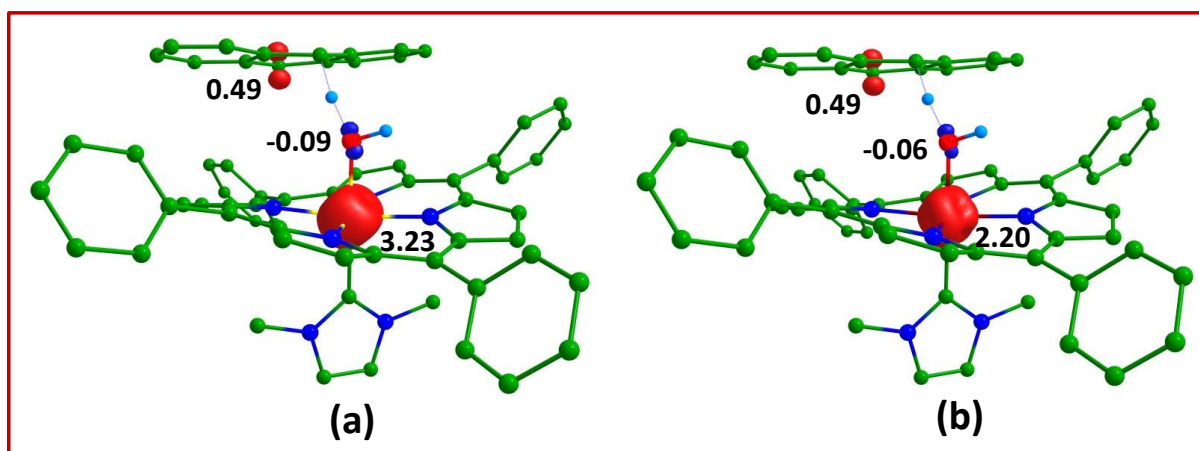
**Table S4** Mulliken atomic charges and spin density of the species **1**, **2** and respective intermediates in the C-H bond activation.

System	Spin State	Mulliken atomic charges				Spin density			
		Fe	O	C <sub>DHA/MHA</sub>	H <sub>DHA/MHA</sub>	Fe	O	C <sub>DHA/MHA</sub>	H <sub>DHA/MHA</sub>
<b>Species 1</b>	HS	0.561	-0.304	-	-	2.950	0.805	-	-
	IS	0.379	-0.285	-	-	1.047	1.034	-	-
	LS	0.353	-0.303	-	-	0.000	0.000	-	-
<b>TS1</b>	HS	0.575	-0.470	-0.461	0.340	2.854	0.553	0.353	-0.064
	IS	0.414	-0.455	-0.452	0.333	0.965	0.707	0.375	-0.076
	LS	0.356	-0.442	-0.436	0.312	0.000	0.000	0.000	0.00
<b>Int1</b>	HS	0.767	-0.658	-	-	4.063	0.395	-	-
	IS	0.569	-0.653	-	-	2.606	0.366	-	-
	LS	0.383	-0.562	-	-	0.924	0.158	-	-
<b>TS2</b>	HS <sub>F</sub>	0.827	-0.721	-0.573	0.415	4.123	0.163	0.055	0.018
	HS <sub>AF</sub>	0.650	-0.660	-0.548	0.381	3.232	-0.092	-0.081	0.042
	IS <sub>F</sub>	0.645	-0.716	-0.562	0.396	2.742	0.172	0.049	0.018
	IS <sub>AF</sub>	0.529	-0.689	-0.561	0.420	1.173	0.012	0.016	0.039
	LS <sub>F</sub>	0.526	-0.686	-0.577	0.421	1.064	0.047	0.039	0.026
	LS <sub>AF</sub>	-	-	-	-	-	-	-	-
<b>P</b>	HS	0.627	-0.653	-	-	3.743	0.028	-	-
	IS	0.518	-0.674	-	-	1.059	0.025	-	-
	LS	0.324	-0.640	-	-	0.000	0.000	-	-
		Co	O	C <sub>DHA/MHA</sub>	H <sub>DHA/MHA</sub>	Co	O	C <sub>DHA/MHA</sub>	H <sub>DHA/MHA</sub>
<b>Species 2</b>	HS	0.607	-0.223	-	-	2.803	1.576	-	-
	IS	0.457	-0.233	-	-	1.610	1.178	-	-
	LS	0.416	-0.325	-	-	-0.061	1.048	-	-
<b>TS1'</b>	HS	0.589	-0.416	-0.455	0.301	2.824	1.192	0.312	-0.062
	IS	0.474	-0.433	-0.453	0.319	1.636	0.786	0.351	-0.069
	LS	0.413	-0.470	-0.436	0.312	-0.037	0.673	0.356	-0.083
<b>Int1'</b>	HS	0.628	-0.594	-	-	2.900	0.501	-	-
	IS	0.460	-0.564	-	-	1.645	0.208	-	-
	LS	0.357	-0.594	-	-	0.000	0.000	-	-
<b>TS2'</b>	HS <sub>F</sub>	0.537	-0.650	-0.515	0.367	2.701	0.309	0.209	-0.005
	HS <sub>AF</sub>	0.545	-0.651	-0.535	0.367	1.787	0.075	-0.010	0.040
	IS <sub>F</sub>	0.545	-0.651	-0.535	0.367	2.202	-0.062	-0.075	0.035
	IS <sub>AF</sub>	-	-	-	-	-	-	-	-
	LS <sub>F</sub>	0.472	-0.672	-0.556	0.405	0.021	0.011	0.041	0.026
<b>P'</b>	HS	0.491	-0.651	-	-	2.679	0.024	-	-
	LS	0.421	-0.634	-	-	-0.006	-0.001	-	-

*LS<sub>AF</sub> (TS2) and IS<sub>AF</sub> (TS2)' = these species have convergence issue*



**Fig. S9** Potential Energy ( $E$ , in kcal mol<sup>-1</sup>) vs. Intrinsic Reaction Coordinate (in amu<sup>1/2</sup> bohr) for **TS2** and **TS2'** by (a) species **1** and (b) **2**, respectively.



**Fig. S10** The computed spin density plots (a) for species **1** and (b) for species **2** of the second transition state (**TS2**). Contour value = 0.03.

**Table S5** Comparison of computed barrier height for C-H bond activation of DHA substrate by  $\text{Fe}^{\text{IV}}=\text{O}$ .

Sr. No.	Species	$\Delta G(\text{kJ/mol})$	References
1	$[\text{Fe}^{\text{IV}}(\text{O})(\text{TMG}_3\text{tren})]^{+2}$	60.3	1
2	$[\text{Fe}^{\text{IV}}(\text{O})(\text{TMG}_2\text{dien})(\text{MeCN})]^{+2}$	45.6	1
3	$[\text{Fe}^{\text{IV}}(\text{O})(\text{tBu}_3\text{tacn})]^{+2}$	111.0	2
4	$[\text{Fe}^{\text{IV}}(\text{O})(\text{H}_3\text{buea})]^-$	119.6	3
5	$[\text{Fe}^{\text{IV}}(\text{O})(\text{H1}^{\text{cvp}})]^-$	88.2	4
6	$[\text{Fe}^{\text{IV}}(\text{O})(\text{TMC})(\text{CH}_3\text{CN})]^{+2}$	108.3	5
7	$[\text{Fe}^{\text{IV}}(\text{O})(\text{TMC})(\text{CH}_2\text{S})]^+$	110.4	5
8	$[\text{Fe}^{\text{IV}}(\text{O})(\text{TMC})(\text{N}_3)]^+$	106.2	5
9	$[\text{Fe}^{\text{IV}}(\text{O})(\text{Bn-TPEN})]^{+2}$	60.2	6
10	$[\text{Fe}^{\text{IV}}(\text{O})(\text{TPP})(1,3\text{-Me}_2\text{Imd})]$	44.6	This work

## References

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## XYZ Coordinates

The coordinates are given in xyz-format, and the specific multiplicity/species/spin state pair for each of the calculations is given in parenthesis in the comment line of the structure.

### Fe-based species

<sup>5</sup>1<sub>(HS)</sub>

Fe	-0.000055000	0.000363000	-0.302007000	C	-5.306421000	0.343689000	-2.294902000
C	-0.000040000	-0.000217000	1.906352000	H	-4.679231000	-0.318320000	-2.882483000
C	0.677989000	-0.026373000	4.107041000	C	-6.636249000	0.573049000	-2.662338000
H	1.391230000	-0.050202000	4.912727000	H	-7.043681000	0.083655000	-3.541620000
C	-0.678097000	0.024096000	4.107057000	C	-7.438008000	1.436622000	-1.904163000
H	-1.391345000	0.047188000	4.912758000	H	-8.469944000	1.615421000	-2.189787000
C	-2.493497000	0.085615000	2.405987000	C	-6.900379000	2.067653000	-0.774675000
H	-3.061958000	0.358848000	3.299381000	H	-7.517441000	2.731830000	-0.177096000
H	-2.645461000	0.836167000	1.637820000	C	-5.570456000	1.837700000	-0.406965000
H	-2.830505000	-0.886046000	2.041563000	H	-5.156160000	2.318396000	0.473076000
C	2.493450000	-0.086268000	2.406003000	C	-0.982166000	-4.792777000	0.366838000
H	3.061940000	-0.359568000	3.299360000	C	-1.792478000	-5.546535000	-0.504325000
H	2.645681000	-0.836574000	1.637648000	H	-2.226516000	-5.060234000	-1.371130000
H	2.830194000	0.885580000	2.041849000	C	-2.019566000	-6.906943000	-0.269957000
N	1.075571000	-0.042381000	2.768551000	H	-2.641248000	-7.474578000	-0.955573000
N	-1.075650000	0.041251000	2.768573000	C	-1.436370000	-7.539083000	0.836188000
N	-1.722108000	-1.115189000	-0.267556000	H	-1.612252000	-8.595013000	1.016715000
N	1.152221000	-1.719192000	-0.198043000	C	-0.619083000	-6.802489000	1.703594000
N	1.722271000	1.115178000	-0.267109000	H	-0.161020000	-7.285613000	2.561327000
N	-1.152431000	1.719394000	-0.197576000	C	-0.392102000	-5.442315000	1.468718000
C	-2.985466000	-0.642311000	-0.546635000	H	0.241868000	-4.868187000	2.136640000
C	-1.804495000	-2.467162000	-0.004395000	C	4.752935000	-0.975441000	-1.163729000
C	0.647702000	-2.994199000	-0.081331000	C	5.306484000	-0.343546000	-2.294879000
C	2.471511000	-1.807195000	-0.603538000	H	4.679339000	0.318515000	-2.882447000
C	2.985594000	0.642431000	-0.546415000	C	6.636318000	-0.572934000	-2.662282000
C	1.804520000	2.467204000	-0.004064000	H	7.043798000	-0.083514000	-3.541527000
C	-0.647779000	2.994342000	-0.080815000	C	7.438019000	-1.436571000	-1.904123000
C	-2.471656000	1.807430000	-0.603170000	H	8.469957000	-1.615396000	-2.189724000
C	-3.927103000	-1.738876000	-0.390288000	C	6.900331000	-2.067636000	-0.774683000
H	-4.995477000	-1.656123000	-0.513353000	H	7.517347000	-2.731871000	-0.177123000
C	-3.209606000	-2.847456000	-0.027108000	C	5.570404000	-1.837653000	-0.407004000
H	-3.590478000	-3.832512000	0.189478000	H	5.156060000	-2.318380000	0.472996000
C	1.708429000	-3.940132000	-0.396292000	C	0.982227000	4.792803000	0.367189000
H	1.593453000	-5.012606000	-0.401926000	C	1.792337000	5.546535000	-0.504174000
C	2.814544000	-3.213619000	-0.743931000	H	2.226205000	5.060202000	-1.371048000
H	3.767793000	-3.588512000	-1.080739000	C	2.019473000	6.906952000	-0.269886000
C	3.927147000	1.739085000	-0.390273000	H	2.641002000	7.474573000	-0.955652000
H	4.995505000	1.656444000	-0.513542000	C	1.436527000	7.539108000	0.836382000
C	3.209597000	2.847626000	-0.027069000	H	1.612446000	8.595042000	1.016849000
H	3.590422000	3.832730000	0.189378000	C	0.619445000	6.802528000	1.703995000
C	-1.708483000	3.940334000	-0.395690000	H	0.161578000	7.285666000	2.561824000
H	-1.593489000	5.012808000	-0.401211000	C	0.392412000	5.442347000	1.469195000
C	-2.814634000	3.213886000	-0.743404000	H	-0.241416000	4.868231000	2.137263000
H	-3.767851000	3.588858000	-1.080214000	O	0.000003000	0.000758000	-1.963900000
C	-3.338249000	0.707515000	-0.778073000				
C	-0.706668000	-3.345695000	0.125635000				
C	3.338252000	-0.707354000	-0.778113000				
C	0.706655000	3.345705000	0.126061000				
C	-4.752926000	0.975555000	-1.163707000				

<sup>3</sup><sub>1</sub>(IS)

Fe	-0.000069000	0.000237000	-0.353750000	H	7.626883000	-2.304193000	-0.562706000
C	-0.000042000	-0.000197000	1.826739000	C	5.618205000	-1.534999000	-0.691640000
C	-0.678748000	0.012762000	4.028561000	H	5.281022000	-2.039610000	0.207563000
H	-1.391881000	0.023856000	4.834793000	C	0.728184000	4.738311000	0.641117000
C	0.678512000	-0.016802000	4.028579000	C	1.518111000	5.622971000	-0.118468000
H	1.391598000	-0.029112000	4.834835000	H	2.002122000	5.257261000	-1.017371000
C	2.492378000	-0.035526000	2.317518000	C	1.659576000	6.961157000	0.264328000
H	3.072551000	-0.315798000	3.201294000	H	2.266958000	7.631040000	-0.336597000
H	2.656584000	-0.765127000	1.531287000	C	1.008933000	7.440377000	1.408906000
H	2.807871000	0.950597000	1.971684000	H	1.118473000	8.479227000	1.704254000
C	-2.492496000	0.035054000	2.317460000	C	0.209754000	6.573078000	2.165307000
H	-3.072414000	0.316331000	3.201090000	H	-0.301084000	6.937275000	3.051489000
H	-2.655869000	0.764501000	1.530932000	C	0.068767000	5.235182000	1.782561000
H	-2.809000000	-0.950895000	1.972023000	H	-0.550495000	4.559667000	2.363892000
N	-1.075968000	0.024608000	2.689183000	C	-4.711758000	0.725460000	-1.403551000
N	1.075829000	-0.026301000	2.689213000	C	-5.168819000	0.052384000	-2.553808000
N	1.608848000	1.160541000	-0.322848000	H	-4.473808000	-0.573876000	-3.103161000
N	-1.176750000	1.601516000	-0.288805000	C	-6.490730000	0.196283000	-2.987464000
N	-1.608820000	-1.160467000	-0.323045000	H	-6.823710000	-0.323163000	-3.880729000
N	1.176594000	-1.601301000	-0.288863000	C	-7.380737000	1.012110000	-2.276342000
C	2.888977000	0.773294000	-0.658392000	H	-8.406573000	1.124514000	-2.613213000
C	1.659873000	2.492494000	0.044343000	C	-6.940110000	1.679801000	-1.126221000
C	-0.771395000	2.895076000	-0.040838000	H	-7.626680000	2.304912000	-0.563317000
C	-2.489736000	1.657119000	-0.731253000	C	-5.618102000	1.535423000	-0.692033000
C	-2.888949000	-0.773179000	-0.658632000	H	-5.280892000	2.040130000	0.207108000
C	-1.659920000	-2.492385000	0.044229000	C	-0.728142000	-4.738103000	0.641458000
C	0.771308000	-2.894865000	-0.040770000	C	-1.517606000	-5.623128000	-0.118191000
C	2.489620000	-1.656934000	-0.731246000	H	-2.001308000	-5.257776000	-1.017402000
C	3.790205000	1.889284000	-0.449919000	C	-1.658951000	-6.961239000	0.264909000
H	4.856320000	1.853429000	-0.608854000	H	-2.265964000	-7.631405000	-0.336073000
C	3.042944000	2.931778000	0.025591000	C	-1.008645000	-7.440028000	1.409856000
H	3.386271000	3.911157000	0.316475000	H	-1.118092000	-8.478822000	1.705438000
C	-1.869830000	3.800050000	-0.321504000	C	-0.209903000	-6.572379000	2.166314000
H	-1.816605000	4.873200000	-0.228741000	H	0.300681000	-6.936245000	3.052777000
C	-2.909072000	3.043928000	-0.786192000	C	-0.069030000	-5.234560000	1.783261000
H	-3.868967000	3.385644000	-1.137837000	H	0.549886000	-4.558772000	2.364641000
C	-3.790221000	-1.889121000	-0.450119000	O	-0.000025000	0.000267000	-2.025338000
H	-4.856334000	-1.853234000	-0.609054000				
C	-3.043011000	-2.931608000	0.025482000				
H	-3.386397000	-3.910933000	0.316468000				
C	1.869750000	-3.799840000	-0.321380000				
H	1.816513000	-4.872984000	-0.228570000				
C	2.908961000	-3.043743000	-0.786151000				
H	3.868839000	-3.385465000	-1.137825000				
C	3.305321000	-0.537605000	-0.951597000				
C	0.539943000	3.313536000	0.247192000				
C	-3.305333000	0.537750000	-0.951744000				
C	-0.540004000	-3.313394000	0.247264000				
C	4.711783000	-0.725275000	-1.403335000				
C	5.168826000	-0.052262000	-2.553631000				
H	4.473770000	0.573854000	-3.103090000				
C	6.490778000	-0.196050000	-2.987201000				
H	6.823742000	0.323330000	-3.880511000				
C	7.380850000	-1.011674000	-2.275931000				
H	8.406720000	-1.123984000	-2.612730000				
C	6.940255000	-1.679262000	-1.125738000				

<sup>1</sup><sub>1</sub>(LS)

Fe	0.000248000	-0.000318000	-0.368970000	H	7.580234000	-2.469138000	-0.605014000
C	0.000358000	-0.001254000	1.809421000	C	5.586226000	-1.660708000	-0.720114000
C	-0.678390000	0.009784000	4.011995000	H	5.250878000	-2.145059000	0.190825000
H	-1.391012000	0.022549000	4.818683000	C	0.845183000	4.701106000	0.676783000
C	0.679083000	-0.026115000	4.011882000	C	1.639455000	5.582692000	-0.081901000
H	1.391676000	-0.043974000	4.818498000	H	2.101051000	5.222640000	-0.994762000
C	2.493402000	-0.052137000	2.303307000	C	1.813138000	6.911534000	0.319737000
H	3.071178000	-0.325549000	3.190819000	H	2.423397000	7.579308000	-0.280632000
H	2.656465000	-0.790210000	1.524935000	C	1.190830000	7.384616000	1.482488000
H	2.813619000	0.928957000	1.948275000	H	1.325366000	8.416288000	1.792326000
C	-2.492592000	0.048681000	2.303597000	C	0.387532000	6.520648000	2.238376000
H	-3.069489000	0.324563000	3.190929000	H	-0.101431000	6.880118000	3.138721000
H	-2.653046000	0.786839000	1.524862000	C	0.214463000	5.192045000	1.836948000
H	-2.815944000	-0.931599000	1.948987000	H	-0.407892000	4.519091000	2.418005000
N	-1.075596000	0.026459000	2.673364000	C	-4.687912000	0.843774000	-1.431270000
N	1.076364000	-0.034004000	2.673195000	C	-5.144883000	0.195251000	-2.595714000
N	1.640230000	1.122458000	-0.350249000	H	-4.455969000	-0.437885000	-3.144843000
N	-1.142336000	1.617014000	-0.266934000	C	-6.458121000	0.372427000	-3.043033000
N	-1.640336000	-1.121274000	-0.350652000	H	-6.790905000	-0.128269000	-3.947006000
N	1.142194000	-1.616198000	-0.268399000	C	-7.339601000	1.197281000	-2.331688000
C	2.906447000	0.708371000	-0.693493000	H	-8.358747000	1.335498000	-2.679112000
C	1.724458000	2.449493000	0.025815000	C	-6.899324000	1.840238000	-1.167417000
C	-0.702003000	2.897405000	-0.002631000	H	-7.579814000	2.471576000	-0.604067000
C	-2.453428000	1.711288000	-0.710726000	C	-5.586008000	1.662682000	-0.719412000
C	-2.906589000	-0.706993000	-0.693709000	H	-5.250418000	2.146923000	0.191494000
C	-1.724552000	-2.448647000	0.024430000	C	-0.845419000	-4.700580000	0.674413000
C	0.701966000	-2.896698000	-0.004131000	C	-1.639504000	-5.581872000	-0.084795000
C	2.453541000	-1.710077000	-0.711624000	H	-2.100800000	-5.221497000	-0.997683000
C	3.835849000	1.804023000	-0.494394000	C	-1.813443000	-6.910815000	0.316407000
H	4.899545000	1.743794000	-0.662323000	H	-2.423566000	-7.578366000	-0.284349000
C	3.116917000	2.860661000	-0.007069000	C	-1.191571000	-7.384280000	1.479237000
H	3.485215000	3.830586000	0.285102000	H	-1.326306000	-8.416025000	1.788743000
C	-1.780591000	3.830323000	-0.261113000	C	-0.388485000	-6.520585000	2.235664000
H	-1.701567000	4.900226000	-0.151632000	H	0.100119000	-6.880348000	3.136087000
C	-2.838366000	3.107111000	-0.738089000	C	-0.215183000	-5.191874000	1.834682000
H	-3.789308000	3.478424000	-1.083694000	H	0.406976000	-4.519118000	2.416182000
C	-3.835899000	-1.802807000	-0.495354000	O	-0.000459000	0.003302000	-2.040266000
H	-4.899598000	-1.742481000	-0.663221000				
C	-3.116956000	-2.859772000	-0.008710000				
H	-3.485268000	-3.829904000	0.282768000				
C	1.780884000	-3.829282000	-0.262212000				
H	1.702137000	-4.899211000	-0.152769000				
C	2.838676000	-3.105816000	-0.738871000				
H	3.789789000	-3.476995000	-1.084147000				
C	3.291883000	-0.615795000	-0.967390000				
C	0.623489000	3.286518000	0.264314000				
C	-3.291971000	0.617266000	-0.966937000				
C	-0.623552000	-3.285857000	0.262450000				
C	4.687855000	-0.841983000	-1.431828000				
C	5.144568000	-0.193255000	-2.596263000				
H	4.455461000	0.439788000	-3.145260000				
C	6.457802000	-0.370094000	-3.043729000				
H	6.790379000	0.130769000	-3.947687000				
C	7.339546000	-1.194802000	-2.332542000				
H	8.358686000	-1.332764000	-2.680084000				
C	6.899539000	-1.837931000	-1.168266000				



<sup>5</sup>RC<sub>(HS)</sub>

Fe	0.000051000	-0.000489000	0.838231000	C	5.952398000	-4.099257000	0.363693000
O	-0.000061000	0.000000000	-0.820778000	H	6.406696000	-4.837762000	1.017231000
C	0.000293000	-0.001130000	3.139967000	C	4.787038000	-3.438778000	0.767080000
C	-0.622838000	0.265544000	5.346466000	H	4.343290000	-3.664919000	1.731672000
H	-1.275268000	0.540331000	6.156896000	C	2.509819000	4.248449000	1.364568000
C	0.623923000	-0.268756000	5.346211000	C	3.392598000	4.740140000	0.383418000
H	1.276536000	-0.543891000	6.156377000	H	3.533868000	4.176099000	-0.532674000
C	2.303232000	-0.967858000	3.645413000	C	4.068908000	5.950087000	0.572147000
H	2.725440000	-1.455704000	4.526968000	H	4.740858000	6.315987000	-0.198050000
H	2.192946000	-1.698838000	2.851193000	C	3.873976000	6.691885000	1.743271000
H	2.973835000	-0.172722000	3.316698000	H	4.399250000	7.630577000	1.888782000
C	-2.302583000	0.965270000	3.646361000	C	2.993554000	6.218139000	2.722902000
H	-2.724732000	1.452475000	4.528296000	H	2.835254000	6.787486000	3.633691000
H	-2.192522000	1.696770000	2.852590000	C	2.315777000	5.009219000	2.533652000
H	-2.973112000	0.170248000	3.317227000	H	1.634254000	4.642653000	3.294818000
N	-0.989487000	0.424781000	4.007557000	C	-4.183186000	2.471966000	-0.058010000
N	0.990264000	-0.427424000	4.007149000	C	-4.778470000	2.184995000	-1.302276000
N	1.999621000	0.500725000	0.869682000	H	-4.314337000	1.455767000	-1.958363000
N	-0.527572000	2.007915000	0.920882000	C	-5.942962000	2.847844000	-1.704034000
N	-1.999472000	-0.501745000	0.869728000	H	-6.383336000	2.619061000	-2.669532000
N	0.527711000	-2.008973000	0.919408000	C	-6.534358000	3.805441000	-0.871546000
C	3.040212000	-0.358983000	0.573516000	H	-7.438259000	4.318459000	-1.184828000
C	2.517150000	1.769412000	1.055945000	C	-5.952225000	4.098704000	0.367201000
C	0.363536000	3.058578000	1.009770000	H	-6.406341000	4.836887000	1.021228000
C	-1.760511000	2.513373000	0.539979000	C	-4.786811000	3.437952000	0.769986000
C	-3.040127000	0.358153000	0.574267000	H	-4.342843000	3.663560000	1.734601000
C	-2.516959000	-1.770566000	1.055173000	C	-2.509597000	-4.249825000	1.362074000
C	-0.363364000	-3.059704000	1.007836000	C	-3.392289000	-4.740929000	0.380552000
C	1.760612000	-2.514192000	0.538092000	H	-3.533505000	-4.176319000	-0.535198000
C	4.283703000	0.392512000	0.638221000	C	-4.068599000	-5.950995000	0.568490000
H	5.266776000	-0.020047000	0.475790000	H	-4.740485000	-6.316434000	-0.201982000
C	3.968247000	1.684183000	0.962345000	C	-3.873751000	-6.693502000	1.739181000
H	4.651235000	2.506201000	1.103433000	H	-4.399024000	-7.632290000	1.884082000
C	-0.351361000	4.292162000	0.715291000	C	-2.993417000	-6.220340000	2.719170000
H	0.090885000	5.275615000	0.700230000	H	-2.835190000	-6.790238000	3.629628000
C	-1.640128000	3.956285000	0.402441000	C	-2.315639000	-5.011295000	2.530712000
H	-2.432174000	4.619901000	0.094264000	H	-1.634183000	-4.645185000	3.292155000
C	-4.283590000	-0.393413000	0.638619000	C	-3.562303000	-0.659463000	-5.101012000
H	-5.266695000	0.019236000	0.476611000	C	-2.420684000	-1.366560000	-4.705493000
C	-3.968067000	-1.685313000	0.961759000	C	-1.264025000	-0.689331000	-4.296968000
H	-4.651002000	-2.507468000	1.102308000	C	-1.249171000	0.720705000	-4.294985000
C	0.351535000	-4.293116000	0.712596000	C	-2.391791000	1.423176000	-4.700715000
H	-0.090701000	-5.276567000	0.697035000	C	-3.548036000	0.740051000	-5.098724000
C	1.640243000	-3.957038000	0.399766000	C	-0.015790000	-1.421552000	-3.838509000
H	2.432275000	-4.620457000	0.091128000	C	0.014961000	1.425549000	-3.837053000
C	2.936941000	-1.752806000	0.359449000	C	1.263216000	0.693783000	-4.296230000
C	1.765244000	2.959949000	1.176212000	C	1.248359000	-0.716245000	-4.295669000
C	-2.936887000	1.752110000	0.361067000	C	2.390977000	-1.418315000	-4.702096000
C	-1.765035000	-2.961188000	1.174538000	H	2.373979000	-2.505091000	-4.709894000
C	4.183178000	-2.472393000	-0.060285000	C	3.547225000	-0.734796000	-5.099414000
C	4.778175000	-2.184739000	-1.304525000	C	3.561492000	0.664719000	-5.100300000
H	4.313845000	-1.455189000	-1.960118000	C	2.419874000	1.371423000	-4.704071000
C	5.942613000	-2.847314000	-1.706890000	H	-0.017099000	-1.445573000	-2.736047000
H	6.382781000	-2.618004000	-2.672357000	H	-4.451523000	-1.196877000	-5.416933000
C	6.534241000	-3.805315000	-0.875030000	H	-2.426013000	-2.453514000	-4.714928000
H	7.438104000	-4.318117000	-1.188777000	H	-2.374808000	2.509959000	-4.707411000

