

Deciphering the Origin of Million-fold Reactivity Observed for the Open Core Diiron [HO-Fe^{III}-O-Fe^{IV}=O]²⁺ Species Towards C-H Bond Activation: Role of Spin-states, Spin-coupling, and Spin-cooperation

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Table S1^a. Computed energy of possible spin states of complexes.

Spin states	B3LYP-D3/def2-TZVP ($\Delta E + GFE$) (kJ/mol)	
1		
¹⁰ 1 _(hs, hs)	6.9	42.9
² 1 _(hs, hs)	0.0	
⁸ 1 _(hs, is)	42.8	
⁴ 1 _(hs, is)	56.2	
⁶ 1 _(hs, ls)	69.9	
⁸ 1 _(is, hs)	38.5	
⁴ 1 _(is, hs)	35.6	
⁶ 1 _(is, is)	79.9	
² 1 _(is, is)	81.5	
⁴ 1 _(is, ls)	118.9	
⁶ 1 _(ls, hs)	51.3	
⁴ 1 _(ls, hs)	86.6	
⁴ 1 _(ls, is)	111.3	
² 1 _(ls, is)	111.6	
² 1 _(ls, ls)	150.8	
RC		
¹⁰ RC _(hs, hs)	14.5	39.7
² RC _(hs, hs)	0.0	
⁸ RC _(hs, is)	29.4	
⁴ RC _(hs, is)	29.6	
⁶ RC _(is, is)	74.7	
² RC _(is, is)	75.9	
⁴ RC _(ls, is)	104.0	
² RC _(ls, is)	106.1	
² RC _(ls, ls)	185.9	
I-TS_H		
I - ¹⁰ TS_H _(hs, hs)	19.5	45.7
I - ² TS_H _(hs, hs)	0.0	
I - ⁸ TS_H _(hs, is)	78.6	
I - ⁴ TS_H _(hs, is)	79.4	
I - ⁶ TS_H _(is, is)	90.8	
I - ² TS_H _(is, is)	113.5	
I - ⁴ TS_H _(ls, is)	149.7	
I - ² TS_H _(ls, is)	158.5	
I - ² TS_H _(ls, ls)	177.6	
I-Int1		
I - ¹² Int1 _(hs, hs)	23.4	
I - ¹⁰ Int1 _(hs, hs)	22.6	
I - ² Int1 _(hs, hs)	0.0	

Table S1^b. Computed energy of possible spin states of complexes.

I-Int1		20.4
I-¹⁰Int1 _(hs, is)	76.9	
I-⁸Int1 _(hs, is)	73.4	
I-⁴Int1 _(hs, is)	61.9	
I-²Int1 _(hs, is)	50.6	
I-⁸Int1 _(is, is)	113.9	
I-⁶Int1 _(is, is)	93.2	
I-²Int1 _(is, is)	88.5	
I-⁴Int1 _(ls, ls)	182.9	
I-²Int1 _(ls, ls)	143.4	
I-²Int1 _(ls, ls)	143.4	
I-⁶Int1 _(ls, is)	119.8	
I-⁴Int1 _(ls, is)	120.7	
I-⁴Int1 _(ls, is)	106.2	
I-²Int1 _(ls, is)	116.9	
Ia-TS_{Reb}		9.2
Ia-¹²TS_{Reb} _(hs, hs)	122.8	
Ia-¹⁰TS_{Reb} _(hs, hs)	16.0	
Ia-²TS_{Reb} _(hs, hs)	0.0	
Ia-¹⁰TS_{Reb} _(hs, is)	45.9	
Ia-⁸TS_{Reb} _(hs, is)	70.9	
Ia-⁴TS_{Reb} _(hs, is)	62.2	
Ia-²TS_{Reb} _(hs, is)	48.7	
Ia-⁸TS_{Reb} _(is, is)	108.9	
Ia-⁶TS_{Reb} _(is, is)	122.3	
Ia-²TS_{Reb} _(is, is)	119.8	
Ia-⁴TS_{Reb} _(ls, ls)	173.5	
Ia-²TS_{Reb} _(ls, ls)	184.4	
Ia-²TS_{Reb} _(ls, ls)	192.8	
Ia-⁶TS_{Reb} _(ls, is)	161.9	
Ia-⁴TS_{Reb} _(ls, is)	136.9	
Ia-⁴TS_{Reb} _(ls, is)	132.7	
Ia-²TS_{Reb} _(ls, is)	163.8	
Ib-TS_{2H}		
Ib-¹²TS_{2H} _(hs, hs)	117.3	
Ib-¹⁰TS_{2H} _(hs, hs)	23.1	
Ib-²TS_{2H} _(hs, hs)	0.0	
Ib-¹⁰TS_{2H} _(hs, is)	44.1	
Ib-⁸TS_{2H} _(hs, is)	66.9	
Ib-⁴TS_{2H} _(hs, is)	99.9	

Table S1^c. Computed energy of possible spin states of complexes.