H	-4.424690000	1.296652000	-5.417236000
H	0.025776000	2.465118000	-4.184485000
H	4.423879000	-1.291079000	-5.418476000
H	4.450703000	1.202458000	-5.415693000
H	2.425222000	2.458385000	-4.712395000
H	-0.026543000	-2.460786000	-4.186984000
H	0.016247000	1.448443000	-2.734562000

<sup>3</sup>RC<sub>(15)</sub>

Fe	0.000476000	0.000699000	0.801932000
O	-0.000116000	-0.000596000	-0.861547000
C	0.001206000	0.002608000	3.085762000
C	-0.666298000	0.120807000	5.294734000
H	-1.364069000	0.238005000	6.105672000
C	0.670501000	-0.110949000	5.294439000
H	1.368895000	-0.226578000	6.105066000
C	2.464587000	-0.398987000	3.586770000
H	2.990190000	-0.794073000	4.459300000
H	2.525421000	-1.119209000	2.777166000
H	2.934415000	0.535889000	3.276042000
C	-2.461767000	0.405141000	3.587842000
H	-2.987005000	0.800755000	4.460342000
H	-2.523366000	1.124610000	2.777606000
H	-2.931408000	-0.530179000	3.278208000
N	-1.059532000	0.189510000	3.955019000
N	1.062649000	-0.182532000	3.954555000
N	1.743804000	0.963274000	0.829665000
N	-0.973623000	1.741044000	0.858014000
N	-1.742860000	-0.961799000	0.832431000
N	0.974614000	-1.739525000	0.860098000
C	2.968637000	0.421753000	0.482396000
C	1.952706000	2.300183000	1.125941000
C	-0.414872000	2.986626000	1.077634000
C	-2.282680000	1.945729000	0.441472000
C	-2.967935000	-0.420786000	0.485160000
C	-1.951555000	-2.298260000	1.130802000
C	0.415984000	-2.984783000	1.081814000
C	2.283367000	-1.944831000	0.442838000
C	3.989647000	1.443705000	0.606411000
H	5.039890000	1.292076000	0.414450000
C	3.374421000	2.583608000	1.042897000
H	3.832014000	3.534531000	1.262269000
C	-1.413989000	4.006984000	0.820587000
H	-1.245889000	5.068737000	0.904710000
C	-2.544637000	3.370833000	0.392253000
H	-3.471724000	3.818852000	0.073033000
C	-3.988849000	-1.442585000	0.611345000
H	-5.039222000	-1.291264000	0.419857000
C	-3.373323000	-2.581830000	1.049111000
H	-3.830762000	-3.532430000	1.270201000
C	1.414882000	-4.005530000	0.825444000
H	1.246804000	-5.067159000	0.911174000
C	2.545236000	-3.370009000	0.395414000
H	3.472090000	-3.818491000	0.076168000
C	3.227091000	-0.932576000	0.211562000
C	0.943424000	3.256878000	1.320256000
C	-3.226588000	0.933115000	0.212453000
C	-0.942137000	-3.254675000	1.325812000

C	4.595042000	-1.301943000	-0.272520000
C	5.024074000	-0.873575000	-1.543846000
H	4.348830000	-0.298082000	-2.168135000
C	6.299895000	-1.204269000	-2.012487000
H	6.608657000	-0.873448000	-2.999090000
C	7.169373000	-1.963004000	-1.220121000
H	8.159280000	-2.218332000	-1.585296000
C	6.754908000	-2.391370000	0.046509000
H	7.424913000	-2.975360000	0.670193000
C	5.478549000	-2.063580000	0.516232000
H	5.164795000	-2.390265000	1.502847000
C	1.322054000	4.666648000	1.655717000
C	2.070062000	5.463374000	0.767184000
H	2.375557000	5.048826000	-0.187852000
C	2.402090000	6.781948000	1.095936000
H	2.974342000	7.382608000	0.395708000
C	1.990352000	7.329572000	2.316689000
H	2.248369000	8.352848000	2.570718000
C	1.239089000	6.551246000	3.204963000
H	0.913887000	6.968427000	4.153083000
C	0.905907000	5.233172000	2.876050000
H	0.324659000	4.630200000	3.566565000
C	-4.594897000	1.301763000	-0.271165000
C	-5.024916000	0.871421000	-1.541487000
H	-4.350182000	0.294918000	-2.165389000
C	-6.301082000	1.201424000	-2.009677000
H	-6.610590000	0.869058000	-2.995527000
C	-7.169931000	1.961431000	-1.217845000
H	-8.160105000	2.216230000	-1.582668000
C	-6.754484000	2.391771000	0.047795000
H	-7.423993000	2.976761000	0.671075000
C	-5.477778000	2.064677000	0.517060000
H	-5.163270000	2.392897000	1.502924000
C	-1.320548000	-4.663961000	1.663538000
C	-2.069239000	-5.461911000	0.776676000
H	-2.375429000	-5.048688000	-0.178712000
C	-2.401068000	-6.780009000	1.107522000
H	-2.973858000	-7.381631000	0.408561000
C	-1.988448000	-7.325932000	2.328741000
H	-2.246312000	-8.348841000	2.584400000
C	-1.236515000	-6.546381000	3.215371000
H	-0.910630000	-6.962240000	4.163837000
C	-0.903534000	-5.228779000	2.884363000
H	-0.321758000	-4.624861000	3.573606000
C	-3.550362000	-0.674267000	-5.219434000
C	-2.413537000	-1.379173000	-4.803798000
C	-1.263156000	-0.698565000	-4.384391000
C	-1.250424000	0.711986000	-4.387600000
C	-2.387289000	1.411397000	-4.812389000

C	-3.536730000	0.725369000	-5.224657000
C	-0.014209000	-1.423295000	-3.914965000
C	0.009950000	1.415949000	-3.916969000
C	1.258605000	0.690561000	-4.386135000
C	1.245878000	-0.719992000	-4.387343000
C	2.382489000	-1.420001000	-4.811830000
H	2.367607000	-2.506709000	-4.819569000
C	3.531687000	-0.734555000	-5.225731000
C	3.545323000	0.665087000	-5.222480000
C	2.408740000	1.370577000	-4.807174000
H	-0.012431000	-1.427817000	-2.812339000
H	-4.433557000	-1.214353000	-5.547860000
H	-2.417855000	-2.466127000	-4.808715000
H	-2.372410000	2.498092000	-4.821665000
H	-4.409298000	1.280260000	-5.556584000
H	0.018913000	2.459732000	-4.251182000
H	4.404071000	-1.289908000	-5.557368000
H	4.428323000	1.204709000	-5.552189000
H	2.413053000	2.457523000	-4.813606000
H	-0.023380000	-2.467543000	-4.247718000
H	0.008866000	1.421980000	-2.814351000

<sup>1</sup>RC<sub>(LS)</sub>

Fe	0.774252000	-0.048337000	0.156863000	C	-2.541057000	-2.551214000	0.749591000
O	0.489342000	-0.015019000	-1.504929000	H	-3.109813000	-3.430289000	0.500636000
C	1.420501000	-0.043581000	2.201037000	C	2.095937000	-4.031917000	-0.435472000
C	1.995673000	-0.720126000	4.325671000	H	1.883983000	-5.079489000	-0.581237000
H	2.155650000	-1.428847000	5.119902000	C	3.312465000	-3.433405000	-0.250506000
C	2.147633000	0.628583000	4.279710000	H	4.282625000	-3.902671000	-0.231895000
H	2.460931000	1.336454000	5.027641000	C	4.655879000	1.336904000	-0.849766000
C	1.812833000	2.437270000	2.597193000	H	5.702100000	1.149858000	-1.033371000
H	2.358400000	2.993047000	3.365003000	C	3.931457000	2.456114000	-1.157785000
H	2.318497000	2.547033000	1.643665000	H	4.280883000	3.359296000	-1.631236000
H	0.797058000	2.828125000	2.517093000	C	1.517646000	3.145198000	-0.731007000
C	1.281155000	-2.521943000	2.758849000	C	-2.115047000	0.912886000	1.648251000
H	1.198969000	-3.060693000	3.707163000	C	-0.295221000	-3.233746000	-0.222693000
H	0.345093000	-2.603632000	2.215991000	C	4.042643000	-0.998092000	-0.117607000
H	2.086700000	-2.953874000	2.162244000	C	1.727618000	4.495334000	-1.320568000
N	1.552124000	-1.114062000	3.061571000	C	0.836173000	4.961064000	-2.306789000
N	1.795929000	1.025276000	2.987765000	H	0.029393000	4.311626000	-2.625916000
N	-0.137508000	1.688368000	0.402660000	C	0.994770000	6.230760000	-2.870787000
N	-0.830586000	-1.002633000	0.710117000	H	0.303557000	6.570658000	-3.636039000
N	1.703501000	-1.787525000	-0.108512000	C	2.045503000	7.059371000	-2.454665000
N	2.479496000	0.931329000	-0.222320000	H	2.169407000	8.045273000	-2.891747000
C	0.288556000	2.900356000	-0.096550000	C	2.934158000	6.609438000	-1.469363000
C	-1.288926000	1.922149000	1.127526000	H	3.744438000	7.249962000	-1.134495000
C	-1.933459000	-0.445379000	1.335628000	C	2.775759000	5.338707000	-0.905607000
C	-1.174073000	-2.304667000	0.349848000	H	3.454882000	4.996706000	-0.131783000
C	1.088899000	-2.993002000	-0.327079000	C	-3.316565000	1.272073000	2.450971000
C	3.068275000	-2.007718000	-0.108911000	C	-4.290871000	2.169920000	1.972636000
C	3.731185000	0.363345000	-0.301984000	H	-4.167955000	2.607243000	0.989222000
C	2.567136000	2.213490000	-0.736925000	C	-5.422037000	2.467742000	2.740156000
C	-0.614443000	3.941597000	0.352995000	H	-6.167053000	3.155618000	2.351587000
H	-0.507710000	4.988494000	0.117932000	C	-5.602660000	1.872456000	3.995318000
C	-1.556059000	3.348158000	1.145852000	H	-6.481616000	2.104068000	4.588943000
H	-2.370282000	3.823023000	1.667269000	C	-4.644522000	0.970610000	4.477182000
C	-2.986089000	-1.435350000	1.399056000	H	-4.777114000	0.502649000	5.447956000
H	-3.969530000	-1.255167000	1.801618000	C	-3.513474000	0.671842000	3.710726000

H	-2.769979000	-0.027888000	4.078632000
C	-0.795372000	-4.558364000	-0.675142000
C	-0.501144000	-4.982032000	-1.987401000
H	0.084494000	-4.329464000	-2.626220000
C	-0.972851000	-6.207181000	-2.467481000
H	-0.744863000	-6.511094000	-3.484476000
C	-1.744930000	-7.036057000	-1.641834000
H	-2.116470000	-7.985486000	-2.014527000
C	-2.026502000	-6.635273000	-0.329472000
H	-2.608966000	-7.279281000	0.322299000
C	-1.550305000	-5.411126000	0.151627000
H	-1.754887000	-5.113245000	1.173819000
C	5.487079000	-1.362976000	-0.095829000
C	6.052311000	-2.229934000	-1.050985000
H	5.418774000	-2.642283000	-1.828495000
C	7.416483000	-2.538210000	-1.015266000
H	7.837314000	-3.203118000	-1.763297000
C	8.240375000	-1.980778000	-0.028618000
H	9.298830000	-2.220377000	-0.002229000
C	7.692108000	-1.105630000	0.918319000
H	8.324596000	-0.665661000	1.683348000
C	6.328444000	-0.796735000	0.881964000
H	5.899017000	-0.116939000	1.611012000
C	-3.676143000	-3.581665000	-2.353944000
C	-2.850835000	-2.470328000	-2.534867000
C	-3.252632000	-1.187914000	-2.124505000
C	-4.516795000	-1.024120000	-1.531482000
C	-5.352871000	-2.140871000	-1.369353000
C	-4.940504000	-3.414837000	-1.769737000
C	-2.297284000	-0.030393000	-2.284928000
C	-4.960814000	0.324376000	-1.003839000
C	-4.190661000	1.506285000	-1.554828000
C	-2.909856000	1.338855000	-2.111132000
C	-2.185012000	2.472024000	-2.520387000
H	-1.182212000	2.326398000	-2.912026000
C	-2.727217000	3.753013000	-2.404432000
C	-4.017267000	3.918967000	-1.880926000
C	-4.737900000	2.798167000	-1.460804000
H	-1.454588000	-0.140515000	-1.577329000
H	-3.331026000	-4.566841000	-2.650016000
H	-1.864559000	-2.592707000	-2.972496000
H	-6.331261000	-2.003587000	-0.914467000
H	-5.596533000	-4.269234000	-1.630501000
H	-6.035695000	0.461292000	-1.188782000
H	-2.152574000	4.619913000	-2.715646000
H	-4.453941000	4.910125000	-1.801504000
H	-5.738187000	2.915943000	-1.049998000
H	-1.812286000	-0.088030000	-3.268182000
H	-4.846005000	0.324320000	0.093868000

<sup>5</sup>TS1<sub>(HS)</sub>

Fe	-0.683817000	-0.065614000	0.306243000
O	-0.384198000	0.085803000	-1.416566000
C	-1.172158000	-0.171795000	2.392357000
C	-1.767878000	0.391539000	4.541973000
H	-2.059816000	1.057148000	5.335728000
C	-1.558542000	-0.949026000	4.522824000
H	-1.625211000	-1.693052000	5.297598000

C	-0.889236000	-2.660620000	2.843937000
H	-1.231013000	-3.310237000	3.654563000
H	-1.414728000	-2.917126000	1.930080000
H	0.184191000	-2.792277000	2.700345000
C	-1.675893000	2.270002000	2.911631000
H	-1.726060000	2.831478000	3.848764000
H	-0.814175000	2.598481000	2.340284000

H	-2.585521000	2.441028000	2.333753000	C	-0.869596000	5.242413000	-1.652578000
N	-1.529834000	0.850990000	3.244796000	H	-1.268023000	4.511684000	-2.347843000
N	-1.199189000	-1.277898000	3.214068000	C	-0.802005000	6.593996000	-2.003902000
N	0.712236000	-1.539920000	0.505594000	H	-1.156495000	6.915826000	-2.978450000
N	0.734263000	1.369893000	0.771399000	C	-0.272232000	7.529478000	-1.104812000
N	-2.063867000	1.418316000	0.041754000	H	-0.217463000	8.578890000	-1.377255000
N	-2.135207000	-1.521165000	-0.039798000	C	0.181933000	7.102420000	0.149627000
C	0.553169000	-2.859114000	0.131993000	H	0.582927000	7.822250000	0.856799000
C	1.942143000	-1.403018000	1.123274000	C	0.110365000	5.750181000	0.501561000
C	2.002363000	1.102975000	1.229340000	H	0.450471000	5.422110000	1.477903000
C	0.672232000	2.699968000	0.401178000	C	-5.588251000	0.008173000	-0.232928000
C	-1.774601000	2.752646000	-0.135184000	C	-6.253773000	0.721167000	-1.249156000
C	-3.431222000	1.248472000	-0.028793000	H	-5.667412000	1.285435000	-1.965967000
C	-3.468411000	-1.252643000	-0.244658000	C	-7.648720000	0.686796000	-1.349653000
C	-1.876198000	-2.803195000	-0.481291000	H	-8.144568000	1.236887000	-2.143634000
C	1.724795000	-3.599435000	0.567418000	C	-8.403395000	-0.065783000	-0.440096000
H	1.872149000	-4.658303000	0.428152000	H	-9.485764000	-0.092644000	-0.519472000
C	2.556600000	-2.719019000	1.203686000	C	-7.752327000	-0.789985000	0.567208000
H	3.503254000	-2.938996000	1.668475000	H	-8.329210000	-1.379120000	1.273683000
C	2.777432000	2.333524000	1.178924000	C	-6.357547000	-0.755580000	0.666901000
H	3.817743000	2.417478000	1.450804000	H	-5.848507000	-1.318345000	1.442751000
C	1.974814000	3.299918000	0.636950000	C	1.854853000	3.792129000	-3.073846000
H	2.250125000	4.307303000	0.374358000	C	1.425853000	2.465702000	-3.105375000
C	-3.030097000	3.478465000	-0.251216000	C	2.251847000	1.424437000	-2.633959000
H	-3.116284000	4.547927000	-0.361755000	C	3.519142000	1.743022000	-2.098599000
C	-4.044327000	2.563770000	-0.152433000	C	3.947622000	3.077438000	-2.088793000
H	-5.104745000	2.756517000	-0.176875000	C	3.127977000	4.101543000	-2.570997000
C	-4.097066000	-2.437427000	-0.811748000	C	1.779513000	0.022507000	-2.696037000
H	-5.136367000	-2.509077000	-1.091868000	C	4.393727000	0.665006000	-1.496143000
C	-3.116511000	-3.376814000	-0.982010000	C	4.054229000	-0.742543000	-1.935620000
H	-3.214813000	-4.355195000	-1.424807000	C	2.780684000	-1.041573000	-2.473112000
C	-0.620549000	-3.445365000	-0.398191000	C	2.494695000	-2.371288000	-2.844958000
C	2.531845000	-0.179641000	1.515069000	H	1.514470000	-2.594292000	-3.257182000
C	-0.495381000	3.353224000	-0.046966000	C	3.442675000	-3.383371000	-2.694802000
C	-4.100203000	0.007324000	-0.117202000	C	4.709280000	-3.081876000	-2.174075000
C	-0.537145000	-4.876369000	-0.806832000	C	5.006044000	-1.765570000	-1.807358000
C	0.449665000	-5.295819000	-1.720260000	H	0.791330000	-0.042465000	-1.861149000
H	1.134103000	-4.557460000	-2.117650000	H	1.203686000	4.583803000	-3.427297000
C	0.548469000	-6.637174000	-2.102249000	H	0.439535000	2.212552000	-3.482104000
H	1.312129000	-6.940036000	-2.812546000	H	4.930962000	3.310953000	-1.687581000
C	-0.337024000	-7.587197000	-1.576107000	H	3.472071000	5.131276000	-2.552000000
H	-0.261479000	-8.628661000	-1.872991000	H	5.450951000	0.875869000	-1.709832000
C	-1.318867000	-7.184479000	-0.661286000	H	3.204499000	-4.400882000	-2.990099000
H	-2.002513000	-7.915485000	-0.240201000	H	5.458645000	-3.860328000	-2.068466000
C	-1.416539000	-5.842571000	-0.278689000	H	5.992783000	-1.517841000	-1.423030000
H	-2.170077000	-5.533275000	0.437818000	H	1.150612000	-0.172060000	-3.572332000
C	3.864305000	-0.202157000	2.185217000	H	4.296380000	0.719032000	-0.400025000
C	4.971453000	-0.873870000	1.629954000				
H	4.852704000	-1.393353000	0.687097000				
C	6.214806000	-0.852967000	2.270517000				
H	7.057655000	-1.371065000	1.822622000				
C	6.378274000	-0.157930000	3.475759000				
H	7.344038000	-0.141889000	3.971338000				
C	5.287250000	0.521005000	4.034517000				
H	5.403660000	1.063559000	4.967828000				
C	4.044199000	0.500349000	3.394162000				
H	3.197939000	1.027360000	3.822403000				
C	-0.409353000	4.798403000	-0.396600000				

<sup>3</sup>TS1<sub>(IS)</sub>

Fe	-0.702839000	-0.004018000	0.195515000	C	-1.990582000	-6.946514000	-0.972722000
O	-0.335471000	0.089008000	-1.531411000	H	-2.707758000	-7.634974000	-0.535990000
C	-1.240331000	-0.076680000	2.256193000	C	-1.958903000	-5.614543000	-0.546041000
C	-1.771046000	0.527298000	4.413766000	H	-2.645400000	-5.270914000	0.220603000
H	-1.978143000	1.213051000	5.217168000	C	3.603636000	-0.659678000	2.409697000
C	-1.742612000	-0.829047000	4.373591000	C	4.692846000	-1.425418000	1.948416000
H	-1.912717000	-1.569338000	5.136209000	H	4.626097000	-1.907476000	0.980457000
C	-1.289512000	-2.584990000	2.661971000	C	5.858024000	-1.541461000	2.713844000
H	-1.751842000	-3.201503000	3.438106000	H	6.689594000	-2.130814000	2.339046000
H	-1.803533000	-2.744882000	1.719888000	C	5.960084000	-0.891924000	3.950826000
H	-0.238527000	-2.860077000	2.555472000	H	6.865335000	-0.982777000	4.543094000
C	-1.428581000	2.399851000	2.803623000	C	4.887756000	-0.118912000	4.415571000
H	-1.409306000	2.956221000	3.745001000	H	4.957932000	0.390324000	5.371994000
H	-0.532577000	2.623742000	2.233854000	C	3.722404000	-0.002998000	3.651243000
H	-2.309076000	2.689364000	2.227018000	H	2.889997000	0.595317000	4.007127000
N	-1.464401000	0.970762000	3.124480000	C	0.138212000	4.722102000	-0.606164000
N	-1.422676000	-1.181759000	3.059899000	C	-0.250227000	5.155455000	-1.890007000
N	0.483337000	-1.571649000	0.421054000	H	-0.714394000	4.440919000	-2.561233000
N	0.801115000	1.190876000	0.665347000	C	-0.025685000	6.472870000	-2.300187000
N	-1.882384000	1.570594000	-0.058067000	H	-0.325432000	6.785952000	-3.295713000
N	-2.233763000	-1.205780000	-0.211641000	C	0.590719000	7.384699000	-1.432431000
C	0.225103000	-2.848492000	-0.039864000	H	0.769139000	8.407026000	-1.750963000
C	1.675484000	-1.617609000	1.121490000	C	0.967787000	6.970546000	-0.148588000
C	1.981061000	0.821064000	1.275236000	H	1.430897000	7.674821000	0.535866000
C	0.923624000	2.523545000	0.299096000	C	0.737907000	5.653059000	0.262729000
C	-1.452026000	2.861145000	-0.273789000	H	1.013276000	5.340188000	1.263888000
C	-3.264321000	1.589191000	-0.049897000	C	-5.561929000	0.594760000	-0.076663000
C	-3.561580000	-0.843688000	-0.287437000	C	-6.237395000	1.380905000	-1.030275000
C	-2.134451000	-2.505195000	-0.678907000	H	-5.661774000	1.891944000	-1.794109000
C	1.282768000	-3.732333000	0.405425000	C	-7.632491000	1.483851000	-1.011372000
H	1.330293000	-4.787833000	0.191740000	H	-8.137339000	2.088980000	-1.758219000
C	2.148213000	-2.987939000	1.156407000	C	-8.377589000	0.797258000	-0.043707000
H	3.035507000	-3.328096000	1.663251000	H	-9.460192000	0.876666000	-0.030774000
C	2.871889000	1.963209000	1.314621000	C	-7.717976000	0.000869000	0.901657000
H	3.875904000	1.944103000	1.707360000	H	-8.288295000	-0.537978000	1.652207000
C	2.243482000	2.990315000	0.670136000	C	-6.323078000	-0.101544000	0.882719000
H	2.648873000	3.957230000	0.427303000	H	-5.807670000	-0.719887000	1.610698000
C	-2.605356000	3.737291000	-0.352336000	C	2.639776000	3.710196000	-2.830477000
H	-2.556262000	4.806194000	-0.487200000	C	2.010394000	2.468998000	-2.921548000
C	-3.717688000	2.962481000	-0.168207000	C	2.631647000	1.300271000	-2.436014000
H	-4.746867000	3.281631000	-0.139063000	C	3.899130000	1.405839000	-1.822164000
C	-4.332096000	-1.957051000	-0.807839000	C	4.533390000	2.654079000	-1.755177000
H	-5.395300000	-1.934878000	-0.987344000	C	3.915701000	3.804144000	-2.254265000
C	-3.449933000	-2.963150000	-1.084865000	C	1.959341000	-0.011946000	-2.586775000
H	-3.660223000	-3.923618000	-1.526871000	C	4.553025000	0.195494000	-1.193585000
C	-0.970493000	-3.288032000	-0.633932000	C	4.038332000	-1.132624000	-1.702881000
C	2.357230000	-0.492278000	1.612033000	C	2.778444000	-1.219969000	-2.339156000
C	-0.120180000	3.311838000	-0.208525000	C	2.330212000	-2.480420000	-2.783214000
C	-4.079324000	0.447705000	-0.086880000	H	1.361340000	-2.539729000	-3.271156000
C	-1.033969000	-4.704783000	-1.094465000	C	3.105168000	-3.627051000	-2.608807000
C	-0.135286000	-5.168466000	-2.073043000	C	4.357978000	-3.535467000	-1.986484000
H	0.581409000	-4.473349000	-2.489389000	C	4.815302000	-2.290314000	-1.545177000
C	-0.165367000	-6.500036000	-2.499781000	H	0.885364000	-0.003842000	-1.861126000
H	0.531881000	-6.837705000	-3.260785000	H	2.140468000	4.600545000	-3.195645000
C	-1.094487000	-7.394333000	-1.952342000	H	1.020585000	2.384277000	-3.360347000
H	-1.118895000	-8.428041000	-2.282980000	H	5.516799000	2.719700000	-1.295609000

H	4.418046000	4.764946000	-2.192690000
H	5.643007000	0.246336000	-1.324680000
H	2.742794000	-4.588673000	-2.959168000
H	4.973609000	-4.420570000	-1.858631000
H	5.795759000	-2.203790000	-1.082345000
H	1.395066000	-0.082111000	-3.524392000
H	4.382091000	0.241853000	-0.106330000

<sup>1</sup>TS1<sub>(LS)</sub>

Fe	-0.665413000	0.016091000	0.234210000	C	-1.296111000	-4.674774000	-1.047182000
O	-0.382413000	0.014277000	-1.495053000	C	-0.408391000	-5.188528000	-2.010543000
C	-1.306150000	-0.006516000	2.244579000	H	0.357705000	-4.535056000	-2.406425000
C	-1.920748000	0.647683000	4.367923000	C	-0.512713000	-6.513153000	-2.446552000
H	-2.132900000	1.351422000	5.154306000	H	0.177621000	-6.890345000	-3.195318000
C	-1.961486000	-0.708930000	4.340062000	C	-1.507381000	-7.350102000	-1.923953000
H	-2.209862000	-1.430525000	5.099159000	H	-1.589943000	-8.378458000	-2.261881000
C	-1.488192000	-2.506532000	2.684783000	C	-2.393834000	-6.852016000	-0.959858000
H	-1.974658000	-3.093026000	3.469401000	H	-3.161669000	-7.496483000	-0.542536000
H	-1.993777000	-2.676546000	1.740407000	C	-2.287773000	-5.526980000	-0.523660000
H	-0.443519000	-2.809763000	2.598169000	H	-2.967019000	-5.144699000	0.230944000
C	-1.366302000	2.481941000	2.779743000	C	3.595582000	-0.909135000	2.399105000
H	-1.327481000	3.034699000	3.722900000	C	4.626907000	-1.720275000	1.885020000
H	-0.440282000	2.633661000	2.235191000	H	4.498825000	-2.180546000	0.912166000
H	-2.205561000	2.840845000	2.181378000	C	5.809806000	-1.913383000	2.606560000
N	-1.520037000	1.060170000	3.095993000	H	6.595916000	-2.537708000	2.192273000
N	-1.587921000	-1.092264000	3.050640000	C	5.987028000	-1.296495000	3.851758000
N	0.392080000	-1.633151000	0.475528000	H	6.905639000	-1.446627000	4.410478000
N	0.874021000	1.119752000	0.708707000	C	4.972622000	-0.479862000	4.369153000
N	-1.745248000	1.672867000	-0.070528000	H	5.101718000	0.003508000	5.332849000
N	-2.280021000	-1.110552000	-0.184155000	C	3.789651000	-0.287021000	3.648483000
C	0.060080000	-2.896334000	0.020864000	H	3.002375000	0.346126000	4.044530000
C	1.583820000	-1.747565000	1.166399000	C	0.456192000	4.702905000	-0.546728000
C	2.034000000	0.673034000	1.316933000	C	0.096972000	5.188320000	-1.820657000
C	1.083061000	2.450510000	0.354371000	H	-0.407349000	4.518348000	-2.508485000
C	-1.247732000	2.934440000	-0.280601000	C	0.397211000	6.499586000	-2.200353000
C	-3.124936000	1.765686000	-0.088061000	H	0.117029000	6.852157000	-3.188401000
C	-3.575877000	-0.655061000	-0.288202000	C	1.063905000	7.354508000	-1.311946000
C	-2.265390000	-2.413125000	-0.643028000	H	1.301398000	8.371922000	-1.606790000
C	1.064645000	-3.840546000	0.468865000	C	1.413088000	6.889865000	-0.037709000
H	1.044723000	-4.899344000	0.266546000	H	1.913709000	7.550409000	0.663744000
C	1.976742000	-3.144112000	1.209509000	C	1.105410000	5.579147000	0.343579000
H	2.844630000	-3.531650000	1.716641000	H	1.356419000	5.230388000	1.339135000
C	2.992333000	1.757849000	1.362353000	C	-5.476346000	0.913871000	-0.128570000
H	3.993747000	1.673656000	1.753319000	C	-6.092076000	1.716049000	-1.108618000
C	2.429395000	2.826921000	0.726378000	H	-5.477842000	2.171973000	-1.877270000
H	2.896047000	3.766800000	0.487139000	C	-7.478140000	1.906102000	-1.107427000
C	-2.348645000	3.874805000	-0.387984000	H	-7.937282000	2.522322000	-1.874448000
H	-2.239760000	4.939274000	-0.521794000	C	-8.273437000	1.293118000	-0.130333000
C	-3.503734000	3.161648000	-0.224533000	H	-9.348982000	1.440586000	-0.130679000
H	-4.514626000	3.535896000	-0.217491000	C	-7.673664000	0.481930000	0.841985000
C	-4.415906000	-1.716527000	-0.813326000	H	-8.283378000	-0.000443000	1.599970000
H	-5.471219000	-1.620162000	-1.013876000	C	-6.287906000	0.291264000	0.839854000
C	-3.602169000	-2.784020000	-1.068684000	H	-5.818523000	-0.340056000	1.587559000
H	-3.871548000	-3.730535000	-1.508655000	C	2.852532000	3.645535000	-2.797042000
C	-1.152412000	-3.266506000	-0.581801000	C	2.125848000	2.459123000	-2.891770000
C	2.337366000	-0.661801000	1.640420000	C	2.655259000	1.243067000	-2.417578000
C	0.107417000	3.304805000	-0.176455000	C	3.930936000	1.241093000	-1.814326000
C	-4.005215000	0.673468000	-0.118567000	C	4.661761000	2.435656000	-1.739470000

C	4.133964000	3.633695000	-2.225840000
C	1.881179000	-0.017169000	-2.585469000
C	4.502738000	-0.026191000	-1.221709000
C	3.900426000	-1.299538000	-1.770166000
C	2.633550000	-1.288759000	-2.393131000
C	2.102196000	-2.498894000	-2.879925000
H	1.122126000	-2.483536000	-3.347818000
C	2.812950000	-3.694228000	-2.764904000
C	4.074279000	-3.701609000	-2.153059000
C	4.608613000	-2.506996000	-1.664817000
H	0.898149000	-0.011829000	-1.862747000
H	2.424328000	4.574773000	-3.154334000
H	1.130315000	2.457242000	-3.325544000
H	5.650373000	2.418926000	-1.287225000
H	4.710681000	4.551360000	-2.160022000
H	5.592918000	-0.043578000	-1.357418000
H	2.395747000	-4.617080000	-3.155441000
H	4.637408000	-4.626068000	-2.069800000
H	5.595480000	-2.497931000	-1.208198000
H	1.323013000	-0.021522000	-3.529154000
H	4.338294000	-0.002766000	-0.133644000

<sup>6</sup>Int1<sub>(HS)</sub>

Fe	0.014361000	0.016516000	-0.472226000	H	3.961379000	-3.438044000	-0.985069000
C	-0.024282000	-0.038687000	2.002059000	C	3.885352000	1.883992000	-0.320982000
C	0.644098000	-0.045873000	4.214158000	H	4.961786000	1.834156000	-0.366751000
H	1.352369000	-0.037797000	5.025167000	C	3.109900000	2.974117000	-0.024050000
C	-0.714889000	-0.066758000	4.207074000	H	3.444127000	3.972449000	0.208595000
H	-1.431420000	-0.087517000	5.010567000	C	-1.862917000	3.884970000	-0.428510000
C	-2.504183000	-0.084614000	2.450917000	H	-1.792481000	4.961148000	-0.434763000
H	-3.126534000	0.124469000	3.325769000	C	-2.957229000	3.116360000	-0.716360000
H	-2.668885000	0.679689000	1.695709000	H	-3.941720000	3.454453000	-0.997510000
H	-2.770356000	-1.060395000	2.039254000	C	-3.390912000	0.597897000	-0.743330000
C	2.451808000	0.011276000	2.478556000	C	-0.581461000	-3.379137000	-0.014814000
H	3.065308000	-0.216142000	3.355108000	C	3.402656000	-0.581488000	-0.719046000
H	2.629557000	-0.732453000	1.706477000	C	0.589731000	3.387708000	0.016841000
H	2.716733000	0.998319000	2.093534000	C	-4.840204000	0.827446000	-1.007218000
N	1.044356000	-0.030913000	2.874165000	C	-5.469309000	0.200827000	-2.101219000
N	-1.101239000	-0.059747000	2.862973000	H	-4.876061000	-0.429630000	-2.755112000
N	-1.684516000	-1.185523000	-0.406064000	C	-6.832348000	0.392818000	-2.348977000
N	1.217523000	-1.675955000	-0.288153000	H	-7.298306000	-0.092215000	-3.201219000
N	1.695473000	1.193211000	-0.348132000	C	-7.592906000	1.213510000	-1.505642000
N	-1.207120000	1.685698000	-0.277210000	H	-8.650696000	1.363297000	-1.698105000
C	-2.981998000	-0.746370000	-0.569403000	C	-6.980422000	1.838715000	-0.411528000
C	-1.712924000	-2.539709000	-0.129269000	H	-7.564587000	2.469075000	0.252041000
C	0.762339000	-2.972712000	-0.187752000	C	-5.617383000	1.645735000	-0.163726000
C	2.564311000	-1.711658000	-0.599497000	H	-5.144274000	2.120842000	0.689196000
C	2.991529000	0.757476000	-0.524892000	C	-0.810140000	-4.834606000	0.221561000
C	1.721148000	2.548060000	-0.083834000	C	-1.615248000	-5.603600000	-0.641425000
C	-0.751977000	2.981317000	-0.170201000	H	-2.076770000	-5.122714000	-1.497166000
C	-2.551557000	1.724232000	-0.603080000	C	-1.806179000	-6.970295000	-0.411941000
C	-3.876799000	-1.870498000	-0.360284000	H	-2.424357000	-7.548998000	-1.091466000
H	-4.953499000	-1.817899000	-0.397187000	C	-1.192491000	-7.593868000	0.682490000
C	-3.101831000	-2.962056000	-0.063827000	H	-1.340262000	-8.654652000	0.859611000
H	-3.437907000	-3.958109000	0.176101000	C	-0.383083000	-6.841551000	1.543869000
C	1.877161000	-3.874071000	-0.438017000	H	0.095992000	-7.317138000	2.394267000
H	1.809307000	-4.950468000	-0.446620000	C	-0.192528000	-5.475104000	1.314033000
C	2.973206000	-3.102478000	-0.713894000	H	0.432515000	-4.888290000	1.979086000



C	4.850667000	-0.805039000	-0.994866000
C	5.465198000	-0.171374000	-2.093027000
H	4.861525000	0.458719000	-2.737642000
C	6.826220000	-0.358372000	-2.355597000
H	7.281768000	0.131864000	-3.210483000
C	7.598066000	-1.180411000	-1.523802000
H	8.654303000	-1.325913000	-1.727930000
C	6.999268000	-1.812728000	-0.426190000
H	7.592446000	-2.444330000	0.228184000
C	5.638163000	-1.625215000	-0.163340000
H	5.175313000	-2.105967000	0.692184000
C	0.817321000	4.844793000	0.245256000
C	1.617775000	5.608407000	-0.626604000
H	2.074069000	5.121891000	-1.481913000
C	1.808205000	6.976725000	-0.406292000
H	2.422525000	7.551858000	-1.092303000
C	1.198718000	7.606507000	0.686993000
H	1.346237000	8.668556000	0.856787000
C	0.393435000	6.859158000	1.556500000
H	-0.082726000	7.339856000	2.405696000
C	0.203088000	5.491039000	1.335918000
H	-0.419269000	4.908021000	2.006946000
O	0.025650000	0.006784000	-2.353579000
H	-0.472060000	-0.649950000	-2.878324000

<sup>4</sup>Int1<sub>(IS)</sub>

Fe	0.008388000	0.005818000	-0.478681000
C	-0.019098000	-0.028088000	2.008125000
C	0.650100000	0.016917000	4.218561000
H	1.357184000	0.037745000	5.030646000
C	-0.710490000	0.014589000	4.211674000
H	-1.425873000	0.025031000	5.016656000
C	-2.492914000	-0.039916000	2.432472000
H	-3.130028000	0.210586000	3.285582000
H	-2.636512000	0.691743000	1.640117000
H	-2.759872000	-1.030039000	2.054899000
C	2.451165000	0.006184000	2.458765000
H	3.075933000	-0.265877000	3.314543000
H	2.592716000	-0.715237000	1.657288000
H	2.735090000	0.998166000	2.098035000
N	1.049391000	-0.012149000	2.877300000
N	-1.096054000	-0.010743000	2.866416000
N	-1.612827000	-1.182762000	-0.416924000
N	1.202373000	-1.610345000	-0.345356000
N	1.620584000	1.178606000	-0.369500000
N	-1.191057000	1.609340000	-0.342570000
C	-2.918267000	-0.784675000	-0.631747000
C	-1.644883000	-2.522285000	-0.060960000
C	0.793631000	-2.915055000	-0.153676000
C	2.541976000	-1.649607000	-0.700803000
C	2.924276000	0.783744000	-0.594451000
C	1.650060000	2.519108000	-0.028362000
C	-0.784142000	2.913291000	-0.151687000
C	-2.526941000	1.649212000	-0.715376000
C	-3.803237000	-1.901448000	-0.379916000
H	-4.878618000	-1.859210000	-0.449537000
C	-3.024157000	-2.958177000	0.007941000
H	-3.347890000	-3.942376000	0.305486000

C	1.910404000	-3.806014000	-0.400606000
H	1.859675000	-4.881734000	-0.343774000
C	2.973482000	-3.030972000	-0.771374000
H	3.956833000	-3.356405000	-1.069659000
C	3.808597000	1.903714000	-0.348999000
H	4.883583000	1.863828000	-0.424756000
C	3.029092000	2.959388000	0.037324000
H	3.350290000	3.946477000	0.327717000
C	-1.896712000	3.805540000	-0.412708000
H	-1.844038000	4.881263000	-0.359211000
C	-2.955768000	3.031540000	-0.793660000
H	-3.934628000	3.357510000	-1.105653000
C	-3.354386000	0.529706000	-0.877170000
C	-0.520232000	-3.347415000	0.095829000
C	3.365790000	-0.525301000	-0.850782000
C	0.525792000	3.346425000	0.112026000
C	-4.792446000	0.721939000	-1.214665000
C	-5.345314000	0.059744000	-2.328414000
H	-4.700780000	-0.563944000	-2.938864000
C	-6.698153000	0.209741000	-2.650053000
H	-7.105464000	-0.301573000	-3.516813000
C	-7.523886000	1.021526000	-1.861121000
H	-8.573815000	1.138581000	-2.110797000
C	-6.987420000	1.679533000	-0.746555000
H	-7.623021000	2.302083000	-0.124170000
C	-5.634390000	1.529026000	-0.424875000
H	-5.220921000	2.027820000	0.445343000
C	-0.712398000	-4.784362000	0.441776000
C	-1.515672000	-5.633850000	-0.343622000
H	-2.005783000	-5.229988000	-1.222926000
C	-1.667169000	-6.983709000	-0.008897000
H	-2.284687000	-7.625952000	-0.629345000

C	-1.014757000	-7.509205000	1.114210000
H	-1.132063000	-8.556959000	1.372799000
C	-0.205650000	-6.676152000	1.898134000
H	0.304093000	-7.075793000	2.769496000
C	-0.054375000	-5.326643000	1.563263000
H	0.570596000	-4.677038000	2.167311000
C	4.801971000	-0.709903000	-1.199772000
C	5.338575000	-0.043057000	-2.318770000
H	4.683293000	0.578356000	-2.920038000
C	6.688405000	-0.187237000	-2.655547000
H	7.083976000	0.327551000	-3.525678000
C	7.526222000	-0.997158000	-1.877370000
H	8.573826000	-1.109278000	-2.138936000
C	7.005275000	-1.659622000	-0.758087000
H	7.650581000	-2.280574000	-0.144108000
C	5.655223000	-1.515382000	-0.420949000
H	5.253663000	-2.017242000	0.453164000
C	0.716150000	4.786123000	0.447400000
C	1.517467000	5.629394000	-0.346493000
H	2.005221000	5.218175000	-1.223633000
C	1.667488000	6.982206000	-0.023086000
H	2.283188000	7.620090000	-0.649793000
C	1.015664000	7.516286000	1.096378000
H	1.131960000	8.566356000	1.346002000
C	0.208028000	6.689168000	1.888014000
H	-0.301669000	7.095733000	2.756232000
C	0.057949000	5.336661000	1.564492000
H	-0.566297000	4.691632000	2.174314000
O	0.037955000	0.011378000	-2.396339000
H	-0.327893000	-0.768270000	-2.862080000

<sup>2</sup>Int1<sub>(LS)</sub>

Fe	0.005347000	0.002223000	-0.275196000	C	-0.213007000	2.994093000	-0.008715000
C	-0.000711000	-0.011220000	1.832575000	C	-2.118308000	2.086791000	-0.714611000
C	0.652058000	-0.165298000	4.034140000	C	-4.067572000	-1.151734000	-0.469100000
H	1.347680000	-0.309545000	4.842733000	H	-5.106543000	-0.910420000	-0.629525000
C	-0.678978000	0.099937000	4.029066000	C	-3.537916000	-2.320267000	0.008227000
H	-1.383912000	0.228703000	4.832190000	H	-4.067170000	-3.213487000	0.298316000
C	-2.453263000	0.450806000	2.311573000	C	1.131753000	-4.084060000	-0.312510000
H	-2.978618000	0.825046000	3.194800000	H	0.887411000	-5.131229000	-0.228308000
H	-2.483194000	1.200942000	1.528233000	C	2.289711000	-3.522079000	-0.775668000
H	-2.936194000	-0.463195000	1.960608000	H	3.171446000	-4.028470000	-1.133647000
C	2.446418000	-0.485200000	2.331786000	C	4.070282000	1.162155000	-0.451416000
H	2.962470000	-0.866541000	3.217479000	H	5.108010000	0.925982000	-0.626588000
H	2.486185000	-1.228821000	1.542482000	C	3.540903000	2.326154000	0.031886000
H	2.932381000	0.431846000	1.993317000	H	4.066829000	3.223801000	0.313994000
N	1.050687000	-0.230961000	2.696415000	C	-1.119538000	4.084126000	-0.315156000
N	-1.061857000	0.191906000	2.688374000	H	-0.868213000	5.129939000	-0.235945000
N	-1.782979000	-0.860615000	-0.343068000	C	-2.273513000	3.527027000	-0.789580000
N	0.844260000	-1.795782000	-0.265237000	H	-3.146550000	4.035759000	-1.165035000
N	1.790696000	0.856001000	-0.291811000	C	-3.125128000	1.139353000	-0.952882000
N	-0.846512000	1.794033000	-0.246020000	C	-1.154273000	-3.173448000	0.251485000
C	-2.967557000	-0.231217000	-0.674437000	C	3.130451000	-1.129562000	-0.937749000
C	-2.097613000	-2.157858000	0.031844000	C	1.153039000	3.167538000	0.278246000
C	0.214970000	-2.999763000	-0.023863000	C	-4.468635000	1.592723000	-1.408638000
C	2.126625000	-2.083588000	-0.712172000	C	-5.040261000	1.028923000	-2.566422000
C	2.968490000	0.236205000	-0.644934000	H	-4.474534000	0.287174000	-3.120367000
C	2.098815000	2.152749000	0.068791000	C	-6.309105000	1.423671000	-3.002637000

H	-6.730130000	0.984610000	-3.901900000
C	-7.032129000	2.386700000	-2.286370000
H	-8.016661000	2.693987000	-2.625088000
C	-6.478442000	2.948366000	-1.128422000
H	-7.037122000	3.686692000	-0.561195000
C	-5.209672000	2.552554000	-0.691950000
H	-4.787148000	2.976437000	0.212840000
C	-1.604275000	-4.537157000	0.644874000
C	-2.554740000	-5.256102000	-0.106200000
H	-2.969527000	-4.805414000	-1.001041000
C	-2.943266000	-6.543878000	0.278173000
H	-3.672323000	-7.085701000	-0.316588000
C	-2.383464000	-7.139934000	1.415864000
H	-2.684543000	-8.139879000	1.712356000
C	-1.426625000	-6.440919000	2.163457000
H	-0.984814000	-6.896868000	3.044282000
C	-1.039291000	-5.153079000	1.779516000
H	-0.298026000	-4.608022000	2.354977000
C	4.472770000	-1.574143000	-1.405892000
C	5.025253000	-1.005152000	-2.570407000
H	4.446302000	-0.267120000	-3.115611000
C	6.291736000	-1.390901000	-3.021531000
H	6.699184000	-0.948015000	-3.925160000
C	7.030324000	-2.348812000	-2.314148000
H	8.013203000	-2.648393000	-2.664486000
C	6.494978000	-2.915092000	-1.149852000
H	7.066128000	-3.649190000	-0.589544000
C	5.228411000	-2.528861000	-0.698234000
H	4.819962000	-2.955899000	0.211651000
C	1.600580000	4.534598000	0.664250000
C	2.541619000	5.254214000	-0.097664000
H	2.949380000	4.801544000	-0.994667000
C	2.927360000	6.545134000	0.279029000
H	3.648852000	7.088190000	-0.323758000
C	2.374300000	7.142732000	1.419285000
H	2.673437000	8.145074000	1.709712000
C	1.426352000	6.442685000	2.177095000
H	0.989387000	6.900228000	3.059538000
C	1.041191000	5.151891000	1.800569000
H	0.306054000	4.606170000	2.383329000
O	0.064462000	0.056530000	-2.112721000
H	-0.450505000	-0.698807000	-2.471506000

<sup>7</sup>TS2<sub>(HS)</sub>

Fe	0.658711000	-0.043458000	0.232681000	H	2.287266000	-2.811786000	2.210372000
O	0.275671000	-0.056505000	-1.747854000	N	1.483466000	-1.176884000	3.281254000
C	1.238160000	-0.091585000	2.474321000	N	1.413770000	0.973262000	3.325590000
C	1.802076000	-0.797353000	4.587837000	N	-0.494083000	1.622723000	0.465852000
H	2.027689000	-1.518534000	5.354598000	N	-0.947070000	-1.242896000	0.677683000
C	1.755543000	0.561974000	4.616374000	N	1.804680000	-1.737292000	-0.127821000
H	1.925553000	1.263862000	5.414725000	N	2.327611000	1.136055000	-0.090311000
C	1.250206000	2.382431000	2.960665000	C	-0.102075000	2.923605000	0.176660000
H	1.632978000	2.996225000	3.780518000	C	-1.736204000	1.669841000	1.079257000
H	1.815478000	2.587960000	2.054525000	C	-2.160948000	-0.800380000	1.162984000
H	0.197688000	2.614947000	2.788439000	C	-1.072357000	-2.595195000	0.370045000
C	1.437029000	-2.577033000	2.853745000	C	1.312430000	-3.026271000	-0.259887000
H	1.464022000	-3.209247000	3.745430000	C	3.188250000	-1.793942000	-0.174328000
H	0.514011000	-2.755199000	2.307292000	C	3.612593000	0.674874000	-0.296861000

C	2.287200000	2.480089000	-0.440581000	H	7.872813000	-2.513093000	-2.204433000
C	-1.128463000	3.820403000	0.646213000	C	8.312786000	-1.276985000	-0.488465000
H	-1.091030000	4.895322000	0.573295000	H	9.386519000	-1.423186000	-0.553087000
C	-2.115354000	3.057345000	1.224606000	C	7.770574000	-0.464759000	0.516313000
H	-3.013917000	3.412743000	1.700602000	H	8.423542000	0.019097000	1.236427000
C	-3.080230000	-1.921623000	1.188685000	C	6.387021000	-0.277426000	0.598206000
H	-4.114522000	-1.861647000	1.483885000	H	5.963392000	0.351343000	1.374693000
C	-2.421603000	-3.008965000	0.681479000	C	-3.214255000	-3.496876000	-2.616397000
H	-2.831814000	-3.984168000	0.483901000	C	-2.433285000	-2.408563000	-3.000849000
C	2.430903000	-3.932669000	-0.369868000	C	-2.800469000	-1.088714000	-2.670052000
H	2.348557000	-5.004747000	-0.460585000	C	-3.995273000	-0.881811000	-1.896162000
C	3.581829000	-3.183762000	-0.281870000	C	-4.786237000	-2.008363000	-1.531966000
H	4.598017000	-3.543655000	-0.299414000	C	-4.410151000	-3.292183000	-1.892870000
C	4.424518000	1.777311000	-0.781479000	C	-1.975849000	0.057751000	-3.053030000
H	5.466091000	1.701031000	-1.050992000	C	-4.382980000	0.438392000	-1.558108000
C	3.607793000	2.871440000	-0.894482000	C	-3.690327000	1.579468000	-2.032867000
H	3.869267000	3.848040000	-1.269421000	C	-2.510793000	1.401113000	-2.838337000
C	1.165005000	3.323143000	-0.311483000	C	-1.877613000	2.541611000	-3.371200000
C	-2.512560000	0.540814000	1.443306000	H	-0.989287000	2.405497000	-3.981493000
C	-0.038635000	-3.419829000	-0.108681000	C	-2.373457000	3.822151000	-3.130707000
C	4.047466000	-0.669417000	-0.221160000	C	-3.521812000	4.003957000	-2.328857000
C	1.339382000	4.771811000	-0.618819000	C	-4.166481000	2.900840000	-1.791707000
C	0.462413000	5.412174000	-1.515593000	H	-0.871510000	0.007576000	-2.294559000
H	-0.325940000	4.829230000	-1.976448000	H	-2.902318000	-4.503978000	-2.875014000
C	0.605024000	6.773052000	-1.803453000	H	-1.519337000	-2.568890000	-3.567298000
H	-0.076253000	7.249241000	-2.502387000	H	-5.696156000	-1.837438000	-0.962545000
C	1.624291000	7.519910000	-1.197530000	H	-5.022111000	-4.142545000	-1.607281000
H	1.734765000	8.576532000	-1.421149000	H	-5.282053000	0.580443000	-0.964977000
C	2.498066000	6.895464000	-0.297664000	H	-1.883460000	4.683497000	-3.575408000
H	3.283943000	7.468969000	0.184570000	H	-3.903192000	5.003693000	-2.145294000
C	2.355430000	5.534021000	-0.009226000	H	-5.072109000	3.026909000	-1.204090000
H	3.024980000	5.051516000	0.695131000	H	-1.455272000	-0.066549000	-4.010878000
C	-3.811150000	0.759890000	2.142116000	H	0.891764000	-0.615286000	-2.259941000
C	-4.800369000	1.621901000	1.629277000				
H	-4.610625000	2.132889000	0.695068000				
C	-6.013353000	1.802722000	2.300667000				
H	-6.764753000	2.466711000	1.883482000				
C	-6.266338000	1.122177000	3.499490000				
H	-7.209090000	1.261443000	4.019470000				
C	-5.293705000	0.258783000	4.019705000				
H	-5.477998000	-0.272001000	4.948969000				
C	-4.079227000	0.081150000	3.348683000				
H	-3.323962000	-0.585357000	3.752059000				
C	-0.362692000	-4.838143000	-0.433327000				
C	-0.104753000	-5.329389000	-1.728090000				
H	0.325247000	-4.658801000	-2.464429000				
C	-0.408912000	-6.652245000	-2.065330000				
H	-0.210395000	-7.011987000	-3.070301000				
C	-0.973087000	-7.509399000	-1.110792000				
H	-1.210850000	-8.535964000	-1.371602000				
C	-1.225414000	-7.034922000	0.182882000				
H	-1.653077000	-7.695856000	0.930656000				
C	-0.920277000	-5.711417000	0.519290000				
H	-1.110319000	-5.344512000	1.522387000				
C	5.516865000	-0.900228000	-0.319381000				
C	6.076676000	-1.705368000	-1.331515000				
H	5.418876000	-2.168107000	-2.059187000				
C	7.460229000	-1.894302000	-1.413312000				

<sup>5</sup>TS2<sub>(HS)</sub>

Fe	0.737432000	0.012779000	0.397202000	C	1.873102000	7.087893000	-0.449284000
O	0.208302000	-0.030509000	-1.482452000	H	2.610229000	7.760759000	-0.021442000
C	1.285967000	0.040827000	2.502339000	C	1.878646000	5.735217000	-0.092346000
C	1.886455000	-0.617294000	4.622864000	H	2.614905000	5.358875000	0.610095000
H	2.156638000	-1.319558000	5.392671000	C	-3.857729000	0.452043000	2.139982000
C	1.745480000	0.734083000	4.646687000	C	-4.881600000	1.191580000	1.516832000
H	1.863843000	1.449359000	5.442382000	H	-4.669003000	1.692360000	0.581504000
C	1.139190000	2.518378000	3.000304000	C	-6.157460000	1.265041000	2.085220000
H	1.523180000	3.145434000	3.809830000	H	-6.935506000	1.836804000	1.587641000
H	1.663964000	2.752351000	2.078209000	C	-6.436566000	0.596466000	3.284697000
H	0.071931000	2.704225000	2.866882000	H	-7.427502000	0.653058000	3.724689000
C	1.673574000	-2.427158000	2.907278000	C	-5.428679000	-0.148744000	3.910558000
H	1.758591000	-3.040232000	3.808797000	H	-5.635106000	-0.670211000	4.840382000
H	0.766076000	-2.690681000	2.371476000	C	-4.152498000	-0.221438000	3.342117000
H	2.538176000	-2.599916000	2.263917000	H	-3.370380000	-0.800348000	3.822385000
N	1.605757000	-1.022772000	3.315658000	C	0.065937000	-4.827249000	-0.387943000
N	1.382479000	1.118308000	3.353449000	C	0.421059000	-5.283286000	-1.673601000
N	-0.554489000	1.580420000	0.612164000	H	0.847366000	-4.576616000	-2.377703000
N	-0.796586000	-1.343078000	0.840045000	C	0.216759000	-6.616390000	-2.043724000
N	1.973129000	-1.563992000	-0.052486000	H	0.490550000	-6.947324000	-3.040984000
N	2.286953000	1.349923000	-0.035185000	C	-0.345283000	-7.521264000	-1.132907000
C	-0.296475000	2.891673000	0.271768000	H	-0.506378000	-8.555790000	-1.419658000
C	-1.805579000	1.517390000	1.195258000	C	-0.694155000	-7.083163000	0.151296000
C	-2.053668000	-0.982128000	1.263236000	H	-1.120119000	-7.780312000	0.866495000
C	-0.832798000	-2.670715000	0.463748000	C	-0.487609000	-5.749767000	0.520729000
C	1.585425000	-2.885294000	-0.172761000	H	-0.752369000	-5.411363000	1.516715000
C	3.354623000	-1.503434000	-0.151949000	C	5.595699000	-0.441435000	-0.426891000
C	3.587958000	0.992310000	-0.306475000	C	6.156631000	-1.205485000	-1.469262000
C	2.114920000	2.670862000	-0.399075000	H	5.495562000	-1.719228000	-2.158741000
C	-1.420524000	3.707400000	0.708302000	C	7.543876000	-1.289822000	-1.628240000
H	-1.486585000	4.777965000	0.599059000	H	7.957514000	-1.878318000	-2.441588000
C	-2.328480000	2.873332000	1.298739000	C	8.397086000	-0.607375000	-0.751089000
H	-3.269833000	3.146308000	1.746453000	H	9.473588000	-0.672498000	-0.875272000
C	-2.919615000	-2.150033000	1.194623000	C	7.852007000	0.164984000	0.283085000
H	-3.970947000	-2.153130000	1.432487000	H	8.505726000	0.699021000	0.966050000
C	-2.177943000	-3.177095000	0.681403000	C	6.464843000	0.249047000	0.441184000
H	-2.522895000	-4.161922000	0.417339000	H	6.038527000	0.848309000	1.239098000
C	2.779041000	-3.701314000	-0.310305000	C	-2.667602000	-3.729548000	-2.686584000
H	2.782390000	-4.776900000	-0.394940000	C	-2.040974000	-2.519313000	-2.975557000
C	3.861128000	-2.861880000	-0.263565000	C	-2.650210000	-1.287848000	-2.670053000
H	4.903375000	-3.134088000	-0.310000000	C	-3.930099000	-1.294212000	-2.020697000
C	4.285978000	2.150767000	-0.841940000	C	-4.555973000	-2.542738000	-1.741410000
H	5.316124000	2.157782000	-1.162454000	C	-3.941957000	-3.737776000	-2.075521000
C	3.376453000	3.172022000	-0.922110000	C	-1.967039000	-0.010086000	-2.950610000
H	3.536264000	4.161851000	-1.319225000	C	-4.563126000	-0.063850000	-1.712881000
C	0.913352000	3.401944000	-0.254805000	C	-4.008796000	1.187134000	-2.084047000
C	-2.496920000	0.333902000	1.539279000	C	-2.736825000	1.229906000	-2.748753000
C	0.273138000	-3.397335000	-0.025850000	C	-2.231876000	2.476288000	-3.166430000
C	4.119346000	-0.319499000	-0.249271000	H	-1.266241000	2.506310000	-3.663253000
C	0.928499000	4.844736000	-0.629892000	C	-2.945557000	3.653733000	-2.950653000
C	-0.032692000	5.348707000	-1.527819000	C	-4.193142000	3.618551000	-2.288257000
H	-0.769030000	4.666113000	-1.935117000	C	-4.713136000	2.407027000	-1.864306000
C	-0.039595000	6.700957000	-1.883193000	H	-0.993282000	0.032464000	-2.169337000
H	-0.785727000	7.070692000	-2.580550000	H	-2.170127000	-4.665838000	-2.917077000
C	0.914663000	7.576168000	-1.347160000	H	-1.058908000	-2.513731000	-3.441315000
H	0.910365000	8.626034000	-1.623554000	H	-5.528495000	-2.536503000	-1.256332000

H	-4.428728000	-4.683010000	-1.855108000
H	-5.527641000	-0.081429000	-1.212631000
H	-2.546155000	4.601603000	-3.298379000
H	-4.743971000	4.538876000	-2.120608000
H	-5.681100000	2.363786000	-1.371419000
H	-1.417645000	-0.017885000	-3.901342000
H	0.846478000	-0.581747000	-1.985552000

<sup>5</sup>TS2<sub>(IS)</sub>

Fe	-0.607732000	-0.121208000	0.156623000	C	-0.747810000	-4.800758000	-1.210590000
O	-0.302415000	-0.090840000	-1.849760000	C	0.273982000	-5.153195000	-2.116858000
C	-1.135244000	-0.226511000	2.461543000	H	1.001632000	-4.399221000	-2.396907000
C	-1.571829000	0.333757000	4.651228000	C	0.346845000	-6.446151000	-2.643763000
H	-1.753631000	0.999832000	5.477527000	H	1.135593000	-6.697707000	-3.346317000
C	-1.522334000	-1.024766000	4.585483000	C	-0.597196000	-7.412764000	-2.272046000
H	-1.643778000	-1.778532000	5.344761000	H	-0.541986000	-8.416470000	-2.681949000
C	-1.107846000	-2.721919000	2.771937000	C	-1.610229000	-7.077851000	-1.363799000
H	-1.551093000	-3.396761000	3.509809000	H	-2.336394000	-7.825588000	-1.059508000
H	-1.623510000	-2.828367000	1.820359000	C	-1.683372000	-5.784713000	-0.835161000
H	-0.051941000	-2.967520000	2.636227000	H	-2.455739000	-5.532816000	-0.116573000
C	-1.333311000	2.220471000	2.998691000	C	3.673480000	-0.628095000	2.434901000
H	-1.313766000	2.808874000	3.920190000	C	4.776939000	-1.449939000	2.131491000
H	-0.451613000	2.444368000	2.401885000	H	4.780187000	-2.001729000	1.201254000
H	-2.226491000	2.471337000	2.421945000	C	5.873116000	-1.524665000	2.997755000
N	-1.333281000	0.799902000	3.354021000	H	6.716646000	-2.158408000	2.740554000
N	-1.260440000	-1.345739000	3.249476000	C	5.893433000	-0.777381000	4.182123000
N	0.626277000	-1.651079000	0.375398000	H	6.746007000	-0.835685000	4.851665000
N	0.866721000	1.131832000	0.605143000	C	4.806562000	0.050434000	4.492963000
N	-1.852057000	1.431253000	-0.048977000	H	4.810743000	0.634210000	5.408531000
N	-2.116981000	-1.390431000	-0.181828000	C	3.710329000	0.124025000	3.628758000
C	0.385160000	-2.948083000	-0.041137000	H	2.865412000	0.760642000	3.869492000
C	1.809153000	-1.659844000	1.103047000	C	0.000537000	4.730641000	-0.328505000
C	2.082646000	0.782815000	1.167905000	C	-0.433850000	5.293422000	-1.544669000
C	0.923844000	2.490698000	0.310586000	H	-0.857779000	4.639495000	-2.297654000
C	-1.485514000	2.763030000	-0.138569000	C	-0.289226000	6.661222000	-1.793562000
C	-3.241033000	1.384564000	0.040203000	H	-0.620056000	7.074321000	-2.741669000
C	-3.454377000	-1.055932000	-0.273920000	C	0.290920000	7.495637000	-0.828283000
C	-1.974340000	-2.673259000	-0.696492000	H	0.407590000	8.557335000	-1.022470000
C	1.437267000	-3.802945000	0.460744000	C	0.714153000	6.951310000	0.390933000
H	1.491488000	-4.867165000	0.296569000	H	1.151481000	7.592331000	1.150474000
C	2.276343000	-3.024469000	1.210352000	C	0.564182000	5.582692000	0.640480000
H	3.143585000	-3.343449000	1.763121000	H	0.877583000	5.165907000	1.591577000
C	2.931118000	1.946516000	1.213949000	C	-5.497987000	0.308170000	0.018862000
H	3.943514000	1.949494000	1.584180000	C	-6.223771000	1.150421000	-0.846666000
C	2.229819000	2.988962000	0.661327000	H	-5.685538000	1.747557000	-1.574557000
H	2.570958000	3.994280000	0.488097000	C	-7.620532000	1.202835000	-0.788574000
C	-2.677516000	3.580944000	-0.081240000	H	-8.162933000	1.853335000	-1.467896000
H	-2.679615000	4.659112000	-0.107666000	C	-8.318874000	0.408544000	0.130164000
C	-3.747250000	2.739524000	0.075254000	H	-9.402785000	0.448805000	0.173716000
H	-4.784635000	3.009101000	0.190791000	C	-7.609847000	-0.444459000	0.986533000
C	-4.178819000	-2.162872000	-0.849022000	H	-8.143094000	-1.066181000	1.699255000
H	-5.238416000	-2.163276000	-1.050473000	C	-6.213717000	-0.496056000	0.928737000
C	-3.262148000	-3.141126000	-1.145872000	H	-5.660804000	-1.156620000	1.588644000
H	-3.443468000	-4.086175000	-1.631285000	C	1.642047000	3.782491000	-3.682726000
C	-0.781287000	-3.419371000	-0.660989000	C	1.430484000	2.413351000	-3.846131000
C	2.476751000	-0.514190000	1.556396000	C	2.217029000	1.467163000	-3.162591000
C	-0.176793000	3.271902000	-0.087384000	C	3.262072000	1.933714000	-2.295975000
C	-4.012821000	0.218114000	-0.030529000	C	3.456339000	3.335925000	-2.145142000

C	2.658342000	4.247150000	-2.821732000
C	1.917787000	0.031170000	-3.232703000
C	4.084148000	0.990297000	-1.630187000
C	3.948009000	-0.409226000	-1.826753000
C	2.890062000	-0.905979000	-2.661482000
C	2.779328000	-2.295776000	-2.859314000
H	1.972525000	-2.666031000	-3.486261000
C	3.675064000	-3.186187000	-2.267264000
C	4.726179000	-2.700828000	-1.460953000
C	4.858992000	-1.335190000	-1.248930000
H	0.867197000	-0.063607000	-2.499782000
H	1.020613000	4.495763000	-4.215361000
H	0.644619000	2.057253000	-4.507764000
H	4.248211000	3.678517000	-1.485200000
H	2.803488000	5.313632000	-2.682829000
H	4.886188000	1.352093000	-0.993049000
H	3.564913000	-4.254488000	-2.428931000
H	5.430201000	-3.394927000	-1.010870000
H	5.665325000	-0.947838000	-0.632698000
H	1.498172000	-0.294684000	-4.192022000
H	-0.987656000	0.419145000	-2.324628000

<sup>3</sup>TS2<sub>(IS)</sub>

Fe	-0.534837000	-0.247745000	0.527147000
O	-0.085412000	0.143248000	-1.313629000
C	-1.062268000	-0.684419000	2.561685000
C	-1.543931000	-0.470602000	4.803634000
H	-1.685787000	0.053359000	5.732660000
C	-1.659092000	-1.785855000	4.493911000
H	-1.913242000	-2.636846000	5.101325000
C	-1.377162000	-3.215600000	2.473452000
H	-1.937683000	-3.907871000	3.105789000
H	-1.866389000	-3.139267000	1.508042000
H	-0.361482000	-3.590992000	2.339173000
C	-0.998482000	1.643551000	3.602219000
H	-0.880719000	1.987396000	4.632245000
H	-0.105817000	1.893485000	3.038259000
H	-1.862872000	2.136168000	3.154021000
N	-1.181220000	0.188809000	3.625898000
N	-1.366905000	-1.905277000	3.132284000
N	0.559072000	-1.901298000	0.398679000
N	1.075892000	0.741057000	1.133142000
N	-1.597918000	1.437136000	0.505866000
N	-2.141015000	-1.221423000	-0.133403000
C	0.219366000	-3.038160000	-0.316863000
C	1.771876000	-2.150843000	1.021714000
C	2.262946000	0.190514000	1.582282000
C	1.284095000	2.110910000	0.998743000
C	-1.072205000	2.722264000	0.571299000
C	-2.985098000	1.559152000	0.523808000
C	-3.449395000	-0.761681000	-0.150191000
C	-2.117742000	-2.420103000	-0.842543000
C	1.243484000	-4.046366000	-0.109065000
H	1.230532000	-5.036772000	-0.535785000
C	2.168500000	-3.520299000	0.749409000
H	3.054696000	-3.998286000	1.134290000
C	3.240233000	1.241979000	1.756026000
H	4.259423000	1.088546000	2.072550000

C	2.653039000	2.413063000	1.356303000
H	3.104252000	3.390750000	1.308377000
C	-2.163583000	3.671448000	0.659728000
H	-2.044567000	4.740781000	0.733586000
C	-3.331340000	2.958878000	0.676198000
H	-4.334158000	3.346027000	0.756882000
C	-4.274293000	-1.706137000	-0.867424000
H	-5.331368000	-1.591579000	-1.046929000
C	-3.450696000	-2.701707000	-1.325175000
H	-3.723172000	-3.544875000	-1.939079000
C	-0.999624000	-3.267084000	-0.976571000
C	2.551724000	-1.185931000	1.677431000
C	0.286143000	3.057463000	0.703874000
C	-3.883141000	0.510252000	0.279497000
C	-1.128767000	-4.520171000	-1.785462000
C	-0.315412000	-4.709021000	-2.920204000
H	0.384802000	-3.929268000	-3.201857000
C	-0.412043000	-5.875520000	-3.685693000
H	0.219269000	-5.998506000	-4.560190000
C	-1.321706000	-6.878133000	-3.329923000
H	-1.396988000	-7.783472000	-3.923899000
C	-2.132400000	-6.706512000	-2.201717000
H	-2.834587000	-7.482750000	-1.913266000
C	-2.036307000	-5.539560000	-1.436535000
H	-2.659046000	-5.418209000	-0.555987000
C	3.806615000	-1.589844000	2.384770000
C	4.898063000	-2.164097000	1.704682000
H	4.842644000	-2.288641000	0.628962000
C	6.056771000	-2.531185000	2.397593000
H	6.891103000	-2.965957000	1.855570000
C	6.149466000	-2.327140000	3.779362000
H	7.049907000	-2.611943000	4.314638000
C	5.076932000	-1.744597000	4.464702000
H	5.141280000	-1.577526000	5.535639000
C	3.918211000	-1.377226000	3.773141000

H	3.086139000	-0.927871000	4.306312000
C	0.655883000	4.506798000	0.627195000
C	0.489164000	5.212679000	-0.580083000
H	0.124458000	4.688307000	-1.456668000
C	0.817583000	6.570001000	-0.663472000
H	0.690580000	7.094754000	-1.605260000
C	1.313849000	7.247240000	0.456494000
H	1.567880000	8.300562000	0.390288000
C	1.481607000	6.557291000	1.662861000
H	1.860977000	7.075420000	2.538375000
C	1.155226000	5.199702000	1.747287000
H	1.279153000	4.671753000	2.687580000
C	-5.356175000	0.765389000	0.323845000
C	-5.974368000	1.701644000	-0.528513000
H	-5.369303000	2.247759000	-1.244628000
C	-7.355760000	1.915420000	-0.475495000
H	-7.813861000	2.636986000	-1.144909000
C	-8.147076000	1.195099000	0.426909000
H	-9.218918000	1.361530000	0.467056000
C	-7.547747000	0.254192000	1.272558000
H	-8.153811000	-0.310827000	1.974130000
C	-6.166897000	0.039753000	1.219177000
H	-5.703838000	-0.689130000	1.876823000
C	-0.249284000	3.029193000	-4.938843000
C	0.099065000	1.738397000	-4.545150000
C	1.282469000	1.485060000	-3.818129000
C	2.146069000	2.591405000	-3.497238000
C	1.762607000	3.900905000	-3.906850000
C	0.587220000	4.118360000	-4.611614000
C	1.608578000	0.157139000	-3.303433000
C	3.368735000	2.341461000	-2.821599000
C	3.819671000	1.029733000	-2.529609000
C	2.964646000	-0.091451000	-2.829073000
C	3.458642000	-1.395088000	-2.611497000
H	2.818447000	-2.242154000	-2.843229000
C	4.742576000	-1.610344000	-2.115570000
C	5.574368000	-0.513283000	-1.799029000
C	5.117226000	0.780034000	-1.996449000
H	0.811420000	0.106083000	-2.153003000
H	-1.161359000	3.196848000	-5.503803000
H	-0.544802000	0.900871000	-4.804041000
H	2.418143000	4.732887000	-3.662897000
H	0.315460000	5.122704000	-4.922941000
H	4.018173000	3.181805000	-2.588997000
H	5.107757000	-2.624690000	-1.981543000
H	6.572741000	-0.684456000	-1.407638000
H	5.755267000	1.628995000	-1.765305000
H	1.145280000	-0.675523000	-3.841232000
H	-0.816246000	0.665535000	-1.700194000

<sup>3</sup>TS2<sub>(LS)</sub>

Fe	-0.630051000	-0.104962000	0.241073000
O	-0.238438000	-0.027677000	-1.621287000
C	-1.089996000	-0.243352000	2.252525000
C	-1.586665000	0.293170000	4.428576000
H	-1.779841000	0.953781000	5.255845000
C	-1.562264000	-1.060958000	4.344682000
H	-1.722985000	-1.825194000	5.085069000

C	-1.146120000	-2.767686000	2.577778000
H	-1.612444000	-3.399019000	3.339218000
H	-1.666692000	-2.895325000	1.634610000
H	-0.098472000	-3.049376000	2.461319000
C	-1.281994000	2.218513000	2.877026000
H	-1.251119000	2.741828000	3.836544000
H	-0.399643000	2.472094000	2.299367000



H	-2.177198000	2.515313000	2.328078000	C	-0.370387000	5.234215000	-1.623133000
N	-1.299094000	0.778753000	3.150933000	H	-0.808174000	4.568342000	-2.357235000
N	-1.262625000	-1.374479000	3.017125000	C	-0.210888000	6.593625000	-1.905443000
N	0.611382000	-1.631640000	0.387703000	H	-0.542939000	6.987989000	-2.861139000
N	0.866071000	1.110016000	0.650918000	C	0.386160000	7.443437000	-0.964277000
N	-1.846819000	1.439264000	-0.008054000	H	0.515409000	8.498625000	-1.184374000
N	-2.126495000	-1.322187000	-0.199506000	C	0.808365000	6.922446000	0.265337000
C	0.380294000	-2.899949000	-0.107963000	H	1.257017000	7.575588000	1.007818000
C	1.783475000	-1.679068000	1.125092000	C	0.641863000	5.562311000	0.548512000
C	2.065974000	0.755768000	1.242486000	H	0.952053000	5.166720000	1.509444000
C	0.948453000	2.458194000	0.323218000	C	-5.504581000	0.360845000	0.120688000
C	-1.453201000	2.756869000	-0.169094000	C	-6.252840000	1.205604000	-0.723263000
C	-3.235620000	1.425760000	0.081319000	H	-5.734468000	1.804242000	-1.464029000
C	-3.469170000	-1.001423000	-0.244191000	C	-7.647785000	1.256945000	-0.630168000
C	-1.982427000	-2.589230000	-0.757768000	H	-8.207059000	1.910176000	-1.293072000
C	1.427599000	-3.784651000	0.365467000	C	-8.323138000	0.457674000	0.301203000
H	1.487448000	-4.837643000	0.142117000	H	-9.405668000	0.497112000	0.371772000
C	2.253502000	-3.049986000	1.168719000	C	-7.592580000	-0.400406000	1.134145000
H	3.117326000	-3.396825000	1.709889000	H	-8.107835000	-1.027773000	1.855194000
C	2.927850000	1.910464000	1.289879000	C	-6.198248000	-0.450166000	1.041834000
H	3.932454000	1.908100000	1.681064000	H	-5.629050000	-1.115589000	1.682941000
C	2.253149000	2.948436000	0.698473000	C	1.727830000	3.774174000	-3.629284000
H	2.615082000	3.942905000	0.506366000	C	1.464023000	2.412590000	-3.761927000
C	-2.631122000	3.601453000	-0.144035000	C	2.224399000	1.450962000	-3.066847000
H	-2.613654000	4.676718000	-0.224634000	C	3.294835000	1.897265000	-2.218178000
C	-3.715914000	2.791985000	0.060098000	C	3.534078000	3.295361000	-2.091341000
H	-4.747126000	3.088408000	0.163816000	C	2.764770000	4.219755000	-2.781267000
C	-4.197597000	-2.094627000	-0.836357000	C	1.892941000	0.028441000	-3.114225000
H	-5.261686000	-2.097569000	-1.013179000	C	4.098099000	0.938439000	-1.553837000
C	-3.278227000	-3.051611000	-1.191998000	C	3.935210000	-0.455868000	-1.754813000
H	-3.464596000	-3.981793000	-1.703554000	C	2.858880000	-0.927424000	-2.583315000
C	-0.788899000	-3.339602000	-0.748229000	C	2.740587000	-2.312069000	-2.816790000
C	2.444818000	-0.548809000	1.624026000	H	1.931226000	-2.658690000	-3.453477000
C	-0.135286000	3.243453000	-0.119694000	C	3.634758000	-3.221087000	-2.254702000
C	-4.021965000	0.268805000	0.036624000	C	4.693664000	-2.762125000	-1.441740000
C	-0.777595000	-4.716475000	-1.314740000	C	4.841065000	-1.403132000	-1.202119000
C	0.227513000	-5.079389000	-2.234259000	H	0.849635000	-0.030291000	-2.271228000
H	0.963724000	-4.336363000	-2.516678000	H	1.129851000	4.499036000	-4.172380000
C	0.278387000	-6.371176000	-2.767079000	H	0.661566000	2.072034000	-4.411936000
H	1.055846000	-6.629193000	-3.479854000	H	4.341063000	3.622841000	-1.441992000
C	-0.671774000	-7.328249000	-2.387022000	H	2.946408000	5.283181000	-2.663781000
H	-0.633909000	-8.330980000	-2.801276000	H	4.912416000	1.283920000	-0.923235000
C	-1.667526000	-6.984654000	-1.463162000	H	3.517725000	-4.284278000	-2.442774000
H	-2.397972000	-7.724847000	-1.150630000	H	5.394443000	-3.472172000	-1.012105000
C	-1.717780000	-5.692680000	-0.929196000	H	5.658436000	-1.035584000	-0.588226000
H	-2.477053000	-5.435023000	-0.198907000	H	1.386883000	-0.296938000	-4.029992000
C	3.631245000	-0.682950000	2.511804000	H	-0.993103000	0.322520000	-2.133135000
C	4.736263000	-1.500801000	2.202776000				
H	4.748614000	-2.033078000	1.261196000				
C	5.824336000	-1.593513000	3.077458000				
H	6.669188000	-2.223872000	2.816176000				
C	5.835724000	-0.867743000	4.275312000				
H	6.682111000	-0.940203000	4.951319000				
C	4.748749000	-0.041648000	4.590401000				
H	4.747182000	0.527468000	5.515216000				
C	3.660535000	0.049790000	3.717755000				
H	2.816411000	0.686919000	3.960372000				
C	0.064710000	4.693106000	-0.397319000				

<sup>5</sup>Int2<sub>(HS)</sub>

Fe	0.030837000	0.035075000	0.030466000	C	7.157112000	1.061767000	-0.328432000
O	0.010062000	0.078011000	-2.098178000	H	7.825761000	1.525885000	0.390335000
C	0.007209000	-0.106438000	2.007379000	C	5.788083000	0.979641000	-0.051555000
C	-0.630392000	-0.466955000	4.202973000	H	5.393099000	1.377944000	0.877436000
H	-1.310702000	-0.726309000	4.996132000	C	-0.381498000	4.956040000	0.129474000
C	0.676916000	-0.101522000	4.223224000	C	0.151600000	5.845925000	-0.822733000
H	1.368071000	0.028661000	5.038450000	H	0.683517000	5.444077000	-1.678468000
C	2.397535000	0.550915000	2.526988000	C	-0.009970000	7.228306000	-0.679188000
H	3.032148000	0.488198000	3.415566000	H	0.404031000	7.899088000	-1.425965000
H	2.795906000	-0.099542000	1.752030000	C	-0.713589000	7.745747000	0.416323000
H	2.381254000	1.578657000	2.158306000	H	-0.839739000	8.818326000	0.526986000
C	-2.380147000	-0.813190000	2.447358000	C	-1.258208000	6.870166000	1.364898000
H	-3.028795000	-0.782905000	3.327663000	H	-1.806715000	7.262435000	2.215957000
H	-2.731082000	-0.090083000	1.715155000	C	-1.095063000	5.488156000	1.220842000
H	-2.406305000	-1.813516000	2.009075000	H	-1.517188000	4.805965000	1.951680000
N	-1.023047000	-0.461703000	2.861685000	C	-4.903840000	-0.327067000	-0.971804000
N	1.050523000	0.113435000	2.893833000	C	-5.379700000	-1.093776000	-2.054444000
N	1.382480000	1.600825000	-0.223113000	H	-4.661765000	-1.586468000	-2.701757000
N	-1.587293000	1.377175000	-0.218256000	C	-6.751373000	-1.218678000	-2.297353000
N	-1.352711000	-1.543318000	-0.413801000	H	-7.097538000	-1.808721000	-3.140521000
N	1.587033000	-1.328197000	-0.281735000	C	-7.676072000	-0.579427000	-1.460906000
C	2.732598000	1.489674000	-0.483175000	H	-8.740822000	-0.675219000	-1.649486000
C	1.068923000	2.939511000	-0.095126000	C	-7.217414000	0.182705000	-0.378402000
C	-1.449700000	2.751819000	-0.166926000	H	-7.927016000	0.674217000	0.280303000
C	-2.897096000	1.087590000	-0.565221000	C	-5.845568000	0.305494000	-0.135382000
C	-2.722150000	-1.427249000	-0.567526000	H	-5.489645000	0.887831000	0.707849000
C	-1.053053000	-2.877004000	-0.182671000	C	0.376670000	-4.894449000	0.117017000
C	1.462630000	-2.698716000	-0.219366000	C	-0.218079000	-5.810943000	-0.772076000
C	2.901362000	-1.024404000	-0.571048000	H	-0.777336000	-5.432003000	-1.620802000
C	3.310446000	2.825166000	-0.478767000	C	-0.082463000	-7.189485000	-0.576297000
H	4.347764000	3.055672000	-0.663418000	H	-0.543441000	-7.880565000	-1.275555000
C	2.301141000	3.709687000	-0.202216000	C	0.654999000	-7.677989000	0.510179000
H	2.378292000	4.781475000	-0.115304000	H	0.760865000	-8.747783000	0.661551000
C	-2.740045000	3.358694000	-0.470930000	C	1.258697000	-6.777068000	1.397486000
H	-2.925928000	4.420068000	-0.522907000	H	1.831918000	-7.146813000	2.242307000
C	-3.617588000	2.343354000	-0.735456000	C	1.121658000	-5.398973000	1.201400000
H	-4.648153000	2.431865000	-1.041379000	H	1.587142000	-4.697573000	1.886036000
C	-3.317352000	-2.740516000	-0.396784000	H	-0.455941000	0.880299000	-2.403063000
H	-4.374626000	-2.952207000	-0.434577000	H	-0.517785000	-0.721500000	-2.300953000
C	-2.299406000	-3.623387000	-0.135499000				
H	-2.386979000	-4.679329000	0.065414000				
C	2.776661000	-3.295550000	-0.442559000				
H	2.980860000	-4.354701000	-0.458020000				
C	3.655074000	-2.271512000	-0.662831000				
H	4.711423000	-2.344167000	-0.869123000				
C	3.441283000	0.278425000	-0.671841000				
C	-0.240424000	3.474433000	-0.013749000				
C	-3.440261000	-0.211607000	-0.709793000				
C	0.251808000	-3.419893000	-0.079975000				
C	4.902951000	0.378047000	-0.966303000				
C	5.426025000	-0.144885000	-2.164314000				
H	4.747431000	-0.609063000	-2.872303000				
C	6.795036000	-0.065003000	-2.441476000				
H	7.180531000	-0.469093000	-3.372627000				
C	7.665475000	0.539607000	-1.524891000				
H	8.727685000	0.602255000	-1.740154000				

<sup>3</sup>Int2<sub>(IS)</sub>

Fe	-0.000169000	0.000273000	-0.259836000	C	4.994555000	-5.119512000	-1.152413000
O	0.000786000	0.000763000	-2.022936000	H	5.279553000	-5.988800000	-0.567172000
C	-0.001076000	-0.000039000	1.953663000	C	3.973575000	-4.280315000	-0.693265000
C	-0.570865000	0.369254000	4.145053000	H	3.481499000	-4.497284000	0.249239000
H	-1.167385000	0.751185000	4.954887000	C	3.183904000	3.661211000	0.638319000
C	0.567632000	-0.370676000	4.145125000	C	4.280959000	4.026559000	-0.167894000
H	1.163738000	-0.753084000	4.955041000	H	4.454311000	3.495858000	-1.097979000
C	2.107533000	-1.340059000	2.428459000	C	5.130623000	5.071848000	0.207353000
H	2.447512000	-1.899147000	3.303045000	H	5.965466000	5.341934000	-0.432291000
H	1.872301000	-2.034045000	1.627001000	C	4.901895000	5.776196000	1.395812000
H	2.897179000	-0.662518000	2.099776000	H	5.562514000	6.587116000	1.686375000
C	-2.109715000	1.339978000	2.428235000	C	3.813042000	5.429449000	2.203642000
H	-2.449618000	1.899131000	3.302812000	H	3.626524000	5.969663000	3.126941000
H	-1.874032000	2.033906000	1.626881000	C	2.963166000	4.383815000	1.827965000
H	-2.899565000	0.662761000	2.099360000	H	2.121800000	4.112899000	2.457745000
N	-0.906554000	0.590085000	2.806657000	C	-3.580575000	3.142129000	-1.427686000
N	0.904027000	-0.590644000	2.806765000	C	-4.266089000	2.865131000	-2.629230000
N	1.987678000	0.158127000	-0.362377000	H	-3.986037000	1.987049000	-3.202557000
N	-0.117988000	1.981298000	-0.266327000	C	-5.288462000	3.700533000	-3.087959000
N	-1.987751000	-0.157900000	-0.362472000	H	-5.795782000	3.468690000	-4.019699000
N	0.117779000	-1.980843000	-0.268289000	C	-5.655022000	4.835263000	-2.353597000
C	2.866946000	-0.876705000	-0.666901000	H	-6.448116000	5.485376000	-2.709556000
C	2.767636000	1.254772000	0.033638000	C	-4.993922000	5.119752000	-1.153500000
C	0.921292000	2.885005000	-0.007347000	H	-5.279191000	5.989101000	-0.568480000
C	-1.218119000	2.727573000	-0.700652000	C	-3.973209000	4.280549000	-0.693768000
C	-2.866673000	0.876847000	-0.667101000	H	-3.481571000	4.497577000	0.248955000
C	-2.767746000	-1.254688000	0.032691000	C	-3.183941000	-3.661062000	0.637629000
C	-0.921353000	-2.884826000	-0.008070000	C	-4.280525000	-4.027023000	-0.168926000
C	1.218364000	-2.727517000	-0.701424000	H	-4.453556000	-3.496803000	-1.099348000
C	4.208030000	-0.427908000	-0.452161000	C	-5.130206000	-5.072246000	0.206490000
H	5.092732000	-1.028734000	-0.591598000	H	-5.964713000	-5.342806000	-0.433391000
C	4.142710000	0.876291000	0.013958000	C	-4.901937000	-5.775885000	1.395452000
H	4.970453000	1.509465000	0.290155000	H	-5.562566000	-6.586749000	1.686148000
C	0.443637000	4.226667000	-0.272235000	C	-3.813559000	-5.428489000	2.203645000
H	1.040135000	5.119940000	-0.173124000	H	-3.627429000	-5.968138000	3.127351000
C	-0.833900000	4.129421000	-0.742178000	C	-2.963673000	-4.382917000	1.827806000
H	-1.466012000	4.931967000	-1.086250000	H	-2.122688000	-4.111472000	2.457866000
C	-4.208005000	0.427936000	-0.453297000	H	0.733623000	0.391694000	-2.526996000
H	-5.092619000	1.028792000	-0.593162000	H	-0.714289000	-0.417935000	-2.530006000
C	-4.142951000	-0.876352000	0.012372000				
H	-4.970780000	-1.509720000	0.287867000				
C	-0.443313000	-4.226428000	-0.271816000				
H	-1.039533000	-5.119798000	-0.171852000				
C	0.834315000	-4.129382000	-0.741742000				
H	1.466626000	-4.932209000	-1.084798000				
C	2.498068000	-2.226476000	-0.957220000				
C	2.251085000	2.559412000	0.250434000				
C	-2.497744000	2.226595000	-0.956847000				
C	-2.251162000	-2.559257000	0.249567000				
C	3.581229000	-3.141966000	-1.427457000				
C	4.267442000	-2.865034000	-2.628622000				
H	3.987904000	-1.986875000	-3.202108000				
C	5.290111000	-3.700393000	-3.086770000				
H	5.797975000	-3.468520000	-4.018206000				
C	5.656292000	-4.835089000	-2.352175000				
H	6.449600000	-5.485191000	-2.707667000				

<sup>1</sup>Int2<sub>(LS)</sub>

Fe	-0.014952000	0.004006000	-0.155042000	C	-6.858456000	1.991109000	-1.042948000
O	-0.001445000	0.007566000	-2.297886000	H	-7.510388000	2.643639000	-0.469963000
C	-0.002164000	-0.000583000	1.829641000	C	-5.540630000	1.783188000	-0.621700000
C	0.685444000	-0.044807000	4.033470000	H	-5.171042000	2.268007000	0.275606000
H	1.401577000	-0.083073000	4.836239000	C	-0.946134000	-4.733349000	0.592851000
C	-0.668803000	0.030881000	4.039980000	C	-1.778942000	-5.569592000	-0.175639000
H	-1.377434000	0.064858000	4.849562000	H	-2.256206000	-5.166304000	-1.062123000
C	-2.490670000	0.118377000	2.343214000	C	-1.976743000	-6.907075000	0.184367000
H	-3.053823000	0.419877000	3.231513000	H	-2.617914000	-7.538653000	-0.423135000
H	-2.635328000	0.853422000	1.558501000	C	-1.340738000	-7.434773000	1.315752000
H	-2.845612000	-0.855864000	2.000549000	H	-1.494229000	-8.472869000	1.593939000
C	2.491225000	-0.119268000	2.319122000	C	-0.500609000	-6.616169000	2.082018000
H	3.064323000	-0.416901000	3.202315000	H	-0.001605000	-7.017486000	2.958942000
H	2.632388000	-0.854709000	1.533971000	C	-0.303654000	-5.279077000	1.721772000
H	2.838559000	0.856067000	1.972062000	H	0.346974000	-4.640924000	2.310912000
N	1.078478000	-0.065767000	2.692786000	C	4.678804000	-0.936743000	-1.345631000
N	-1.074420000	0.059670000	2.703393000	C	5.200166000	-0.291361000	-2.484286000
N	-1.658593000	-1.096157000	-0.290627000	H	4.556202000	0.375731000	-3.048248000
N	1.080855000	-1.654805000	-0.293287000	C	6.523690000	-0.500534000	-2.885458000
N	1.645286000	1.103199000	-0.320624000	H	6.904875000	0.002033000	-3.769210000
N	-1.097487000	1.658721000	-0.262727000	C	7.353914000	-1.358215000	-2.151992000
C	-2.924675000	-0.649117000	-0.620524000	H	8.381151000	-1.521987000	-2.462441000
C	-1.780751000	-2.435866000	0.046540000	C	6.851057000	-1.999580000	-1.012376000
C	0.630565000	-2.944542000	-0.060156000	H	7.491153000	-2.656410000	-0.431097000
C	2.404067000	-1.765347000	-0.719075000	C	5.527560000	-1.788294000	-0.611481000
C	2.918922000	0.653968000	-0.641322000	H	5.142469000	-2.274267000	0.278512000
C	1.769750000	2.442746000	0.030215000	C	0.938311000	4.736030000	0.593105000
C	-0.644024000	2.945459000	-0.045082000	C	1.774107000	5.571799000	-0.172882000
C	-2.413205000	1.766862000	-0.696351000	H	2.250866000	5.169359000	-1.060014000
C	-3.879666000	-1.725731000	-0.434319000	C	1.973846000	6.908523000	0.188700000
H	-4.942845000	-1.639316000	-0.594765000	H	2.616767000	7.539646000	-0.417438000
C	-3.183177000	-2.811618000	0.019324000	C	1.336702000	7.436367000	1.319339000
H	-3.573300000	-3.780321000	0.286986000	H	1.491365000	8.473981000	1.598649000
C	1.693554000	-3.888541000	-0.347031000	C	0.493189000	6.618645000	2.082904000
H	1.598691000	-4.960336000	-0.269546000	H	-0.007275000	7.020230000	2.958858000
C	2.767042000	-3.168887000	-0.791067000	C	0.294323000	5.282395000	1.721046000
H	3.715943000	-3.546448000	-1.136575000	H	-0.359406000	4.645228000	2.307731000
C	3.870947000	1.728551000	-0.443155000	H	0.263172000	-0.905892000	-2.524605000
H	4.935590000	1.642578000	-0.593931000	H	0.728956000	0.627673000	-2.495908000
C	3.171390000	2.812871000	0.012795000				
H	3.562736000	3.777973000	0.291700000				
C	-1.705163000	3.892840000	-0.341375000				
H	-1.605782000	4.964985000	-0.276040000				
C	-2.777162000	3.171058000	-0.780785000				
H	-3.723881000	3.544871000	-1.136075000				
C	-3.277545000	0.682508000	-0.904482000				
C	-0.697238000	-3.310632000	0.224107000				
C	3.272318000	-0.679774000	-0.922450000				
C	0.687261000	3.314402000	0.223495000				
C	-4.678387000	0.936996000	-1.345565000				
C	-5.176792000	0.294542000	-2.495928000				
H	-4.517330000	-0.362539000	-3.053120000				
C	-6.494257000	0.501657000	-2.917482000				
H	-6.858853000	0.003267000	-3.810577000				
C	-7.339824000	1.352423000	-2.193236000				
H	-8.362506000	1.513838000	-2.519818000				

## Co-based species

 ${}^6_2(\text{HS})$ 

Co	-0.027279000	0.016008000	-0.254893000	H	8.594487000	-1.574138000	-1.753697000
O	0.066798000	0.080659000	-2.175445000	C	6.932324000	-2.004799000	-0.441165000
C	0.023608000	-0.018940000	2.021024000	H	7.511115000	-2.645862000	0.216867000
C	-0.652295000	-0.129947000	4.219761000	C	5.577751000	-1.779051000	-0.175216000
H	-1.362685000	-0.184633000	5.026886000	H	5.105405000	-2.240327000	0.685782000
C	0.707361000	-0.096148000	4.218239000	C	0.949570000	4.827603000	0.188548000
H	1.421300000	-0.108989000	5.023967000	C	1.754279000	5.549003000	-0.715222000
C	2.502102000	0.030579000	2.466285000	H	2.175759000	5.032474000	-1.570771000
H	3.128262000	-0.148220000	3.344695000	C	1.993086000	6.914212000	-0.525929000
H	2.690121000	-0.737235000	1.719637000	H	2.609616000	7.456270000	-1.236435000
H	2.737168000	1.008728000	2.042735000	C	1.428755000	7.583813000	0.567967000
C	-2.454209000	-0.100070000	2.470864000	H	1.613827000	8.643537000	0.713741000
H	-3.074295000	0.091022000	3.351134000	C	0.619525000	6.879354000	1.469102000
H	-2.621007000	0.677990000	1.730297000	H	0.177917000	7.391151000	2.318777000
H	-2.717129000	-1.068652000	2.040525000	C	0.380593000	5.514303000	1.279335000
N	-1.049380000	-0.078626000	2.880797000	H	-0.245627000	4.964465000	1.974299000
N	1.099144000	-0.029697000	2.878277000	C	-4.819943000	0.962520000	-0.993506000
N	1.703373000	1.139460000	-0.394266000	C	-5.444754000	0.374828000	-2.111462000
N	-1.186341000	1.725942000	-0.195982000	H	-4.854984000	-0.255116000	-2.768956000
N	-1.700445000	-1.129574000	-0.408259000	C	-6.798244000	0.605720000	-2.377630000
N	1.159929000	-1.712876000	-0.252277000	H	-7.261059000	0.150393000	-3.247795000
C	2.988907000	0.670140000	-0.564189000	C	-7.552889000	1.427994000	-1.530407000
C	1.769507000	2.498668000	-0.142135000	H	-8.603182000	1.608053000	-1.737563000
C	-0.689419000	3.010152000	-0.132196000	C	-6.944049000	2.016335000	-0.413973000
C	-2.522483000	1.802767000	-0.534242000	H	-7.523659000	2.648668000	0.251755000
C	-2.992700000	-0.654932000	-0.577435000	C	-5.590699000	1.784187000	-0.147409000
C	-1.775434000	-2.495229000	-0.170238000	H	-5.119853000	2.232020000	0.721518000
C	0.676789000	-2.997630000	-0.185318000	C	-0.953967000	-4.823932000	0.156631000
C	2.504298000	-1.784535000	-0.578396000	C	-1.758748000	-5.552849000	-0.740807000
C	3.912425000	1.770742000	-0.378956000	H	-2.184624000	-5.042402000	-1.597896000
H	4.987073000	1.690639000	-0.423005000	C	-1.992195000	-6.918053000	-0.543985000
C	3.166491000	2.886388000	-0.092435000	H	-2.609360000	-7.465760000	-1.249627000
C	3.529047000	3.875685000	0.136414000	C	-1.421444000	-7.580368000	0.550929000
H	-1.773741000	3.944804000	-0.401762000	H	-1.602049000	-8.640058000	0.702476000
H	-1.667903000	5.017553000	-0.436246000	C	-0.611214000	-6.868584000	1.445422000
C	-2.890801000	3.204519000	-0.669908000	H	-0.164137000	-7.374775000	2.295629000
H	-3.864705000	3.563811000	-0.961520000	C	-0.378296000	-5.503537000	1.248331000
C	-3.914761000	-1.758961000	-0.409256000	H	0.248869000	-4.948275000	1.938178000
H	-4.989232000	-1.677066000	-0.453994000				
C	-3.172627000	-2.878833000	-0.134112000				
H	-3.538785000	-3.870668000	0.077421000				
C	1.764390000	-3.929875000	-0.452822000				
H	1.662009000	-5.003036000	-0.486868000				
C	2.878568000	-3.185219000	-0.716811000				
H	3.855054000	-3.540433000	-1.004643000				
C	3.368368000	-0.683304000	-0.729561000				
C	0.667848000	3.375571000	-0.006838000				
C	-3.380671000	0.696927000	-0.711480000				
C	-0.678747000	-3.371633000	-0.044879000				
C	4.808230000	-0.946281000	-1.011401000				
C	5.435406000	-0.339701000	-2.117879000				
H	4.846705000	0.299953000	-2.766842000				
C	6.789884000	-0.564978000	-2.383814000				
H	7.254591000	-0.095556000	-3.245419000				
C	7.543291000	-1.398929000	-1.546967000				

<sup>4</sup>2<sub>(IS)</sub>

Co	-0.000020000	0.000369000	-0.233426000	C	-5.878715000	4.137742000	-0.850139000
O	0.000162000	0.000325000	-1.932304000	H	-6.269526000	4.964894000	-0.265231000
C	-0.000154000	-0.000090000	1.882395000	C	-4.690162000	3.512041000	-0.459802000
C	0.636011000	-0.235035000	4.079855000	H	-4.160327000	3.848142000	0.425266000
H	1.306485000	-0.479823000	4.885254000	C	-2.469538000	-4.222602000	0.394845000
C	-0.636980000	0.233582000	4.079801000	C	-3.486185000	-4.669345000	-0.471850000
H	-1.307695000	0.477913000	4.885139000	H	-3.738775000	-4.069413000	-1.339329000
C	-2.346675000	0.860371000	2.389482000	C	-4.148319000	-5.878368000	-0.233310000
H	-2.803601000	1.268997000	3.295047000	H	-4.924744000	-6.210155000	-0.915886000
H	-2.262010000	1.643564000	1.643620000	C	-3.802014000	-6.666324000	0.872382000
H	-2.965544000	0.048715000	2.005098000	H	-4.315491000	-7.605015000	1.056005000
C	2.346323000	-0.860537000	2.389680000	C	-2.783507000	-6.239544000	1.734525000
H	2.803280000	-1.269092000	3.295260000	H	-2.506105000	-6.845877000	2.591500000
H	2.262011000	-1.643678000	1.643725000	C	-2.121731000	-5.030668000	1.495373000
H	2.964958000	-0.048636000	2.005445000	H	-1.330179000	-4.698000000	2.159077000
N	1.010661000	-0.373782000	2.742213000	C	4.167557000	-2.432773000	-1.199320000
N	-1.011207000	0.373157000	2.742131000	C	4.872388000	-1.993408000	-2.337729000
N	-1.928535000	-0.499385000	-0.273370000	H	4.471952000	-1.164672000	-2.911900000
N	0.547707000	-2.029264000	-0.152352000	C	6.061160000	-2.618388000	-2.727720000
N	1.928717000	0.499232000	-0.273108000	H	6.586835000	-2.271150000	-3.611912000
N	-0.547659000	2.029384000	-0.152024000	C	6.568716000	-3.693373000	-1.985746000
C	-2.978159000	0.355490000	-0.559061000	H	7.491157000	-4.178881000	-2.288837000
C	-2.453027000	-1.753340000	0.000161000	C	5.879062000	-4.137537000	-0.849928000
C	-0.332836000	-3.074224000	-0.045259000	H	6.269984000	-4.964534000	-0.264877000
C	1.758105000	-2.532735000	-0.578884000	C	4.690470000	-3.511872000	-0.459653000
C	2.978337000	-0.355563000	-0.558914000	H	4.160723000	-3.847840000	0.425516000
C	2.453160000	1.753247000	0.000436000	C	2.469620000	4.222604000	0.395048000
C	0.332930000	3.074291000	-0.044931000	C	3.485691000	4.669813000	-0.472091000
C	-1.758059000	2.532807000	-0.578608000	H	3.737904000	4.070200000	-1.339896000
C	-4.219884000	-0.377796000	-0.402653000	C	4.147694000	5.878916000	-0.233595000
H	-5.203147000	0.046565000	-0.528722000	H	4.923665000	6.211056000	-0.916514000
C	-3.901582000	-1.653928000	-0.024846000	C	3.801812000	6.666515000	0.872482000
H	-4.581252000	-2.458825000	0.202969000	H	4.315180000	7.605274000	1.056068000
C	0.360588000	-4.313217000	-0.375162000	C	2.783831000	6.239314000	1.735035000
H	-0.094948000	-5.291121000	-0.387824000	H	2.506738000	6.845381000	2.592298000
C	1.637558000	-3.976142000	-0.732069000	C	2.122182000	5.030360000	1.495922000
H	2.416717000	-4.631596000	-1.087672000	H	1.331031000	4.697375000	2.159943000
C	4.220049000	0.377695000	-0.402279000				
H	5.203318000	-0.046678000	-0.528250000				
C	3.901725000	1.653780000	-0.024349000				
H	4.581404000	2.458600000	0.203687000				
C	-0.360514000	4.313273000	-0.374816000				
H	0.094995000	5.291189000	-0.387457000				
C	-1.637526000	3.976217000	-0.731647000				
H	-2.416706000	4.631703000	-1.087152000				
C	-2.909159000	1.749708000	-0.787176000				
C	-1.725187000	-2.953012000	0.149863000				
C	2.909301000	-1.749726000	-0.787260000				
C	1.725308000	2.952965000	0.150105000				
C	-4.167393000	2.432752000	-1.199287000				
C	-4.872304000	1.993246000	-2.337591000				
H	-4.471965000	1.164367000	-2.911624000				
C	-6.061037000	2.618261000	-2.727642000				
H	-6.586783000	2.270905000	-3.611746000				
C	-6.568463000	3.693428000	-1.985842000				
H	-7.490872000	4.178965000	-2.288982000				

<sup>2</sup><sub>2(LS)</sub>

Co	-0.000014000	-0.000037000	-0.245467000	C	6.543535000	-2.673443000	-1.413530000
O	-0.000102000	-0.000326000	-2.100013000	H	7.160422000	-3.400142000	-0.893560000
C	0.000087000	0.000263000	1.813073000	C	5.281145000	-2.345897000	-0.907376000
C	-0.667592000	0.123212000	4.009378000	H	4.922269000	-2.809659000	0.005260000
H	-1.369549000	0.248199000	4.815758000	C	1.418230000	4.531797000	0.798012000
C	0.667953000	-0.122218000	4.009347000	C	2.343702000	5.319469000	0.085890000
H	1.369980000	-0.247029000	4.815694000	H	2.782686000	4.924484000	-0.823530000
C	2.456647000	-0.429331000	2.293403000	C	2.673716000	6.605555000	0.526602000
H	2.982839000	-0.817820000	3.169913000	H	3.383783000	7.201784000	-0.038272000
H	2.499109000	-1.159422000	1.491768000	C	2.079539000	7.130189000	1.681962000
H	2.929080000	0.498826000	1.965195000	H	2.335739000	8.128757000	2.022051000
C	-2.456430000	0.429956000	2.293519000	C	1.145907000	6.362273000	2.390210000
H	-2.982531000	0.818710000	3.169968000	H	0.676776000	6.763277000	3.283534000
H	-2.498945000	1.159822000	1.491682000	C	0.816286000	5.076406000	1.949730000
H	-2.928916000	-0.498282000	1.965618000	H	0.093098000	4.477352000	2.493805000
N	-1.059561000	0.197309000	2.670184000	C	-4.467138000	1.401248000	-1.562521000
N	1.059807000	-0.196608000	2.670136000	C	-4.957122000	0.781560000	-2.729198000
N	1.732708000	0.900754000	-0.312668000	H	-4.332287000	0.052454000	-3.234106000
N	-0.901082000	1.740910000	-0.271177000	C	-6.219306000	1.109027000	-3.234844000
N	-1.732741000	-0.900853000	-0.312225000	H	-6.577727000	0.628461000	-4.139931000
N	0.901051000	-1.740990000	-0.270714000	C	-7.016231000	2.057627000	-2.580210000
C	2.925585000	0.334828000	-0.708320000	H	-7.995696000	2.312341000	-2.972960000
C	2.003665000	2.193764000	0.098977000	C	-6.543611000	2.673112000	-1.413742000
C	-0.325390000	2.955841000	0.026023000	H	-7.160399000	3.400035000	-0.893969000
C	-2.165076000	1.997726000	-0.778196000	C	-5.281169000	2.345702000	-0.907628000
C	-2.925658000	-0.335054000	-0.707944000	H	-4.922150000	2.809799000	0.004782000
C	-2.003661000	-2.193726000	0.099869000	C	-1.418146000	-4.531515000	0.799667000
C	0.325388000	-2.955821000	0.026955000	C	-2.343671000	-5.319451000	0.087909000
C	2.164993000	-1.997973000	-0.777775000	H	-2.782743000	-4.924795000	-0.821612000
C	3.994610000	1.289144000	-0.498197000	C	-2.673628000	-6.605385000	0.529110000
H	5.035790000	1.095384000	-0.702339000	H	-3.383737000	-7.201826000	-0.035487000
C	3.435481000	2.413795000	0.045737000	C	-2.079341000	-7.129597000	1.684604000
H	3.936320000	3.316354000	0.356117000	H	-2.335498000	-8.128046000	2.025074000
C	-1.262555000	4.018492000	-0.283328000	C	-1.145656000	-6.361416000	2.392495000
H	-1.055017000	5.070090000	-0.163032000	H	-0.676440000	-6.762094000	3.285920000
C	-2.373064000	3.431716000	-0.822501000	C	-0.816090000	-5.075702000	1.951525000
H	-3.251598000	3.916134000	-1.216568000	H	-0.092861000	-4.476442000	2.495317000
C	-3.994662000	-1.289307000	-0.497429000				
H	-5.035859000	-1.095617000	-0.701548000				
C	-3.435481000	-2.413777000	0.046826000				
H	-3.936289000	-3.316239000	0.357540000				
C	1.262518000	-4.018575000	-0.282142000				
H	1.054988000	-5.070133000	-0.161475000				
C	2.372959000	-3.431982000	-0.821653000				
H	3.251437000	-3.916536000	-1.215675000				
C	3.128953000	-1.016001000	-1.037761000				
C	1.026485000	3.168565000	0.347147000				
C	-3.129055000	1.015671000	-1.037783000				
C	-1.026454000	-3.168439000	0.348282000				
C	4.466985000	-1.401726000	-1.562520000				
C	4.956798000	-0.782452000	-2.729489000				
H	4.331869000	-0.053563000	-3.234593000				
C	6.218930000	-1.110055000	-3.235175000				
H	6.577214000	-0.629813000	-4.140489000				
C	7.015979000	-2.058376000	-2.580290000				
H	7.995405000	-2.313196000	-2.973070000				

<sup>6</sup>RC<sub>(HS)</sub>

Co	0.107883000	0.336327000	0.869087000	C	5.534515000	-4.386524000	1.546421000
O	-0.080716000	-0.054482000	-1.007506000	H	5.916826000	-4.936519000	2.400953000
C	0.185340000	0.968521000	3.181891000	C	4.456419000	-3.510349000	1.710811000
C	-0.300998000	1.839786000	5.263956000	H	4.007336000	-3.382274000	2.690831000
H	-0.893067000	2.354288000	6.001044000	C	3.107107000	4.205549000	-0.005348000
C	0.920085000	1.250581000	5.352899000	C	3.975639000	4.280338000	-1.112025000
H	1.602499000	1.159527000	6.180311000	H	3.981273000	3.472251000	-1.836166000
C	2.452009000	0.027474000	3.786727000	C	4.809386000	5.388763000	-1.293484000
H	2.932436000	-0.246983000	4.728647000	H	5.466925000	5.431157000	-2.156308000
H	2.239630000	-0.872996000	3.215894000	C	4.789903000	6.444009000	-0.373721000
H	3.124796000	0.666350000	3.211115000	H	5.437174000	7.303811000	-0.515238000
C	-2.027985000	2.152185000	3.470412000	C	3.926833000	6.385473000	0.726811000
H	-2.430131000	2.846800000	4.211354000	H	3.904840000	7.199402000	1.445009000
H	-1.898400000	2.670939000	2.523791000	C	3.091774000	5.278063000	0.907536000
H	-2.728378000	1.326217000	3.333288000	H	2.424873000	5.233454000	1.762769000
N	-0.731851000	1.662802000	3.945233000	C	-3.841906000	3.083136000	-0.486756000
N	1.199919000	0.725380000	4.087284000	C	-4.609732000	2.587874000	-1.560522000
N	2.101875000	0.557333000	0.538414000	H	-4.322369000	1.651481000	-2.028145000
N	-0.193499000	2.367902000	0.368949000	C	-5.720097000	3.296237000	-2.030519000
N	-1.944084000	0.077626000	0.870190000	H	-6.294678000	2.902584000	-2.863170000
N	0.388879000	-1.648809000	1.375923000	C	-6.087051000	4.509450000	-1.436061000
C	3.043713000	-0.467234000	0.546072000	H	-6.949364000	5.058181000	-1.801512000
C	2.783706000	1.759533000	0.363598000	C	-5.335284000	5.010540000	-0.366868000
C	0.808184000	3.276576000	0.112551000	H	-5.616667000	5.947266000	0.104498000
C	-1.391258000	2.934072000	-0.044784000	C	-4.223179000	4.304383000	0.103007000
C	-2.899766000	1.007226000	0.497906000	H	-3.648692000	4.693223000	0.937731000
C	-2.601092000	-1.038021000	1.366636000	C	-2.897699000	-3.362306000	2.223832000
C	-0.619625000	-2.543958000	1.688897000	C	-3.868700000	-3.916367000	1.366306000
C	1.549586000	-2.374619000	1.174467000	H	-3.960206000	-3.535654000	0.354269000
C	4.360471000	0.117481000	0.403217000	C	-4.695044000	-4.957960000	1.800617000
H	5.286907000	-0.434405000	0.399177000	H	-5.432689000	-5.376873000	1.123123000
C	4.204471000	1.476740000	0.316897000	C	-4.566873000	-5.465651000	3.099051000
H	4.984155000	2.215967000	0.228064000	H	-5.208975000	-6.273676000	3.435248000
C	0.219745000	4.488938000	-0.443216000	C	-3.602970000	-4.927262000	3.959561000
H	0.771866000	5.362086000	-0.752449000	H	-3.497116000	-5.314216000	4.968423000
C	-1.123012000	4.270411000	-0.559955000	C	-2.774737000	-3.887210000	3.525114000
H	-1.859620000	4.935965000	-0.980229000	H	-2.030110000	-3.468679000	4.194766000
C	-4.209499000	0.470159000	0.803588000	C	-4.017382000	-2.364636000	-4.184413000
H	-5.145337000	0.981687000	0.644986000	C	-2.837365000	-2.875852000	-3.631974000
C	-4.025801000	-0.771280000	1.358884000	C	-1.641570000	-2.147400000	-3.694338000
H	-4.788318000	-1.438146000	1.727683000	C	-1.628127000	-0.890290000	-4.332318000
C	-0.053305000	-3.884630000	1.740257000	C	-2.811290000	-0.387886000	-4.891428000
H	-0.608463000	-4.785020000	1.949656000	C	-4.004765000	-1.115789000	-4.815621000
C	1.267740000	-3.783331000	1.405815000	C	-0.351825000	-2.662785000	-3.081858000
H	1.979567000	-4.586082000	1.298593000	C	-0.323618000	-0.115353000	-4.376884000
C	2.794367000	-1.836894000	0.782274000	C	0.873782000	-1.031662000	-4.555125000
C	2.198581000	3.031003000	0.197954000	C	0.860589000	-2.287591000	-3.914685000
C	-2.655346000	2.312740000	0.004264000	C	1.962354000	-3.143362000	-4.051384000
C	-1.997725000	-2.254192000	1.768345000	H	1.945690000	-4.114853000	-3.564200000
C	3.946919000	-2.780968000	0.619145000	C	3.076201000	-2.760948000	-4.809002000
C	4.546382000	-2.954796000	-0.643938000	C	3.088483000	-1.514654000	-5.445721000
H	4.150942000	-2.414315000	-1.497842000	C	1.987816000	-0.659561000	-5.319962000
C	5.623784000	-3.831898000	-0.807149000	H	-0.237977000	-2.209853000	-2.082844000
H	6.068595000	-3.958061000	-1.789364000	H	-4.936688000	-2.940065000	-4.128774000
C	6.122485000	-4.549535000	0.286559000	H	-2.841946000	-3.850314000	-3.150061000
H	6.958868000	-5.229505000	0.158410000	H	-2.795680000	0.577114000	-5.391644000



H	-4.913596000	-0.716211000	-5.255919000
H	-0.351378000	0.640836000	-5.170037000
H	3.920820000	-3.436035000	-4.911294000
H	3.944276000	-1.214067000	-6.042952000
H	1.991581000	0.305586000	-5.819957000
H	-0.399588000	-3.748484000	-2.938227000
H	-0.210680000	0.419596000	-3.419839000

<sup>4</sup>RC<sub>(15)</sub>

Co	0.007385000	-0.001464000	0.923686000
O	-0.000876000	0.000373000	-0.797502000
C	0.017851000	-0.004133000	3.112337000
C	-0.550780000	0.345979000	5.318844000
H	-1.153642000	0.710478000	6.132109000
C	0.607313000	-0.359599000	5.312508000
H	1.217837000	-0.726100000	6.119129000
C	2.161979000	-1.295077000	3.610596000
H	2.520541000	-1.818311000	4.499888000
H	1.939431000	-2.019916000	2.834665000
H	2.934327000	-0.609259000	3.260442000
C	-2.121427000	1.285616000	3.634015000
H	-2.471284000	1.807089000	4.527801000
H	-1.906265000	2.012006000	2.857458000
H	-2.897267000	0.600658000	3.289955000
N	-0.898559000	0.557029000	3.982609000
N	0.942420000	-0.567393000	3.972522000
N	1.981041000	0.186229000	0.853737000
N	-0.206927000	2.108595000	0.975365000
N	-1.966863000	-0.189314000	0.872082000
N	0.222210000	-2.111828000	0.968615000
C	2.881229000	-0.828358000	0.552721000
C	2.703696000	1.356086000	1.064062000
C	0.829074000	3.006885000	1.056020000
C	-1.334757000	2.795445000	0.574187000
C	-2.869877000	0.826009000	0.582095000
C	-2.687500000	-1.359611000	1.086730000
C	-0.812985000	-3.010297000	1.057213000
C	1.346063000	-2.797768000	0.554827000
C	4.222869000	-0.283424000	0.631928000
H	5.127289000	-0.847872000	0.471783000
C	4.117161000	1.035206000	0.977767000
H	4.921947000	1.733101000	1.140988000
C	0.324837000	4.339657000	0.746995000
H	0.917981000	5.240405000	0.725169000
C	-0.997490000	4.204958000	0.423681000
H	-1.673732000	4.978364000	0.095525000
C	-4.210712000	0.280886000	0.672865000
H	-5.116600000	0.845696000	0.522607000
C	-4.101732000	-1.038515000	1.014702000
H	-4.904934000	-1.736781000	1.184026000
C	-0.311841000	-4.342341000	0.740138000
H	-0.905184000	-5.243035000	0.721929000
C	1.007253000	-4.206880000	0.404180000
H	1.680128000	-4.979527000	0.067433000
C	2.601623000	-2.198155000	0.335923000
C	2.188885000	2.663301000	1.208569000
C	-2.592358000	2.196326000	0.365977000
C	-2.171314000	-2.667117000	1.223493000

C	3.732043000	-3.067364000	-0.121207000
C	4.355425000	-2.823766000	-1.361513000
H	3.997890000	-2.010812000	-1.985177000
C	5.409272000	-3.631704000	-1.800627000
H	5.872127000	-3.432712000	-2.762240000
C	5.861502000	-4.695232000	-1.010406000
H	6.679783000	-5.321084000	-1.352583000
C	5.251034000	-4.947202000	0.223741000
H	5.598306000	-5.766587000	0.845773000
C	4.196080000	-4.140889000	0.663916000
H	3.731807000	-4.335063000	1.625700000
C	3.151460000	3.796389000	1.401641000
C	4.106326000	4.132292000	0.421884000
H	4.148972000	3.555368000	-0.496071000
C	4.979921000	5.207790000	0.613652000
H	5.705003000	5.454923000	-0.155653000
C	4.914178000	5.969739000	1.786317000
H	5.592557000	6.804142000	1.934083000
C	3.964213000	5.652369000	2.764017000
H	3.904493000	6.238995000	3.675660000
C	3.089190000	4.578103000	2.571522000
H	2.353319000	4.333139000	3.330923000
C	-3.727166000	3.066708000	-0.077970000
C	-4.362034000	2.826752000	-1.313112000
H	-4.010188000	2.015845000	-1.942637000
C	-5.420118000	3.635785000	-1.739883000
H	-5.891869000	3.439570000	-2.697734000
C	-5.865149000	4.696777000	-0.942215000
H	-6.686739000	5.323476000	-1.274782000
C	-5.243184000	4.945154000	0.286923000
H	-5.584767000	5.762592000	0.914642000
C	-4.183987000	4.137753000	0.714737000
H	-3.710686000	4.329143000	1.672675000
C	-3.131936000	-3.800679000	1.423317000
C	-4.096422000	-4.134260000	0.452223000
H	-4.148133000	-3.555135000	-0.463876000
C	-4.968053000	-5.210267000	0.649990000
H	-5.700681000	-5.455567000	-0.112723000
C	-4.890707000	-5.975063000	1.820088000
H	-5.567562000	-6.809864000	1.972516000
C	-3.931141000	-5.660020000	2.789128000
H	-3.862408000	-6.248867000	3.698703000
C	-3.058094000	-4.585244000	2.590620000
H	-2.314767000	-4.342087000	3.343307000
C	-3.631338000	-0.480357000	-5.119048000
C	-2.522300000	-1.242040000	-4.733192000
C	-1.330204000	-0.622227000	-4.334496000
C	-1.246827000	0.785205000	-4.332652000
C	-2.357745000	1.542522000	-4.729104000

C	-3.548999000	0.916714000	-5.117222000
C	-0.116277000	-1.418209000	-3.889613000
C	0.052653000	1.431316000	-3.886773000
C	1.263050000	0.636424000	-4.343063000
C	1.179679000	-0.770988000	-4.343941000
C	2.287557000	-1.527355000	-4.750544000
H	2.217202000	-2.611978000	-4.760590000
C	3.475821000	-0.900617000	-5.146172000
C	3.558130000	0.496478000	-5.145370000
C	2.452070000	1.257230000	-4.749324000
H	-0.113787000	-1.460393000	-2.788113000
H	-4.548265000	-0.973820000	-5.427155000
H	-2.580481000	-2.327417000	-4.742676000
H	-2.287421000	2.627165000	-4.737286000
H	-4.400405000	1.515175000	-5.428004000
H	0.112403000	2.465039000	-4.246432000
H	4.324857000	-1.498319000	-5.464803000
H	4.472825000	0.990612000	-5.459001000
H	2.510189000	2.342626000	-4.756605000
H	-0.178891000	-2.451024000	-4.251406000
H	0.059177000	1.470680000	-2.785186000

<sup>2</sup>RC<sub>(LS)</sub>

Co	-0.001044000	-0.001826000	0.931527000
O	0.000308000	0.001158000	-0.925480000
C	-0.002580000	-0.005293000	3.038604000
C	-0.536802000	0.410909000	5.242307000
H	-1.096206000	0.844269000	6.053000000
C	0.527837000	-0.429396000	5.241718000
H	1.085874000	-0.865620000	6.051816000
C	1.975288000	-1.535821000	3.541693000
H	2.237835000	-2.136502000	4.415594000
H	1.693533000	-2.195098000	2.727351000
H	2.837888000	-0.937259000	3.243752000
C	-1.981331000	1.523397000	3.543790000
H	-2.244245000	2.122276000	4.418821000
H	-1.698757000	2.184330000	2.731108000
H	-2.843957000	0.925806000	3.243913000
N	-0.849220000	0.663432000	3.903468000
N	0.842605000	-0.677080000	3.902525000
N	1.960410000	0.023628000	0.841277000
N	-0.021716000	1.971165000	0.896313000
N	-1.962378000	-0.026968000	0.838341000
N	0.019677000	-1.974682000	0.890041000
C	2.771770000	-1.022258000	0.437910000
C	2.791488000	1.077589000	1.189744000
C	1.049421000	2.803401000	1.156767000
C	-1.048426000	2.768663000	0.408765000
C	-2.773145000	1.020195000	0.437121000
C	-2.793968000	-1.082035000	1.182219000
C	-1.051845000	-2.807738000	1.146238000
C	1.047085000	-2.770604000	0.401391000
C	4.158179000	-0.624933000	0.574703000
H	5.004053000	-1.252807000	0.344952000
C	4.171265000	0.644990000	1.081612000
H	5.031789000	1.244982000	1.329066000
C	0.674661000	4.173341000	0.860203000
H	1.326983000	5.025932000	0.962065000

C	-0.595208000	4.145250000	0.357920000
H	-1.174764000	4.974671000	-0.013618000
C	-4.159756000	0.622436000	0.570578000
H	-5.005288000	1.251039000	0.341557000
C	-4.173585000	-0.649074000	1.073470000
H	-5.034471000	-1.249836000	1.317771000
C	-0.676665000	-4.176717000	0.845781000
H	-1.329142000	-5.029625000	0.943928000
C	0.593922000	-4.147007000	0.345406000
H	1.173997000	-4.975219000	-0.028008000
C	2.349352000	-2.327075000	0.132072000
C	2.365518000	2.392661000	1.430480000
C	-2.350286000	2.325986000	0.136086000
C	-2.368352000	-2.397877000	1.419331000
C	3.363353000	-3.282883000	-0.411717000
C	3.951894000	-3.033610000	-1.667389000
H	3.642975000	-2.162868000	-2.236265000
C	4.908652000	-3.908994000	-2.191593000
H	5.345069000	-3.703973000	-3.164162000
C	5.298011000	-5.044438000	-1.471348000
H	6.041011000	-5.722518000	-1.879426000
C	4.724352000	-5.299628000	-0.220234000
H	5.026328000	-6.173361000	0.349236000
C	3.766449000	-4.426188000	0.305465000
H	3.335238000	-4.621832000	1.282178000
C	3.359181000	3.440624000	1.821416000
C	4.429567000	3.801161000	0.979470000
H	4.534727000	3.313136000	0.016227000
C	5.336946000	4.794338000	1.362928000
H	6.151828000	5.063102000	0.697896000
C	5.189994000	5.448148000	2.592020000
H	5.894707000	6.218772000	2.888146000
C	4.124688000	5.106808000	3.433305000
H	4.001091000	5.610877000	4.386911000
C	3.216343000	4.114779000	3.049865000

H	2.391491000	3.849911000	3.703891000
C	-3.363471000	3.283534000	-0.406164000
C	-3.949926000	3.038443000	-1.663632000
H	-3.639981000	2.169662000	-2.234943000
C	-4.905884000	3.915525000	-2.186458000
H	-5.340681000	3.713760000	-3.160433000
C	-5.296511000	5.048512000	-1.463035000
H	-6.038888000	5.727911000	-1.870054000
C	-4.724928000	5.299533000	-0.210130000
H	-5.027898000	6.171326000	0.361779000
C	-3.767826000	4.424391000	0.314199000
H	-3.338228000	4.616771000	1.292270000
C	-3.362606000	-3.447120000	1.805314000
C	-4.431742000	-3.804832000	0.960577000
H	-4.535465000	-3.313591000	-0.001186000
C	-5.339687000	-4.799285000	1.339357000
H	-6.153576000	-5.065819000	0.672215000
C	-5.194558000	-5.457211000	2.566467000
H	-5.899707000	-6.228822000	2.858961000
C	-4.130501000	-5.118697000	3.410471000
H	-4.008318000	-5.625962000	4.362562000
C	-3.221592000	-4.125389000	3.031707000
H	-2.397708000	-3.862724000	3.687839000
C	-3.559308000	-0.476589000	-5.276766000
C	-2.466941000	-1.239788000	-4.846158000
C	-1.288361000	-0.620279000	-4.411044000
C	-1.201479000	0.787805000	-4.413388000
C	-2.293411000	1.546011000	-4.856179000
C	-3.471980000	0.919872000	-5.283745000
C	-0.080645000	-1.403612000	-3.928337000
C	0.089095000	1.418369000	-3.921900000
C	1.297856000	0.637191000	-4.405500000
C	1.210990000	-0.770872000	-4.414251000
C	2.303882000	-1.527114000	-4.858033000
H	2.229138000	-2.611420000	-4.877584000
C	3.483365000	-0.899089000	-5.280294000
C	3.570657000	0.497326000	-5.266962000
C	2.477353000	1.258619000	-4.835351000
H	-0.073948000	-1.381026000	-2.824484000
H	-4.466672000	-0.969270000	-5.613486000
H	-2.528268000	-2.325039000	-4.850582000
H	-2.218630000	2.630391000	-4.870752000
H	-4.309474000	1.517996000	-5.631431000
H	0.080014000	1.390808000	-2.818179000
H	4.321618000	-1.495669000	-5.628803000
H	4.478738000	0.991492000	-5.599549000
H	2.538672000	2.343879000	-4.834873000
H	-0.144767000	-2.451889000	-4.241280000
H	0.153890000	2.468036000	-4.230006000

<sup>6</sup>TS1<sub>(HS)</sub>

Co	-0.723445000	-0.010873000	0.184253000
O	-0.410236000	0.141678000	-1.676490000
C	-1.172022000	-0.070441000	2.467614000
C	-1.640542000	0.559524000	4.634852000
H	-1.835498000	1.253141000	5.434935000
C	-1.584783000	-0.798794000	4.615106000
H	-1.714106000	-1.528839000	5.395810000

C	-1.161428000	-2.558207000	2.878812000
H	-1.561615000	-3.196924000	3.671427000
H	-1.724550000	-2.716670000	1.962819000
H	-0.112196000	-2.804544000	2.704560000
C	-1.389564000	2.397499000	2.948338000
H	-1.394684000	2.998541000	3.862025000
H	-0.496227000	2.617997000	2.370245000

H	-2.270913000	2.633362000	2.348744000	C	-0.281138000	5.350706000	-1.595021000
N	-1.387235000	0.984034000	3.326996000	H	-0.756418000	4.695330000	-2.317121000
N	-1.303688000	-1.162648000	3.295090000	C	-0.050803000	6.695550000	-1.901523000
N	0.508281000	-1.654972000	0.389363000	H	-0.353250000	7.087640000	-2.867835000
N	0.867243000	1.229414000	0.647421000	C	0.573404000	7.533356000	-0.967318000
N	-1.920177000	1.630069000	-0.034968000	H	0.754675000	8.577009000	-1.204771000
N	-2.323886000	-1.259818000	-0.128022000	C	0.956951000	7.016709000	0.276959000
C	0.167761000	-2.952296000	0.082030000	H	1.429743000	7.661898000	1.011253000
C	1.745363000	-1.667273000	1.004692000	C	0.723292000	5.671747000	0.583536000
C	2.098375000	0.814787000	1.099677000	H	1.010326000	5.275593000	1.551615000
C	0.945905000	2.574490000	0.352411000	C	-5.586153000	0.656386000	-0.296631000
C	-1.481637000	2.936599000	-0.151590000	C	-6.165276000	1.446984000	-1.308326000
C	-3.298962000	1.629236000	-0.101619000	H	-5.517799000	1.934000000	-2.029417000
C	-3.624890000	-0.846908000	-0.310863000	C	-7.554189000	1.589514000	-1.396706000
C	-2.240377000	-2.591148000	-0.508690000	H	-7.983488000	2.197575000	-2.187214000
C	1.226161000	-3.832604000	0.540293000	C	-8.389750000	0.940195000	-0.478362000
H	1.223200000	-4.906951000	0.446931000	H	-9.467507000	1.050546000	-0.547951000
C	2.176842000	-3.048503000	1.138911000	C	-7.826291000	0.142383000	0.526243000
H	3.082818000	-3.379212000	1.619210000	H	-8.466621000	-0.365939000	1.240828000
C	2.999137000	1.957674000	1.101638000	C	-6.437513000	-0.000026000	0.613872000
H	4.042063000	1.922592000	1.373724000	H	-5.996649000	-0.618617000	1.388973000
C	2.301842000	3.027241000	0.612367000	C	2.557842000	3.728738000	-2.769261000
H	2.682002000	4.011763000	0.400038000	C	1.936687000	2.483683000	-2.860837000
C	-2.643335000	3.805067000	-0.238331000	C	2.619331000	1.304369000	-2.500739000
H	-2.607320000	4.881197000	-0.304882000	C	3.936395000	1.395015000	-2.005851000
C	-3.756357000	3.008663000	-0.175988000	C	4.560674000	2.648892000	-1.939520000
H	-4.787806000	3.323003000	-0.188291000	C	3.884471000	3.811185000	-2.318902000
C	-4.405715000	-1.967583000	-0.814262000	C	1.940589000	-0.009854000	-2.665026000
H	-5.452929000	-1.923539000	-1.069248000	C	4.666399000	0.169448000	-1.503929000
C	-3.552477000	-3.026392000	-0.961221000	C	4.068173000	-1.154003000	-1.926968000
H	-3.781032000	-4.002629000	-1.357932000	C	2.752886000	-1.232066000	-2.432665000
C	-1.082143000	-3.388663000	-0.423425000	C	2.218639000	-2.493929000	-2.765647000
C	2.479684000	-0.518635000	1.382478000	H	1.198968000	-2.543749000	-3.136951000
C	-0.145059000	3.377986000	-0.054446000	C	2.973582000	-3.655902000	-2.616115000
C	-4.108356000	0.477002000	-0.193901000	C	4.290000000	-3.575099000	-2.137597000
C	-1.180191000	-4.824685000	-0.809248000	C	4.827046000	-2.329335000	-1.803737000
C	-0.271433000	-5.362764000	-1.741658000	H	0.946533000	-0.009563000	-1.968858000
H	0.478151000	-4.708512000	-2.170783000	H	2.013126000	4.628791000	-3.031996000
C	-0.334159000	-6.710775000	-2.107359000	H	0.907007000	2.402262000	-3.195934000
H	0.370261000	-7.106187000	-2.833136000	H	5.583489000	2.708634000	-1.575311000
C	-1.306582000	-7.548329000	-1.544762000	H	4.380747000	4.775099000	-2.257199000
H	-1.356627000	-8.595028000	-1.828293000	H	5.722128000	0.211953000	-1.807595000
C	-2.212773000	-7.026957000	-0.611862000	H	2.549302000	-4.620533000	-2.876047000
H	-2.963077000	-7.671437000	-0.163864000	H	4.890907000	-4.473339000	-2.033936000
C	-2.148865000	-5.678259000	-0.245956000	H	5.850348000	-2.257363000	-1.443164000
H	-2.842819000	-5.276610000	0.484759000	H	1.406851000	-0.065101000	-3.622843000
C	3.781143000	-0.694870000	2.088660000	H	4.674131000	0.205278000	-0.401670000
C	4.803337000	-1.526951000	1.590254000				
H	4.644486000	-2.053050000	0.657757000				
C	6.017448000	-1.656971000	2.272667000				
H	6.794801000	-2.297550000	1.866634000				
C	6.236411000	-0.958473000	3.466920000				
H	7.179012000	-1.060454000	3.995754000				
C	5.230280000	-0.124157000	3.972165000				
H	5.388768000	0.420640000	4.897925000				
C	4.017061000	0.006778000	3.289632000				
H	3.235867000	0.650850000	3.679078000				
C	0.108743000	4.815988000	-0.350410000				

**<sup>4</sup>TS1<sub>(IS)</sub>**

Co	-0.694101000	-0.056487000	0.291492000	H	-1.959239000	-7.893848000	-0.243526000
C	-1.166814000	-0.177579000	2.358803000	C	-1.396588000	-5.815314000	-0.311447000
C	-1.766536000	0.366374000	4.511648000	H	-2.134419000	-5.509165000	0.422563000
H	-2.061107000	1.024805000	5.310385000	C	3.839967000	-0.214323000	2.213836000
C	-1.553498000	-0.973368000	4.481791000	C	4.954478000	-0.890770000	1.679222000
H	-1.619279000	-1.724055000	5.250182000	H	4.854448000	-1.402272000	0.730347000
C	-0.881102000	-2.669638000	2.789188000	C	6.183470000	-0.884586000	2.347231000
H	-1.209491000	-3.324729000	3.600945000	H	7.031587000	-1.406803000	1.914214000
H	-1.417359000	-2.923244000	1.880768000	C	6.326500000	-0.198978000	3.560353000
H	0.190807000	-2.795901000	2.631815000	H	7.281160000	-0.194538000	4.077238000
C	-1.675138000	2.258754000	2.898354000	C	5.229075000	0.485975000	4.098786000
H	-1.737415000	2.810128000	3.840761000	H	5.329186000	1.022137000	5.037680000
H	-0.808216000	2.595495000	2.339773000	C	4.000515000	0.479767000	3.430974000
H	-2.579634000	2.432919000	2.313523000	H	3.149712000	1.011639000	3.843792000
N	-1.528358000	0.837034000	3.218455000	C	-0.406023000	4.775874000	-0.437169000
N	-1.191653000	-1.290367000	3.170756000	C	-0.873211000	5.187757000	-1.701749000
N	0.678363000	-1.479935000	0.456431000	H	-1.270324000	4.438400000	-2.377758000
N	0.748828000	1.384693000	0.789680000	C	-0.815437000	6.530936000	-2.085237000
N	-2.035254000	1.372907000	0.036732000	H	-1.175885000	6.827420000	-3.065656000
N	-2.159797000	-1.518496000	-0.068370000	C	-0.287899000	7.490729000	-1.210663000
C	0.522786000	-2.800355000	0.062623000	H	-0.240511000	8.533730000	-1.507999000
C	1.911151000	-1.362810000	1.086610000	C	0.172907000	7.096057000	0.051918000
C	2.009588000	1.124167000	1.250461000	H	0.571489000	7.834861000	0.740673000
C	0.692479000	2.708957000	0.414459000	C	0.110396000	5.752178000	0.436320000
C	-1.742419000	2.713559000	-0.138860000	H	0.454089000	5.449911000	1.419626000
C	-3.410165000	1.218153000	-0.018420000	C	-5.599447000	0.019749000	-0.195609000
C	-3.495322000	-1.264584000	-0.247010000	C	-6.272779000	0.745115000	-1.197994000
C	-1.905458000	-2.794219000	-0.518124000	H	-5.691547000	1.307263000	-1.920646000
C	1.692902000	-3.544554000	0.485065000	C	-7.669302000	0.725597000	-1.278053000
H	1.839116000	-4.600419000	0.325947000	H	-8.171059000	1.285436000	-2.061467000
C	2.519311000	-2.679244000	1.144666000	C	-8.418335000	-0.024866000	-0.362068000
H	3.460062000	-2.910270000	1.615061000	H	-9.501979000	-0.040208000	-0.425671000
C	2.791196000	2.353233000	1.208377000	C	-7.759926000	-0.762007000	0.630912000
H	3.829346000	2.435594000	1.490013000	H	-8.332313000	-1.349933000	1.342062000
C	1.992726000	3.317231000	0.656728000	C	-6.363529000	-0.742182000	0.710311000
H	2.268366000	4.324133000	0.391902000	H	-5.848898000	-1.314983000	1.475045000
C	-2.993223000	3.442431000	-0.239953000	O	-0.378668000	0.170054000	-1.433962000
H	-3.072801000	4.512809000	-0.343546000	C	1.900235000	3.778083000	-3.049313000
C	-4.011531000	2.535437000	-0.126687000	C	1.468683000	2.452100000	-3.073272000
H	-5.070756000	2.734543000	-0.131714000	C	2.293356000	1.413462000	-2.595971000
C	-4.133504000	-2.450066000	-0.804779000	C	3.559151000	1.731431000	-2.059423000
H	-5.178235000	-2.525822000	-1.063709000	C	3.990459000	3.065069000	-2.056912000
C	-3.150085000	-3.381608000	-0.997150000	C	3.173541000	4.087105000	-2.547425000
H	-3.247655000	-4.360011000	-1.440425000	C	1.817360000	0.008164000	-2.656693000
C	-0.640106000	-3.410838000	-0.462833000	C	4.429645000	0.656748000	-1.446454000
C	2.521498000	-0.165097000	1.518977000	C	4.091384000	-0.752477000	-1.878883000
C	-0.475019000	3.338337000	-0.056440000	C	2.821273000	-1.055151000	-2.419130000
C	-4.110683000	-0.003960000	-0.103274000	C	2.535760000	-2.384604000	-2.786807000
C	-0.542709000	-4.842358000	-0.868927000	H	1.558011000	-2.605606000	-3.205392000
C	0.422042000	-5.258129000	-1.806599000	C	3.480199000	-3.397843000	-2.624979000
H	1.087134000	-4.517133000	-2.228997000	C	4.744476000	-3.093688000	-2.100844000
C	0.525424000	-6.600901000	-2.182744000	C	5.042214000	-1.775657000	-1.741923000
H	1.272246000	-6.899730000	-2.912419000	H	0.847654000	-0.046348000	-1.857085000
C	-0.334196000	-7.557256000	-1.626371000	H	1.250234000	4.569003000	-3.406113000
H	-0.255160000	-8.599795000	-1.918500000	H	0.481670000	2.198323000	-3.447057000
C	-1.294974000	-7.158681000	-0.687780000	H	4.972982000	3.299307000	-1.654458000

H	3.519782000	5.116198000	-2.534302000
H	4.325221000	0.717665000	-0.351277000
H	3.240983000	-4.417448000	-2.911295000
H	5.492307000	-3.872363000	-1.986451000
H	6.027731000	-1.526883000	-1.355534000
H	1.217922000	-0.186721000	-3.554042000
H	5.488089000	0.865363000	-1.655518000

<sup>2</sup>TS1<sub>(LS)</sub>

Co	-0.733785000	0.034887000	0.220883000
O	-0.303526000	0.113843000	-1.601196000
C	-1.269594000	-0.027908000	2.203255000
C	-1.763067000	0.583806000	4.363402000
H	-1.922453000	1.271398000	5.176021000
C	-1.837358000	-0.770435000	4.303325000
H	-2.066979000	-1.506442000	5.054369000
C	-1.513514000	-2.531591000	2.565782000
H	-2.049399000	-3.118313000	3.317304000
H	-2.010850000	-2.631751000	1.606899000
H	-0.486718000	-2.893249000	2.483433000
C	-1.277984000	2.450193000	2.780422000
H	-1.222439000	2.990515000	3.729565000
H	-0.367091000	2.618486000	2.215175000
H	-2.134174000	2.808675000	2.206004000
N	-1.417803000	1.022483000	3.082486000
N	-1.539315000	-1.128188000	2.986053000
N	0.343366000	-1.586204000	0.396387000
N	0.825548000	1.119582000	0.671900000
N	-1.779765000	1.660114000	-0.068903000
N	-2.295739000	-1.046577000	-0.262655000
C	0.040161000	-2.825586000	-0.129868000
C	1.500865000	-1.724506000	1.139856000
C	1.946952000	0.680298000	1.341642000
C	1.062808000	2.426735000	0.278139000
C	-1.266185000	2.911908000	-0.320904000
C	-3.157172000	1.777691000	-0.028615000
C	-3.604465000	-0.617224000	-0.292901000
C	-2.272257000	-2.326974000	-0.788495000
C	1.030186000	-3.782560000	0.316593000
H	1.031119000	-4.828107000	0.054431000
C	1.898805000	-3.118646000	1.136272000
H	2.746506000	-3.525364000	1.661329000
C	2.914139000	1.757545000	1.401237000
H	3.895725000	1.674009000	1.839646000
C	2.395109000	2.807008000	0.698112000
H	2.885160000	3.728898000	0.438846000
C	-2.355224000	3.865303000	-0.393348000
H	-2.231226000	4.924738000	-0.552316000
C	-3.514552000	3.176658000	-0.160652000
H	-4.517292000	3.568982000	-0.111417000
C	-4.440546000	-1.666341000	-0.842577000
H	-5.504587000	-1.581427000	-0.996994000
C	-3.615225000	-2.699574000	-1.187370000
H	-3.880632000	-3.628289000	-1.665904000
C	-1.158608000	-3.176454000	-0.769559000
C	2.225964000	-0.654225000	1.685984000
C	0.091392000	3.273632000	-0.272709000
C	-4.046067000	0.693956000	-0.048071000

C	-1.292843000	-4.566626000	-1.290773000
C	-0.424388000	-5.029213000	-2.296184000
H	0.318954000	-4.351218000	-2.692500000
C	-0.521125000	-6.338470000	-2.778894000
H	0.153391000	-6.675382000	-3.560377000
C	-1.487526000	-7.210523000	-2.261158000
H	-1.563256000	-8.226873000	-2.635000000
C	-2.354985000	-6.763158000	-1.255886000
H	-3.101476000	-7.434846000	-0.842825000
C	-2.256964000	-5.453539000	-0.773623000
H	-2.921172000	-5.110511000	0.012718000
C	3.422036000	-0.905394000	2.535163000
C	4.488012000	-1.723494000	2.110836000
H	4.442940000	-2.184320000	1.131222000
C	5.607373000	-1.915172000	2.927700000
H	6.422485000	-2.543696000	2.581600000
C	5.686347000	-1.290442000	4.179084000
H	6.556277000	-1.440343000	4.810942000
C	4.637968000	-0.465015000	4.606733000
H	4.691461000	0.026309000	5.573541000
C	3.518392000	-0.272926000	3.791061000
H	2.704194000	0.366134000	4.117280000
C	0.451381000	4.637383000	-0.740186000
C	0.070298000	5.031261000	-2.039490000
H	-0.467915000	4.322744000	-2.659934000
C	0.400334000	6.297532000	-2.530432000
H	0.106252000	6.578627000	-3.537053000
C	1.116846000	7.197629000	-1.729719000
H	1.379244000	8.179412000	-2.111361000
C	1.483550000	6.825598000	-0.430046000
H	2.021665000	7.523904000	0.203762000
C	1.146955000	5.560392000	0.062976000
H	1.412141000	5.285760000	1.077660000
C	-5.515676000	0.923222000	0.013678000
C	-6.179507000	1.767925000	-0.897234000
H	-5.604487000	2.264228000	-1.671003000
C	-7.565539000	1.944505000	-0.826620000
H	-8.061861000	2.594038000	-1.541161000
C	-8.313791000	1.274293000	0.150049000
H	-9.389410000	1.411136000	0.202795000
C	-7.666971000	0.419132000	1.051869000
H	-8.240071000	-0.108363000	1.808332000
C	-6.281213000	0.243126000	0.981529000
H	-5.775876000	-0.420794000	1.675681000
C	3.063231000	3.615228000	-2.670388000
C	2.332345000	2.432937000	-2.795938000
C	2.832267000	1.210317000	-2.306717000
C	4.084203000	1.199568000	-1.654975000
C	4.822858000	2.386674000	-1.553130000

C	4.323987000	3.591624000	-2.055951000
C	2.048642000	-0.040667000	-2.495764000
C	4.608027000	-0.066272000	-1.014533000
C	4.009928000	-1.339987000	-1.568670000
C	2.771462000	-1.316196000	-2.248140000
C	2.244754000	-2.527058000	-2.737187000
H	1.291582000	-2.497045000	-3.257144000
C	2.923397000	-3.734278000	-2.565727000
C	4.155797000	-3.753483000	-1.898762000
C	4.690185000	-2.557490000	-1.411154000
H	0.980082000	0.016392000	-1.841577000
H	2.650993000	4.548859000	-3.036958000
H	1.351888000	2.440887000	-3.262432000
H	5.793629000	2.361090000	-1.063342000
H	4.906743000	4.503821000	-1.967490000
H	5.703306000	-0.103501000	-1.095737000
H	2.499955000	-4.657560000	-2.949032000
H	4.697176000	-4.686103000	-1.771795000
H	5.657462000	-2.556871000	-0.913424000
H	1.547244000	-0.051960000	-3.471525000
H	4.390484000	-0.017775000	0.064491000

<sup>5</sup>Int1<sub>(HS)</sub>

Co	0.022155000	0.023371000	-0.399139000
O	-0.015490000	-0.008488000	-2.263870000
C	-0.037019000	-0.059921000	1.972406000
C	0.628426000	-0.085721000	4.180928000
H	1.336152000	-0.079606000	4.992185000
C	-0.729651000	-0.120694000	4.171611000
H	-1.447654000	-0.158050000	4.972943000
C	-2.521884000	-0.129882000	2.426462000
H	-3.136083000	0.063116000	3.310603000
H	-2.697905000	0.644703000	1.685290000
H	-2.784902000	-1.101724000	2.005123000
C	2.442899000	0.013545000	2.462225000
H	3.047672000	-0.203462000	3.347282000
H	2.642100000	-0.727941000	1.694261000
H	2.695582000	1.004694000	2.081153000
N	1.031782000	-0.050403000	2.842956000
N	-1.115801000	-0.101645000	2.828265000
N	-1.665858000	-1.190378000	-0.394000000
N	1.231086000	-1.655503000	-0.261043000
N	1.676844000	1.200793000	-0.320456000
N	-1.210879000	1.676655000	-0.241308000
C	-2.965014000	-0.763348000	-0.572056000
C	-1.689606000	-2.546410000	-0.128690000
C	0.784921000	-2.956953000	-0.172826000
C	2.573713000	-1.685553000	-0.586433000
C	2.977818000	0.779950000	-0.513591000
C	1.698786000	2.559828000	-0.065652000
C	-0.770053000	2.976058000	-0.142928000
C	-2.553571000	1.706342000	-0.581041000
C	-3.854701000	-1.894885000	-0.384521000
H	-4.931142000	-1.850362000	-0.436988000
C	-3.075017000	-2.982020000	-0.083786000
H	-3.406006000	-3.982220000	0.145685000
C	1.901796000	-3.851772000	-0.438407000
H	1.837744000	-4.928315000	-0.457617000

C	2.990797000	-3.072448000	-0.717356000
H	3.977795000	-3.399196000	-1.003232000
C	3.864278000	1.913887000	-0.326213000
H	4.940347000	1.873097000	-0.387179000
C	3.083547000	2.998018000	-0.022984000
H	3.411952000	4.000001000	0.202041000
C	-1.884092000	3.872679000	-0.413324000
H	-1.819477000	4.949223000	-0.426418000
C	-2.969732000	3.094942000	-0.705784000
H	-3.953557000	3.423437000	-1.000328000
C	-3.383525000	0.577945000	-0.741618000
C	-0.553594000	-3.377290000	-0.004785000
C	3.402872000	-0.551191000	-0.715559000
C	0.567129000	3.394489000	0.042220000
C	-4.830123000	0.798056000	-1.026887000
C	-5.438541000	0.171788000	-2.132793000
H	-4.831257000	-0.451877000	-2.780295000
C	-6.799096000	0.354699000	-2.400189000
H	-7.248573000	-0.130129000	-3.261379000
C	-7.578362000	1.166079000	-1.564973000
H	-8.634252000	1.308877000	-1.772615000
C	-6.986789000	1.791074000	-0.459281000
H	-7.585341000	2.414501000	0.198017000
C	-5.626237000	1.606957000	-0.191921000
H	-5.169256000	2.082535000	0.669502000
C	-0.769543000	-4.834970000	0.228737000
C	-1.562883000	-5.612316000	-0.637729000
H	-2.025649000	-5.136209000	-1.495429000
C	-1.740594000	-6.980989000	-0.409423000
H	-2.349911000	-7.565837000	-1.091714000
C	-1.124889000	-7.598678000	0.687221000
H	-1.262420000	-8.661000000	0.863421000
C	-0.326337000	-6.838356000	1.551688000
H	0.154855000	-7.309357000	2.403468000
C	-0.149064000	-5.469971000	1.322891000

H	0.468226000	-4.877111000	1.989833000
C	4.848262000	-0.761999000	-1.013195000
C	5.442770000	-0.120289000	-2.117734000
H	4.825531000	0.508002000	-2.751165000
C	6.801129000	-0.296541000	-2.400662000
H	7.240774000	0.200157000	-3.260166000
C	7.590743000	-1.116391000	-1.583496000
H	8.644884000	-1.253785000	-1.803510000
C	7.012116000	-1.757198000	-0.480021000
H	7.618912000	-2.387532000	0.163034000
C	5.653711000	-1.580026000	-0.196771000
H	5.206530000	-2.068027000	0.663001000
C	0.784052000	4.853490000	0.267663000
C	1.573803000	5.624037000	-0.607920000
H	2.031591000	5.140994000	-1.464394000
C	1.752021000	6.994395000	-0.390031000
H	2.358503000	7.574427000	-1.078932000
C	1.140129000	7.619932000	0.704342000
H	1.277997000	8.683596000	0.872201000
C	0.344516000	6.866069000	1.577116000
H	-0.134105000	7.343453000	2.426830000
C	0.166691000	5.495882000	1.358899000
H	-0.448946000	4.908102000	2.032018000
H	-0.597207000	-0.676890000	-2.682676000

### <sup>3</sup>Int1<sub>(IS)</sub>

Co	0.010671000	0.000968000	-0.231534000
O	0.107046000	-0.006081000	-2.059512000
C	0.000462000	-0.004644000	1.906839000
C	0.618835000	-0.246998000	4.108885000
H	1.278980000	-0.503778000	4.919210000
C	-0.644982000	0.247889000	4.100087000
H	-1.315121000	0.508106000	4.901070000
C	-2.328990000	0.898064000	2.384439000
H	-2.798165000	1.310468000	3.281996000
H	-2.219451000	1.681287000	1.641141000
H	-2.951448000	0.096015000	1.985454000
C	2.321162000	-0.914121000	2.418582000
H	2.770135000	-1.336203000	3.322015000
H	2.216656000	-1.692348000	1.669287000
H	2.958353000	-0.116539000	2.033829000
N	0.997772000	-0.396668000	2.773174000
N	-1.007537000	0.390648000	2.759130000
N	-1.907326000	-0.459442000	-0.316819000
N	0.503789000	-2.048167000	-0.149635000
N	1.920050000	0.451318000	-0.248999000
N	-0.505098000	2.038642000	-0.156897000
C	-2.947651000	0.421290000	-0.587011000
C	-2.468377000	-1.698178000	-0.012750000
C	-0.392617000	-3.076437000	-0.036297000
C	1.703032000	-2.576449000	-0.573058000
C	2.950249000	-0.420804000	-0.547901000
C	2.474502000	1.690818000	0.026979000
C	0.395460000	3.064046000	-0.033882000
C	-1.696651000	2.573853000	-0.593854000
C	-4.201535000	-0.280286000	-0.410918000
H	-5.175207000	0.168148000	-0.527178000
C	-3.910627000	-1.559712000	-0.022090000

H	-4.607760000	-2.343718000	0.224802000
C	0.275198000	-4.330687000	-0.359624000
H	-0.199073000	-5.299830000	-0.366548000
C	1.557765000	-4.017994000	-0.720339000
H	2.325137000	-4.688480000	-1.073593000
C	4.209261000	0.284746000	-0.395006000
H	5.181785000	-0.160533000	-0.530929000
C	3.921012000	1.562797000	-0.005160000
H	4.617556000	2.352810000	0.223316000
C	-0.263575000	4.320407000	-0.366883000
H	0.215411000	5.287143000	-0.369796000
C	-1.543226000	4.014325000	-0.741222000
H	-2.302779000	4.687998000	-1.105110000
C	-2.860014000	1.814826000	-0.812368000
C	-1.780492000	-2.918087000	0.154224000
C	2.863261000	-1.811540000	-0.783400000
C	1.780120000	2.909106000	0.176077000
C	-4.106920000	2.520644000	-1.219010000
C	-4.830597000	2.093286000	-2.350274000
H	-4.454487000	1.253221000	-2.924539000
C	-6.008490000	2.742250000	-2.733856000
H	-6.548355000	2.403027000	-3.612612000
C	-6.486836000	3.830909000	-1.992463000
H	-7.400665000	4.335320000	-2.290623000
C	-5.779117000	4.263467000	-0.863320000
H	-6.147587000	5.100569000	-0.278109000
C	-4.601815000	3.613224000	-0.479397000
H	-4.059244000	3.940178000	0.401257000
C	-2.558001000	-4.162656000	0.419981000
C	-3.596350000	-4.591930000	-0.429799000
H	-3.843373000	-3.995479000	-1.301273000
C	-4.287859000	-5.779925000	-0.170071000



H	-5.080835000	-6.098280000	-0.839911000
C	-3.949791000	-6.564750000	0.940375000
H	-4.486125000	-7.487123000	1.140534000
C	-2.909966000	-6.156112000	1.785706000
H	-2.638728000	-6.760226000	2.646195000
C	-2.219037000	-4.968206000	1.525377000
H	-1.411182000	-4.649424000	2.176045000
C	4.107329000	-2.510360000	-1.210622000
C	4.802167000	-2.077938000	-2.357782000
H	4.404486000	-1.242458000	-2.924004000
C	5.976397000	-2.719129000	-2.765165000
H	6.495057000	-2.377301000	-3.655604000
C	6.478715000	-3.802968000	-2.032395000
H	7.390108000	-4.300631000	-2.348991000
C	5.798487000	-4.240108000	-0.888202000
H	6.185726000	-5.073842000	-0.310269000
C	4.624191000	-3.598591000	-0.480491000
H	4.101866000	-3.928920000	0.411246000
C	2.553351000	4.159266000	0.431323000
C	3.578590000	4.590924000	-0.432703000
H	3.817217000	3.992461000	-1.305083000
C	4.265857000	5.784038000	-0.185074000
H	5.048741000	6.104925000	-0.865488000
C	3.936385000	6.570522000	0.926851000
H	4.469496000	7.496833000	1.117378000
C	2.909300000	6.158811000	1.786082000
H	2.644679000	6.764495000	2.647558000
C	2.222193000	4.965932000	1.537780000
H	1.423503000	4.644976000	2.198749000
H	-0.759926000	-0.285655000	-2.426767000

<sup>1</sup>Int1<sub>(LS)</sub>

Co	0.004315000	0.001197000	-0.237281000
O	0.051771000	0.069732000	-2.129214000
C	-0.006485000	-0.012088000	1.813208000
C	0.643355000	-0.178795000	4.011756000
H	1.335840000	-0.335858000	4.820661000
C	-0.682421000	0.113695000	4.006581000
H	-1.384559000	0.256004000	4.809871000
C	-2.450311000	0.496411000	2.286521000
H	-2.965278000	0.899432000	3.163145000
H	-2.465201000	1.230485000	1.487785000
H	-2.952916000	-0.414190000	1.954206000
C	2.432134000	-0.532036000	2.307413000
H	2.937027000	-0.942987000	3.186244000
H	2.457570000	-1.258865000	1.502175000
H	2.938228000	0.381512000	1.988959000
N	1.040887000	-0.254173000	2.674358000
N	-1.063644000	0.214229000	2.666182000
N	-1.756288000	-0.852564000	-0.319454000
N	0.845461000	-1.768092000	-0.276089000
N	1.763912000	0.845006000	-0.270248000
N	-0.845752000	1.766046000	-0.254223000
C	-2.933313000	-0.245883000	-0.707697000
C	-2.070291000	-2.136693000	0.096146000
C	0.235536000	-2.968273000	0.021599000
C	2.106726000	-2.059223000	-0.773483000
C	2.935445000	0.249861000	-0.678237000

C	2.071003000	2.128970000	0.134932000
C	-0.232417000	2.961782000	0.037561000
C	-2.093977000	2.061064000	-0.776189000
C	-4.031655000	-1.164360000	-0.494233000
H	-5.066802000	-0.936198000	-0.693825000
C	-3.508020000	-2.308262000	0.046975000
H	-4.038612000	-3.193391000	0.358421000
C	1.144607000	-4.054681000	-0.284727000
H	0.908988000	-5.100499000	-0.165053000
C	2.274394000	-3.497827000	-0.818000000
H	3.141862000	-4.006605000	-1.205964000
C	4.034324000	1.173687000	-0.471711000
H	5.068393000	0.951389000	-0.682877000
C	3.510022000	2.311323000	0.077193000
H	4.036525000	3.200087000	0.384948000
C	-1.129569000	4.054700000	-0.289578000
H	-0.886382000	5.099410000	-0.176324000
C	-2.253280000	3.501886000	-0.835197000
H	-3.110503000	4.012345000	-1.243093000
C	-3.090330000	1.111978000	-1.036001000
C	-1.122721000	-3.141425000	0.342483000
C	3.099712000	-1.102419000	-1.020304000
C	1.122174000	3.133873000	0.371339000
C	-4.416193000	1.543321000	-1.556385000
C	-4.934935000	0.940103000	-2.719216000
H	-4.339851000	0.188426000	-3.226971000

C	-6.187455000	1.311114000	-3.218696000
H	-6.567626000	0.842317000	-4.121110000
C	-6.946611000	2.288382000	-2.561431000
H	-7.918533000	2.577123000	-2.949332000
C	-6.445802000	2.888349000	-1.398647000
H	-7.033378000	3.637572000	-0.876715000
C	-5.193077000	2.517011000	-0.898936000
H	-4.812585000	2.969714000	0.010420000
C	-1.554221000	-4.491854000	0.794847000
C	-2.510444000	-5.249222000	0.090362000
H	-2.944634000	-4.840046000	-0.815063000
C	-2.878221000	-6.524349000	0.532977000
H	-3.611915000	-7.096817000	-0.026289000
C	-2.291663000	-7.068945000	1.682924000
H	-2.577009000	-8.059028000	2.024589000
C	-1.328004000	-6.331879000	2.383740000
H	-0.864731000	-6.748401000	3.273012000
C	-0.961070000	-5.056822000	1.941530000
H	-0.214890000	-4.481675000	2.480268000
C	4.424782000	-1.522693000	-1.551750000
C	4.926144000	-0.910398000	-2.717551000
H	4.319443000	-0.160638000	-3.214365000
C	6.176452000	-1.270177000	-3.230797000
H	6.544330000	-0.794345000	-4.134618000
C	6.949662000	-2.244228000	-2.585052000
H	7.919996000	-2.523689000	-2.983653000
C	6.465581000	-2.852649000	-1.419585000
H	7.064528000	-3.598946000	-0.906400000
C	5.215025000	-2.492982000	-0.905767000
H	4.847813000	-2.951386000	0.006291000
C	1.551376000	4.487392000	0.817660000
C	2.500393000	5.245556000	0.104614000
H	2.929644000	4.834454000	-0.802239000
C	2.865011000	6.523907000	0.540589000
H	3.592872000	7.097572000	-0.025023000
C	2.282494000	7.070231000	1.691839000
H	2.565514000	8.062828000	2.028202000
C	1.325429000	6.332167000	2.400520000
H	0.864808000	6.750441000	3.290375000
C	0.961103000	5.054065000	1.964688000
H	0.219173000	4.478428000	2.508885000
H	-0.362234000	-0.765323000	-2.437877000

<sup>6</sup>TS2<sub>(HS)</sub>

Co	0.671140000	-0.047474000	0.372505000	H	2.161707000	-2.918889000	2.284578000
O	0.442028000	0.079005000	-1.707212000	N	1.444185000	-1.257797000	3.375542000
C	1.244009000	-0.161037000	2.568898000	N	1.472149000	0.889705000	3.429018000
C	1.784485000	-0.900171000	4.684525000	N	-0.399875000	1.689308000	0.521098000
H	1.978561000	-1.634253000	5.447879000	N	-1.049923000	-1.135357000	0.689902000
C	1.800142000	0.459128000	4.718782000	N	1.699371000	-1.824835000	-0.088428000
H	2.005931000	1.149099000	5.519302000	N	2.410828000	1.027110000	-0.052317000
C	1.372626000	2.303158000	3.063496000	C	0.083096000	2.956245000	0.263651000
H	1.787865000	2.902232000	3.878757000	C	-1.666550000	1.820325000	1.056799000
H	1.941615000	2.478705000	2.152988000	C	-2.258434000	-0.618782000	1.096318000
H	0.331549000	2.585780000	2.893743000	C	-1.238534000	-2.482608000	0.424202000
C	1.328686000	-2.648714000	2.936972000	C	1.139015000	-3.077101000	-0.165953000
H	1.330481000	-3.292518000	3.821051000	C	3.070868000	-1.963819000	-0.181808000
H	0.394644000	-2.775920000	2.394071000	C	3.642899000	0.484321000	-0.348175000

C	2.446152000	2.363720000	-0.385496000	H	7.564236000	-3.002944000	-2.453521000
C	-0.904821000	3.930566000	0.701122000	C	8.178866000	-1.773796000	-0.786842000
H	-0.787457000	5.000954000	0.648292000	H	9.235528000	-1.990421000	-0.909047000
C	-1.967633000	3.235221000	1.208199000	C	7.749133000	-0.913919000	0.232603000
H	-2.868876000	3.641405000	1.636934000	H	8.472105000	-0.464285000	0.906262000
C	-3.252346000	-1.681831000	1.101537000	C	6.388089000	-0.632802000	0.386998000
H	-4.296927000	-1.550825000	1.329747000	H	6.050763000	0.035367000	1.172373000
C	-2.632961000	-2.817631000	0.670488000	C	-3.305564000	-3.454950000	-2.486087000
H	-3.088219000	-3.772257000	0.472965000	C	-2.422204000	-2.406460000	-2.782627000
C	2.200269000	-4.062785000	-0.276526000	C	-2.773890000	-1.068053000	-2.564631000
H	2.053706000	-5.130455000	-0.328249000	C	-4.056713000	-0.773848000	-1.993891000
C	3.390856000	-3.380388000	-0.255370000	C	-4.941182000	-1.845330000	-1.712845000
H	4.384642000	-3.797271000	-0.292172000	C	-4.575473000	-3.167147000	-1.961813000
C	4.504386000	1.532051000	-0.879551000	C	-1.843491000	0.033912000	-2.913282000
H	5.517104000	1.387291000	-1.221687000	C	-4.434708000	0.582647000	-1.767348000
C	3.763113000	2.680759000	-0.921265000	C	-3.620998000	1.678406000	-2.180773000
H	4.064957000	3.642908000	-1.303253000	C	-2.346375000	1.424616000	-2.785619000
C	1.375717000	3.275102000	-0.215307000	C	-1.574324000	2.505417000	-3.229859000
C	-2.534223000	0.745657000	1.353262000	H	-0.599943000	2.303701000	-3.664373000
C	-0.240885000	-3.378749000	-0.008326000	C	-2.034093000	3.825216000	-3.110293000
C	3.986094000	-0.888442000	-0.291825000	C	-3.280446000	4.082079000	-2.516804000
C	1.646533000	4.711044000	-0.509815000	C	-4.062346000	3.021929000	-2.060762000
C	0.807279000	5.426293000	-1.386510000	H	-0.798190000	0.004361000	-2.188870000
H	-0.027668000	4.908705000	-1.843569000	H	-3.000148000	-4.482499000	-2.654456000
C	1.047846000	6.775964000	-1.661248000	H	-1.440004000	-2.629099000	-3.192100000
H	0.395274000	7.310337000	-2.345135000	H	-5.919988000	-1.614585000	-1.300183000
C	2.128285000	7.436642000	-1.061269000	H	-5.268142000	-3.973613000	-1.739462000
H	2.314537000	8.484706000	-1.274474000	H	-5.399514000	0.787064000	-1.312053000
C	2.966060000	6.737343000	-0.182330000	H	-1.431769000	4.644462000	-3.490809000
H	3.799676000	7.244368000	0.294039000	H	-3.640961000	5.102154000	-2.423796000
C	2.727767000	5.386434000	0.090587000	H	-5.042105000	3.210722000	-1.628769000
H	3.372290000	4.844991000	0.775005000	H	-1.344769000	-0.137391000	-3.877640000
C	-3.867029000	1.055531000	1.947234000	H	0.977230000	-0.636365000	-2.114830000
C	-4.755223000	1.960687000	1.335405000				
H	-4.459856000	2.434617000	0.408457000				
C	-6.004756000	2.227892000	1.903549000				
H	-6.680168000	2.923094000	1.413726000				
C	-6.390277000	1.595629000	3.093397000				
H	-7.360831000	1.803589000	3.533193000				
C	-5.515943000	0.691528000	3.710195000				
H	-5.804633000	0.198269000	4.633384000				
C	-4.266575000	0.422996000	3.141074000				
H	-3.588000000	-0.278626000	3.614823000				
C	-0.641780000	-4.787946000	-0.284073000				
C	-0.378966000	-5.353840000	-1.547137000				
H	0.113870000	-4.747097000	-2.299230000				
C	-0.757574000	-6.668906000	-1.834886000				
H	-0.555704000	-7.085444000	-2.816905000				
C	-1.399772000	-7.444901000	-0.860245000				
H	-1.695022000	-8.465561000	-1.082382000				
C	-1.655023000	-6.897084000	0.403555000				
H	-2.142753000	-7.495381000	1.167035000				
C	-1.278013000	-5.580564000	0.689605000				
H	-1.473112000	-5.156124000	1.668559000				
C	5.430456000	-1.213313000	-0.468658000				
C	5.875978000	-2.069783000	-1.494747000				
H	5.148210000	-2.501279000	-2.173146000				
C	7.237778000	-2.347582000	-1.651910000				

<sup>4</sup>TS2<sub>(HS)</sub>

Co	0.752857000	-0.001490000	0.357183000	C	2.141992000	6.999024000	-0.620414000
O	0.234010000	-0.023362000	-1.498148000	H	2.892122000	7.664023000	-0.202982000
C	1.303137000	0.037625000	2.464043000	C	2.106541000	5.657623000	-0.224574000
C	1.878809000	-0.623541000	4.590477000	H	2.823800000	5.281969000	0.497576000
H	2.119577000	-1.329071000	5.367025000	C	-3.789265000	0.653882000	2.176127000
C	1.798219000	0.732618000	4.599679000	C	-4.790754000	1.443384000	1.578300000
H	1.949819000	1.450913000	5.386947000	H	-4.577563000	1.935089000	0.638422000
C	1.272070000	2.524392000	2.934952000	C	-6.048586000	1.576131000	2.175447000
H	1.689585000	3.140985000	3.735952000	H	-6.809016000	2.186346000	1.696512000
H	1.803132000	2.722139000	2.008263000	C	-6.332793000	0.918151000	3.379480000
H	0.214262000	2.759710000	2.804516000	H	-7.309639000	1.021099000	3.842056000
C	1.579558000	-2.441014000	2.896693000	C	-5.348019000	0.123058000	3.980387000
H	1.626484000	-3.046325000	3.806267000	H	-5.558303000	-0.391068000	4.913455000
H	0.665141000	-2.666063000	2.355651000	C	-4.089933000	-0.008755000	3.383275000
H	2.440461000	-2.663598000	2.263678000	H	-3.326034000	-0.626002000	3.844646000
N	1.576373000	-1.030196000	3.287999000	C	-0.126898000	-4.778374000	-0.419038000
N	1.450051000	1.118508000	3.302321000	C	0.216464000	-5.231943000	-1.709047000
N	-0.456449000	1.594608000	0.574351000	H	0.680202000	-4.535459000	-2.399555000
N	-0.835677000	-1.269802000	0.828524000	C	-0.046570000	-6.548362000	-2.100997000
N	1.917632000	-1.598742000	-0.053409000	H	0.219166000	-6.876693000	-3.101328000
N	2.371232000	1.254890000	-0.073213000	C	-0.656973000	-7.439815000	-1.208078000
C	-0.142826000	2.887842000	0.207447000	H	-0.864359000	-8.461146000	-1.511924000
C	-1.701993000	1.605750000	1.174026000	C	-0.992103000	-7.005721000	0.081147000
C	-2.070569000	-0.863843000	1.270249000	H	-1.453334000	-7.693394000	0.783556000
C	-0.932107000	-2.595316000	0.460445000	C	-0.725901000	-5.689236000	0.472510000
C	1.468871000	-2.901442000	-0.176545000	H	-0.978660000	-5.355307000	1.473029000
C	3.303573000	-1.611030000	-0.138961000	C	5.604924000	-0.668910000	-0.387404000
C	3.661318000	0.854410000	-0.319514000	C	6.148796000	-1.472085000	-1.409319000
C	2.254931000	2.575109000	-0.455381000	H	5.477269000	-1.964733000	-2.104032000
C	-1.221205000	3.762658000	0.639330000	C	7.533314000	-1.621361000	-1.542093000
H	-1.237516000	4.832826000	0.509288000	H	7.933804000	-2.239664000	-2.339793000
C	-2.157129000	2.984624000	1.261591000	C	8.401443000	-0.965535000	-0.659278000
H	-3.075975000	3.310154000	1.720611000	H	9.475870000	-1.081162000	-0.763174000
C	-2.986221000	-1.995122000	1.219426000	C	7.874155000	-0.154139000	-0.353996000
H	-4.032912000	-1.955221000	1.474273000	H	8.539514000	0.359925000	1.041068000
C	-2.293602000	-3.050677000	0.698296000	C	6.489706000	-0.005363000	0.486059000
H	-2.681058000	-4.021491000	0.441982000	H	6.077142000	0.623805000	1.268025000
C	2.620370000	-3.774954000	-0.300733000	C	-2.880764000	-3.712930000	-2.555431000
H	2.570410000	-4.849558000	-0.382043000	C	-2.210688000	-2.524580000	-2.841069000
C	3.742354000	-2.991022000	-0.240411000	C	-2.790668000	-1.273668000	-2.566466000
H	4.770244000	-3.314868000	-0.272008000	C	-4.083120000	-1.235938000	-1.946827000
C	4.412843000	1.978755000	-0.857804000	C	-4.753203000	-2.460922000	-1.666852000
H	5.447993000	1.943397000	-1.160169000	C	-4.168489000	-3.677426000	-1.975327000
C	3.540922000	3.028441000	-0.967692000	C	-2.063254000	-0.016170000	-2.865827000
H	3.739457000	4.006577000	-1.376233000	C	-4.686669000	0.015111000	-1.663522000
C	1.079816000	3.346586000	-0.334897000	C	-4.085142000	1.248119000	-2.022546000
C	-2.449949000	0.467722000	1.547153000	C	-2.798886000	1.252597000	-2.655518000
C	0.137737000	-3.363060000	-0.039017000	C	-2.238886000	2.483329000	-3.043175000
C	4.134151000	-0.474673000	-0.236906000	H	-1.257275000	2.485119000	-3.508147000
C	1.139074000	4.777772000	-0.748069000	C	-2.917142000	3.683011000	-2.831724000
C	0.203042000	5.281368000	-1.672279000	C	-4.184020000	3.684658000	-2.207663000
H	-0.546110000	4.606342000	-2.068279000	C	-4.756446000	2.487537000	-1.811037000
C	0.236775000	6.622239000	-2.066981000	H	-1.085204000	0.008453000	-2.166197000
H	-0.490044000	6.991574000	-2.784683000	H	-2.403453000	-4.665206000	-2.761044000
C	1.207997000	7.486657000	-1.544045000	H	-1.215250000	-2.554621000	-3.275235000
H	1.235715000	8.527726000	-1.850672000	H	-5.735162000	-2.419464000	-1.203018000

H	-4.688274000	-4.605333000	-1.757091000
H	-5.662143000	0.029778000	-1.184499000
H	-2.473769000	4.620967000	-3.151022000
H	-4.707046000	4.621849000	-2.045110000
H	-5.736426000	2.471638000	-1.340983000
H	-1.581939000	-0.047412000	-3.854143000
H	0.901147000	-0.516815000	-2.022659000

<sup>4</sup>TS2<sub>(IS)</sub>

Co	0.752927000	-0.001311000	0.357342000
O	0.233531000	-0.023360000	-1.497888000
C	1.303514000	0.038064000	2.464038000
C	1.880097000	-0.622849000	4.590302000
H	2.121456000	-1.328271000	5.366765000
C	1.798747000	0.733264000	4.599569000
H	1.950129000	1.451616000	5.386827000
C	1.271007000	2.524793000	2.935076000
H	1.688086000	3.141615000	3.736127000
H	1.801886000	2.723039000	2.008383000
H	0.213020000	2.759333000	2.804708000
C	1.581493000	-2.440421000	2.896499000
H	1.628718000	-3.045764000	3.806037000
H	0.667204000	-2.665897000	2.355428000
H	2.442522000	-2.662513000	2.263480000
N	1.577549000	-1.029629000	3.287889000
N	1.450029000	1.119005000	3.302313000
N	-0.457303000	1.594046000	0.574686000
N	-0.834701000	-1.270667000	0.828830000
N	1.918717000	-1.597650000	-0.053627000
N	2.370455000	1.256216000	-0.073190000
C	-0.144579000	2.887498000	0.207797000
C	-1.702759000	1.604350000	1.174572000
C	-2.069860000	-0.865492000	1.270515000
C	-0.930355000	-2.596147000	0.460419000
C	1.470777000	-2.900637000	-0.176828000
C	3.304662000	-1.609059000	-0.139200000
C	3.660793000	0.856603000	-0.319566000
C	2.253258000	2.576349000	-0.455378000
C	-1.223428000	3.761605000	0.639935000
H	-1.240442000	4.831771000	0.509955000
C	-2.158738000	2.982938000	1.262328000
H	-3.077697000	3.307858000	1.721551000
C	-2.984853000	-1.997294000	1.219408000
H	-4.031586000	-1.958041000	1.474187000
C	-2.291592000	-3.052350000	0.698111000
H	-2.678468000	-4.023335000	0.441559000
C	2.622822000	-3.773401000	-0.301148000
H	2.573541000	-4.848031000	-0.382552000
C	3.744311000	-2.988762000	-0.240787000
H	4.772406000	-3.311950000	-0.272456000
C	4.411549000	1.981448000	-0.857885000
H	5.446709000	1.946766000	-1.160299000
C	3.538917000	3.030541000	-0.967763000
H	3.736769000	4.008802000	-1.376338000
C	1.077656000	3.347047000	-0.334772000
C	-2.450025000	0.465823000	1.547582000
C	0.139945000	-3.363120000	-0.039244000
C	4.134508000	-0.472165000	-0.237057000

C	1.135855000	4.778236000	-0.748075000
C	0.199326000	5.281071000	-1.672196000
H	-0.549402000	4.605470000	-2.068011000
C	0.232049000	6.621925000	-2.067042000
H	-0.495139000	6.990670000	-2.784674000
C	1.202736000	7.487085000	-1.544338000
H	1.229670000	8.528142000	-1.851075000
C	2.137213000	7.000210000	-0.620795000
H	2.886929000	7.665786000	-0.203540000
C	2.102776000	5.658824000	-0.224814000
H	2.820406000	5.283760000	0.497273000
C	-3.789527000	0.651134000	2.176401000
C	-4.791329000	1.440220000	1.578538000
H	-4.578217000	1.932219000	0.638787000
C	-6.049333000	1.572199000	2.175487000
H	-6.810000000	2.182103000	1.696530000
C	-6.333402000	0.913855000	3.379356000
H	-7.310381000	1.016208000	3.841783000
C	-5.348312000	0.119177000	3.980298000
H	-5.558488000	-0.395217000	4.913242000
C	-4.090053000	-0.011873000	3.383382000
H	-3.325905000	-0.628789000	3.844781000
C	-0.123820000	-4.778550000	-0.419437000
C	0.219708000	-5.231733000	-1.709537000
H	0.682921000	-4.534859000	-2.400004000
C	-0.042511000	-6.548275000	-2.101621000
H	0.223335000	-6.876312000	-3.102019000
C	-0.652242000	-7.440233000	-1.208747000
H	-0.858987000	-8.461663000	-1.512696000
C	-0.987542000	-7.006513000	0.080559000
H	-1.448268000	-7.694569000	0.782924000
C	-0.722166000	-5.689900000	0.472054000
H	-0.975066000	-5.356245000	1.472629000
C	5.605400000	-0.665441000	-0.387596000
C	6.149772000	-1.468154000	-1.409607000
H	5.478550000	-1.961158000	-2.104361000
C	7.534384000	-1.616528000	-1.542412000
H	7.935262000	-2.234486000	-2.340184000
C	8.402100000	-0.960248000	-0.659529000
H	9.476600000	-1.075179000	-0.763447000
C	7.874306000	-0.149303000	0.353842000
H	8.539345000	0.365107000	1.040965000
C	6.489763000	-0.001421000	0.485932000
H	6.076802000	0.627398000	1.267969000
C	-2.878697000	-3.713676000	-2.556304000
C	-2.209498000	-2.524799000	-2.841814000
C	-2.790225000	-1.274354000	-2.566669000
C	-4.082573000	-1.237648000	-1.946751000
C	-4.751748000	-2.463158000	-1.666914000

C	-4.166278000	-3.679190000	-1.975819000
C	-2.063571000	-0.016300000	-2.865497000
C	-4.686922000	0.012930000	-1.663077000
C	-4.086301000	1.246418000	-2.021963000
C	-2.800103000	1.251912000	-2.655058000
C	-2.240993000	2.483120000	-3.042497000
H	-1.259433000	2.485692000	-3.507579000
C	-2.920048000	3.682292000	-2.830698000
C	-4.186866000	3.682931000	-2.206514000
C	-4.758435000	2.485325000	-1.810104000
H	-1.085938000	0.008665000	-2.165226000
H	-2.400815000	-4.665578000	-2.762327000
H	-1.214164000	-2.554049000	-3.276277000
H	-5.733635000	-2.422492000	-1.202856000
H	-4.685372000	-4.607502000	-1.757669000
H	-5.662333000	0.026846000	-1.183904000
H	-2.477313000	4.620632000	-3.149754000
H	-4.710510000	4.619728000	-2.043683000
H	-5.738349000	2.468644000	-1.339935000
H	-1.581682000	-0.046945000	-3.853531000
H	0.900240000	-0.517159000	-2.022615000

<sup>2</sup>TS2<sub>(LS)</sub>

Co	-0.739336000	0.054057000	0.229924000
O	-0.166699000	0.028686000	-1.626086000
C	-1.301612000	0.034650000	2.143818000
C	-1.794215000	0.682078000	4.286790000
H	-1.900598000	1.377515000	5.101050000
C	-2.021482000	-0.653526000	4.208531000
H	-2.359173000	-1.364103000	4.942697000
C	-1.839523000	-2.435968000	2.478253000
H	-2.437796000	-2.959914000	3.228793000
H	-2.340003000	-2.488482000	1.517223000
H	-0.855551000	-2.901987000	2.405295000
C	-1.041841000	2.497185000	2.756485000
H	-0.935224000	3.004032000	3.719387000
H	-0.109738000	2.567363000	2.206750000
H	-1.842296000	2.967183000	2.182812000
N	-1.355382000	1.089763000	3.025474000
N	-1.720951000	-1.036101000	2.899846000
N	0.170702000	-1.655931000	0.407237000
N	0.910812000	0.983500000	0.692647000
N	-1.617176000	1.773810000	-0.099523000
N	-2.385026000	-0.855306000	-0.300026000
C	-0.234766000	-2.849721000	-0.152937000
C	1.293812000	-1.915283000	1.177350000
C	1.984886000	0.428439000	1.361374000
C	1.288894000	2.254048000	0.282765000
C	-0.981423000	2.979926000	-0.315563000
C	-2.983988000	2.028790000	-0.020969000
C	-3.656175000	-0.310512000	-0.309268000
C	-2.473713000	-2.122595000	-0.852182000
C	0.647519000	-3.904191000	0.304312000
H	0.553870000	-4.940768000	0.023505000
C	1.548596000	-3.340294000	1.165136000
H	2.341092000	-3.833994000	1.701957000
C	3.062881000	1.387492000	1.402249000
H	4.035091000	1.193567000	1.825083000

C	2.657410000	2.484122000	0.692045000
H	3.245967000	3.342023000	0.422065000
C	-1.972136000	4.031913000	-0.346873000
H	-1.746639000	5.077996000	-0.480799000
C	-3.194457000	3.454201000	-0.111500000
H	-4.150670000	3.945855000	-0.034674000
C	-4.576146000	-1.268506000	-0.876901000
H	-5.629874000	-1.090219000	-1.024177000
C	-3.842409000	-2.363932000	-1.252605000
H	-4.191362000	-3.256219000	-1.746682000
C	-1.437112000	-3.070427000	-0.840059000
C	2.114301000	-0.922830000	1.729776000
C	0.410619000	3.202397000	-0.268695000
C	-3.970872000	1.034436000	-0.042550000
C	-1.671689000	-4.419782000	-1.425916000
C	-0.822401000	-4.896747000	-2.441517000
H	-0.023789000	-4.256270000	-2.792414000
C	-1.009796000	-6.168687000	-2.992636000
H	-0.348718000	-6.517126000	-3.780500000
C	-2.050373000	-6.987880000	-2.535156000
H	-2.196858000	-7.975174000	-2.962130000
C	-2.900461000	-6.525532000	-1.521845000
H	-3.704383000	-7.157210000	-1.155968000
C	-2.711273000	-5.253411000	-0.970645000
H	-3.362477000	-4.899975000	-0.177943000
C	3.255361000	-1.277662000	2.615411000
C	4.244331000	-2.205315000	2.237437000
H	4.181834000	-2.671941000	1.263047000
C	5.313360000	-2.494076000	3.092516000
H	6.071449000	-3.206772000	2.781419000
C	5.417450000	-1.857925000	4.336303000
H	6.248605000	-2.082632000	4.997646000
C	4.446102000	-0.922691000	4.717519000
H	4.520507000	-0.420757000	5.677523000
C	3.377543000	-0.633379000	3.863188000

H	2.624621000	0.093037000	4.151782000
C	0.902598000	4.528741000	-0.720658000
C	0.533531000	4.995842000	-1.999552000
H	-0.095982000	4.368234000	-2.621249000
C	0.985616000	6.229811000	-2.474113000
H	0.698135000	6.563857000	-3.466462000
C	1.817322000	7.028145000	-1.676818000
H	2.176363000	7.983717000	-2.046047000
C	2.171842000	6.588280000	-0.394885000
H	2.797764000	7.209414000	0.238738000
C	1.711532000	5.356678000	0.081743000
H	1.970009000	5.033934000	1.083619000
C	-5.410688000	1.397201000	0.054227000
C	-6.007474000	2.335437000	-0.810556000
H	-5.401890000	2.805431000	-1.577403000
C	-7.368628000	2.640381000	-0.703174000
H	-7.813522000	3.361227000	-1.382329000
C	-8.159421000	2.008147000	0.265204000
H	-9.215594000	2.245232000	0.347087000
C	-7.581006000	1.061583000	1.121167000
H	-8.187896000	0.563249000	1.870995000
C	-6.220409000	0.756775000	1.013614000
H	-5.767814000	0.022227000	1.671930000
C	3.507577000	3.480148000	-2.613580000
C	2.706451000	2.366759000	-2.857898000
C	3.064652000	1.082172000	-2.399739000
C	4.277739000	0.944772000	-1.639457000
C	5.078719000	2.096456000	-1.399023000
C	4.709096000	3.341243000	-1.885527000
C	2.225813000	-0.091301000	-2.663437000
C	4.670242000	-0.336806000	-1.181422000
C	3.966951000	-1.513577000	-1.536475000
C	2.764410000	-1.409179000	-2.320471000
C	2.117898000	-2.596441000	-2.719584000
H	1.204288000	-2.510865000	-3.301328000
C	2.620246000	-3.849265000	-2.373259000
C	3.803002000	-3.955734000	-1.610331000
C	4.461978000	-2.807251000	-1.200951000
H	1.056332000	0.011570000	-1.991515000
H	3.195126000	4.458047000	-2.963343000
H	1.777936000	2.481815000	-3.411159000
H	5.994655000	1.976116000	-0.825615000
H	5.332611000	4.210485000	-1.698501000
H	5.586171000	-0.429382000	-0.602709000
H	2.103747000	-4.750032000	-2.688913000
H	4.195745000	-4.934636000	-1.351931000
H	5.388391000	-2.872953000	-0.635606000
H	1.739515000	-0.064776000	-3.647742000
H	-0.695937000	0.668960000	-2.143030000

<sup>4</sup>Int2<sub>(HS)</sub>

Co	-0.019301211	0.015890664	-0.220201237
O	0.306062891	0.332389460	-2.368165029
C	-0.041287996	-0.083728541	2.072522167
C	0.631064507	-0.151148368	4.279189707
H	1.339272474	-0.147050420	5.090313653
C	-0.727421334	-0.223373654	4.271578022
H	-1.440730040	-0.302346480	5.074355784

C	-2.512479073	-0.245857867	2.503496818
H	-3.151536274	-0.036596840	3.366402875
H	-2.683309660	0.499143265	1.730417542
H	-2.746809872	-1.235310312	2.104117223
C	2.428620884	0.049455318	2.536092020
H	3.061195134	-0.189448630	3.396007696
H	2.626764954	-0.650236599	1.728190764

H	2.645553393	1.062231780	2.189665076	C	5.546585623	0.409714956	-1.915182953
N	1.028204624	-0.068472890	2.941500532	H	4.924708162	1.028167053	-2.554046475
N	-1.115514108	-0.177800381	2.929719459	C	6.928444166	0.345621537	-2.122365372
N	-1.578708246	-1.330138875	-0.384571628	H	7.379008959	0.914535234	-2.929996747
N	1.360865023	-1.539116262	-0.384917710	C	7.728364370	-0.453710223	-1.295160259
N	1.588742505	1.341664355	-0.272917874	H	8.800792867	-0.504345077	-1.455843872
N	-1.382815295	1.559688557	-0.308137266	C	7.135643517	-1.185262844	-0.257628356
C	-2.921905098	-1.025318492	-0.503020018	H	7.749197020	-1.800125532	0.393956587
C	-1.468178994	-2.690735604	-0.169289623	C	5.753755870	-1.119246395	-0.050523198
C	1.035772388	-2.880222865	-0.337757963	H	5.294645922	-1.678680941	0.757725728
C	2.721986696	-1.441635992	-0.640140956	C	0.334948561	4.906439376	0.124193138
C	2.925531550	1.049987147	-0.420245054	C	1.085180080	5.710732172	-0.755487308
C	1.466985170	2.699453800	-0.066980610	H	1.613115350	5.237745080	-1.576502635
C	-1.042205596	2.892876022	-0.260450458	C	1.140445765	7.098240211	-0.584592161
C	-2.726683673	1.472400770	-0.614308110	H	1.718889416	7.703341695	-1.276187667
C	-3.696144860	-2.237696378	-0.289206479	C	0.443303953	7.707346508	0.467198422
H	-4.773493117	-2.293178496	-0.284064464	H	0.485889492	8.784123783	0.599181049
C	-2.806236477	-3.254113579	-0.062329142	C	-0.312738992	6.918987768	1.344668494
H	-3.032193574	-4.286148917	0.154520286	H	-0.855838365	7.382885712	2.162553738
C	2.233849789	-3.662586556	-0.603917185	C	-0.367840631	5.531880846	1.172680597
H	2.270036516	-4.739477604	-0.658099644	H	-0.952467718	4.917275868	1.849312028
C	3.261526823	-2.781914432	-0.809528476	H	1.158201778	-0.129601329	-2.499264459
H	4.284692092	-3.014680453	-1.058825466	H	-0.390630708	-0.098388338	-2.901828642
C	3.698498111	2.268400300	-0.217105021				
H	4.775207652	2.332829747	-0.235782861				
C	2.804554751	3.276685105	0.021810040				
H	3.024932733	4.311290658	0.231663745				
C	-2.226637632	3.688942229	-0.560028812				
H	-2.249636733	4.765870319	-0.618488081				
C	-3.254579255	2.817924944	-0.795478291				
H	-4.266631802	3.057396699	-1.081152512				
C	-3.464219172	0.267977476	-0.688154266				
C	-0.257940042	-3.420451451	-0.143521866				
C	3.463736563	-0.237443419	-0.656494649				
C	0.253575388	3.424848914	-0.050955006				
C	-4.935954237	0.360271809	-0.908388841				
C	-5.551018541	-0.364709489	-1.948620076				
H	-4.932173266	-0.979049879	-2.594112601				
C	-6.932805115	-0.293906632	-2.152894136				
H	-7.386976252	-0.855146201	-2.963886317				
C	-7.728221493	0.503396263	-1.319322492				
H	-8.800713490	0.559357286	-1.477863996				
C	-7.130599400	1.226786325	-0.278819788				
H	-7.740439137	1.840548323	0.377271099				
C	-5.748789013	1.154277929	-0.074634101				
H	-5.285975353	1.707672445	0.735557434				
C	-0.340100101	-4.900136346	0.039516840				
C	-1.100747417	-5.707975159	-0.828287281				
H	-1.636484876	-5.238918796	-1.646641375				
C	-1.159437936	-7.094234339	-0.648844863				
H	-1.746587082	-7.701264145	-1.331376091				
C	-0.454945323	-7.699612583	0.400101922				
H	-0.499884642	-8.775418288	0.538789754				
C	0.310539731	-6.908278279	1.266740265				
H	0.858270463	-7.368995338	2.083320557				
C	0.367978217	-5.522386348	1.086775550				
H	0.957940998	-4.905303762	1.756389561				
C	4.936792983	-0.324234838	-0.878522077				



$^2\text{Int2}_{(LS)}$ 

Co	-0.012034000	0.000068000	-0.213195000	C	-6.998498000	-0.906097000	-1.504426000
O	0.006304000	0.007052000	-2.282376000	H	-7.899158000	-0.564251000	-1.003175000
C	-0.006369000	-0.004582000	1.723842000	C	-5.744382000	-0.563201000	-0.987107000
C	0.644280000	0.210492000	3.902343000	H	-5.672735000	0.031078000	-0.082693000
H	1.320960000	0.444569000	4.705308000	C	1.042237000	-4.608007000	0.914486000
C	-0.640311000	-0.227507000	3.906254000	C	0.597582000	-5.783178000	0.274219000
H	-1.311172000	-0.464232000	4.713305000	H	-0.018110000	-5.698101000	-0.613911000
C	-2.366338000	-0.844089000	2.219605000	C	0.964627000	-7.044210000	0.754606000
H	-2.989138000	-0.774598000	3.115546000	H	0.616869000	-7.936324000	0.242190000
H	-2.788816000	-0.224896000	1.435832000	C	1.790682000	-7.159953000	1.880855000
H	-2.318614000	-1.881680000	1.884891000	H	2.074753000	-8.139706000	2.252380000
C	2.358240000	0.831971000	2.205564000	C	2.252318000	-6.001395000	2.518984000
H	2.987028000	0.759562000	3.097077000	H	2.895884000	-6.079648000	3.390296000
H	2.776138000	0.214964000	1.417499000	C	1.881265000	-4.740551000	2.040587000
H	2.309192000	1.870514000	1.874203000	H	2.233685000	-3.840565000	2.534501000
N	1.022428000	0.341712000	2.565629000	C	4.563065000	1.001419000	-1.610324000
N	-1.028337000	-0.354153000	2.572119000	C	4.689002000	1.821578000	-2.750409000
N	-1.042249000	-1.652163000	-0.332799000	H	3.788474000	2.185998000	-3.234121000
N	1.625269000	-1.065994000	-0.301239000	C	5.947009000	2.168616000	-3.251632000
N	1.030318000	1.654759000	-0.343589000	H	6.020805000	2.795217000	-4.135349000
N	-1.642056000	1.059410000	-0.264060000	C	7.109555000	1.708260000	-2.618147000
C	-2.370008000	-1.755275000	-0.732175000	H	8.086917000	1.976920000	-3.006761000
C	-0.653169000	-2.902738000	0.138190000	C	7.000637000	0.907762000	-1.474160000
C	1.746558000	-2.403064000	0.060220000	H	7.895321000	0.561773000	-0.965188000
C	2.866272000	-0.653794000	-0.813336000	C	5.740805000	0.563393000	-0.972059000
C	2.365915000	1.759261000	-0.740059000	H	5.659533000	-0.034961000	-0.071298000
C	0.643902000	2.904397000	0.136014000	C	-1.050811000	4.606751000	0.919272000
C	-1.755619000	2.397422000	0.072374000	C	-0.598918000	5.782591000	0.284590000
C	-2.870288000	0.651918000	-0.799463000	H	0.022478000	5.698147000	-0.599579000
C	-2.826105000	-3.083283000	-0.484339000	C	-0.968111000	7.043648000	0.763049000
H	-3.827321000	-3.435267000	-0.677979000	H	-0.614825000	7.935668000	0.254179000
C	-1.777043000	-3.783576000	0.094460000	C	-1.804215000	7.159843000	1.881823000
H	-1.780535000	-4.809052000	0.425682000	H	-2.090105000	8.139673000	2.251763000
C	3.098480000	-2.842846000	-0.234834000	C	-2.274073000	6.001143000	2.513820000
H	3.456805000	-3.847698000	-0.074171000	H	-2.926064000	6.079371000	3.378876000
C	3.755718000	-1.801935000	-0.823532000	C	-1.900720000	4.740350000	2.037553000
H	4.758085000	-1.798945000	-1.220605000	H	-2.260150000	3.840615000	2.526870000
C	2.819857000	3.084558000	-0.484278000	H	0.510119000	0.809570000	-2.527734000
H	3.821491000	3.438232000	-0.672748000	H	0.481099000	-0.805227000	-2.547441000
C	1.769731000	3.781486000	0.098927000				
H	1.775901000	4.804030000	0.438969000				
C	-3.102280000	2.845293000	-0.243675000				
H	-3.453868000	3.854984000	-0.100130000				
C	-3.756413000	1.802353000	-0.830269000				
H	-4.751872000	1.799443000	-1.244358000				
C	-3.213781000	-0.663317000	-1.080469000				
C	0.698617000	-3.251593000	0.415213000				
C	3.210593000	0.664826000	-1.089387000				
C	-0.706085000	3.250372000	0.423161000				
C	-4.560353000	-0.997019000	-1.615934000				
C	-4.671275000	-1.808411000	-2.763605000				
H	-3.763509000	-2.160589000	-3.242064000				
C	-5.923834000	-2.152628000	-3.280154000				
H	-5.987983000	-2.771219000	-4.170278000				
C	-7.093638000	-1.699146000	-2.654799000				
H	-8.066552000	-1.966462000	-3.055546000				

**9,10-dihydroanthracene (DHA)**

C	3.725398000	0.701597000	0.000000000
C	2.511681000	1.389179000	0.000000000
C	1.283565000	0.702240000	0.000000000
C	1.283565000	-0.702240000	0.000000000
C	2.511681000	-1.389179000	0.000000000
C	3.725398000	-0.701597000	0.000000000
C	0.000000000	1.508234000	0.000000000
C	0.000000000	-1.508234000	0.000000000
C	-1.283565000	-0.702240000	0.000000000
C	-1.283565000	0.702240000	0.000000000
C	-2.511681000	1.389179000	0.000000000
H	-2.504187000	2.476441000	0.000000000
C	-3.725398000	0.701597000	0.000000000
C	-3.725398000	-0.701597000	0.000000000
C	-2.511681000	-1.389179000	0.000000000
H	0.000000000	2.177600000	0.874972000
H	4.662698000	1.249235000	0.000000000
H	2.504187000	2.476441000	0.000000000
H	2.504187000	-2.476441000	0.000000000
H	4.662698000	-1.249235000	0.000000000
H	0.000000000	-2.177600000	-0.874972000
H	-4.662698000	1.249235000	0.000000000
H	-4.662698000	-1.249235000	0.000000000
H	-2.504187000	-2.476441000	0.000000000
H	0.000000000	2.177600000	-0.874972000
H	0.000000000	-2.177600000	0.874972000

**mono-hydroanthracene (MHA)**

C	-3.697725000	0.757749000	-0.011799000
C	-2.480025000	1.429029000	-0.000148000
C	-1.250063000	0.717114000	0.008353000
C	-1.285051000	-0.710195000	0.006172000
C	-2.519501000	-1.365435000	-0.006911000
C	-3.723473000	-0.648423000	-0.015977000
C	0.000000000	1.404111000	0.014906000
C	0.000000000	-1.517199000	0.025420000
C	1.285051000	-0.710195000	0.006172000
C	1.250063000	0.717114000	0.008353000
C	2.480025000	1.429029000	-0.000148000
H	2.450590000	2.515196000	0.001755000
C	3.697725000	0.757749000	-0.011799000
C	3.723473000	-0.648423000	-0.015977000
C	2.519501000	-1.365435000	-0.006911000
H	-4.627319000	1.318410000	-0.018326000
H	-2.450590000	2.515196000	0.001755000
H	-2.539759000	-2.452666000	-0.009530000
H	-4.671072000	-1.177487000	-0.026094000
H	0.000000000	-2.164287000	0.918447000
H	4.627319000	1.318410000	-0.018326000
H	4.671072000	-1.177487000	-0.026094000
H	2.539759000	-2.452666000	-0.009530000
H	0.000000000	2.490690000	0.017096000
H	0.000000000	-2.212850000	-0.829388000

**Anthracene**

C	0.000037000	0.715128000	3.668102000
C	0.000003000	1.411675000	2.482779000
C	-0.000040000	0.725049000	1.225423000
C	-0.000040000	-0.725049000	1.225423000
C	0.000003000	-1.411675000	2.482779000

C	0.000037000	-0.715128000	3.668102000
C	-0.000034000	1.409011000	0.000000000
C	-0.000034000	-1.409011000	0.000000000
C	-0.000040000	-0.725049000	-1.225423000
C	-0.000040000	0.725049000	-1.225423000
C	0.000003000	1.411675000	-2.482779000
H	0.000032000	2.498196000	-2.477097000
C	0.000037000	0.715128000	-3.668102000
C	0.000037000	-0.715128000	-3.668102000
C	0.000003000	-1.411675000	-2.482779000
H	-0.000061000	2.496319000	0.000000000
H	0.000093000	1.247068000	4.614328000
H	0.000032000	2.498196000	2.477097000
H	0.000032000	-2.498196000	2.477097000
H	0.000093000	-1.247068000	4.614328000
H	-0.000054000	-2.496319000	0.000000000
H	0.000093000	1.247068000	-4.614328000
H	0.000093000	-1.247068000	-4.614328000
H	0.000032000	-2.498196000	-2.477097000

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