Ib-TS_{2H}		-170.9
Ib-²TS_{2H}(hs, is)	32.7	
Ib-⁸TS_{2H}(is, is)	93.4	
Ib-⁶TS_{2H}(is, is)	143.5	
Ib-²TS_{2H}(is, is)	198.3	
Ib-⁴TS_{2H}(ls, ls)	199.6	
Ib-²TS_{2H}(ls, ls)	199.1	
Ib-²TS_{2H}(ls, ls)	176.7	
Ib-⁶TS_{2H}(ls, is)	173.5	
Ib-⁴TS_{2H}(ls, is)	153.2	
Ib-⁴TS_{2H}(ls, is)	137.2	
Ib-²TS_{2H}(ls, is)	154.7	
Ia-P_{Reb}		11.1
Ia-¹⁰P_{Reb}(hs, hs)	11.4	
Ia-²P_{Reb}(hs, hs)	0.0	
Ia-⁸P_{Reb}(hs, is)	49.2	
Ia-⁴P_{Reb}(hs, is)	54.9	
Ia-⁶P_{Reb}(is, is)	115.5	
Ia-²P_{Reb}(is, is)	109.6	
Ia-⁴P_{Reb}(is, ls)	147.3	
Ia-²P_{Reb}(is, ls)	164.1	
Ia-²P_{Reb}(ls, ls)	169.6	
Ib-P_{2H}		
Ib-¹⁰P_{2H}(hs, hs)	19.3	
Ib-²P_{2H}(hs, hs)	0.0	
Ib-⁸P_{2H}(hs, is)	58.7	
Ib-⁴P_{2H}(hs, is)	62.1	
Ib-⁶P_{2H}(is, is)	125.3	
Ib-²P_{2H}(is, is)	114.6	
Ib-⁴P_{2H}(is, ls)	111.3	
Ib-²P_{2H}(ls, ls)	149.5	

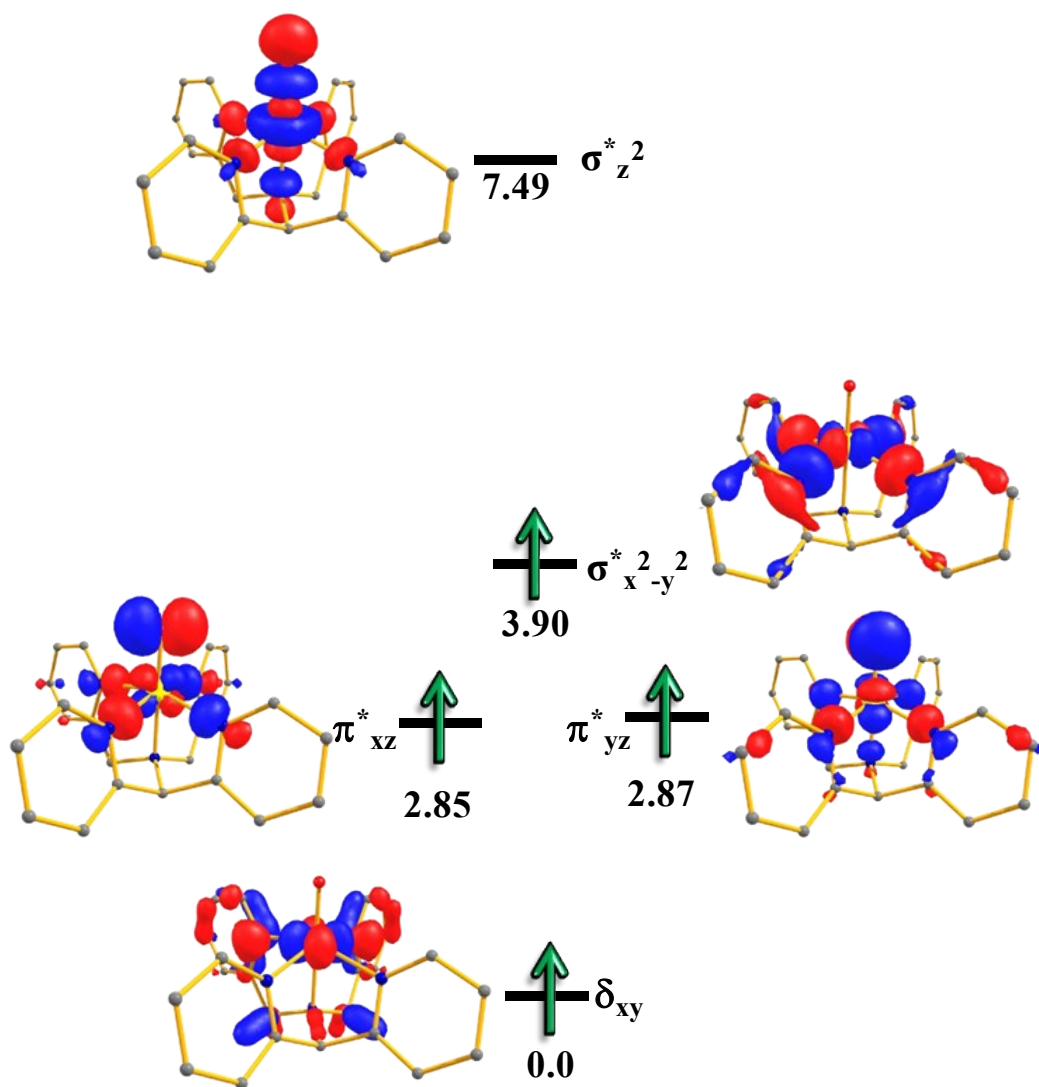


Figure S1. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the quintet state of the $[(\text{N4Py})\text{Fe}^{\text{IV}}=\text{O}]^{2+}$ complex (energies are given in eV).

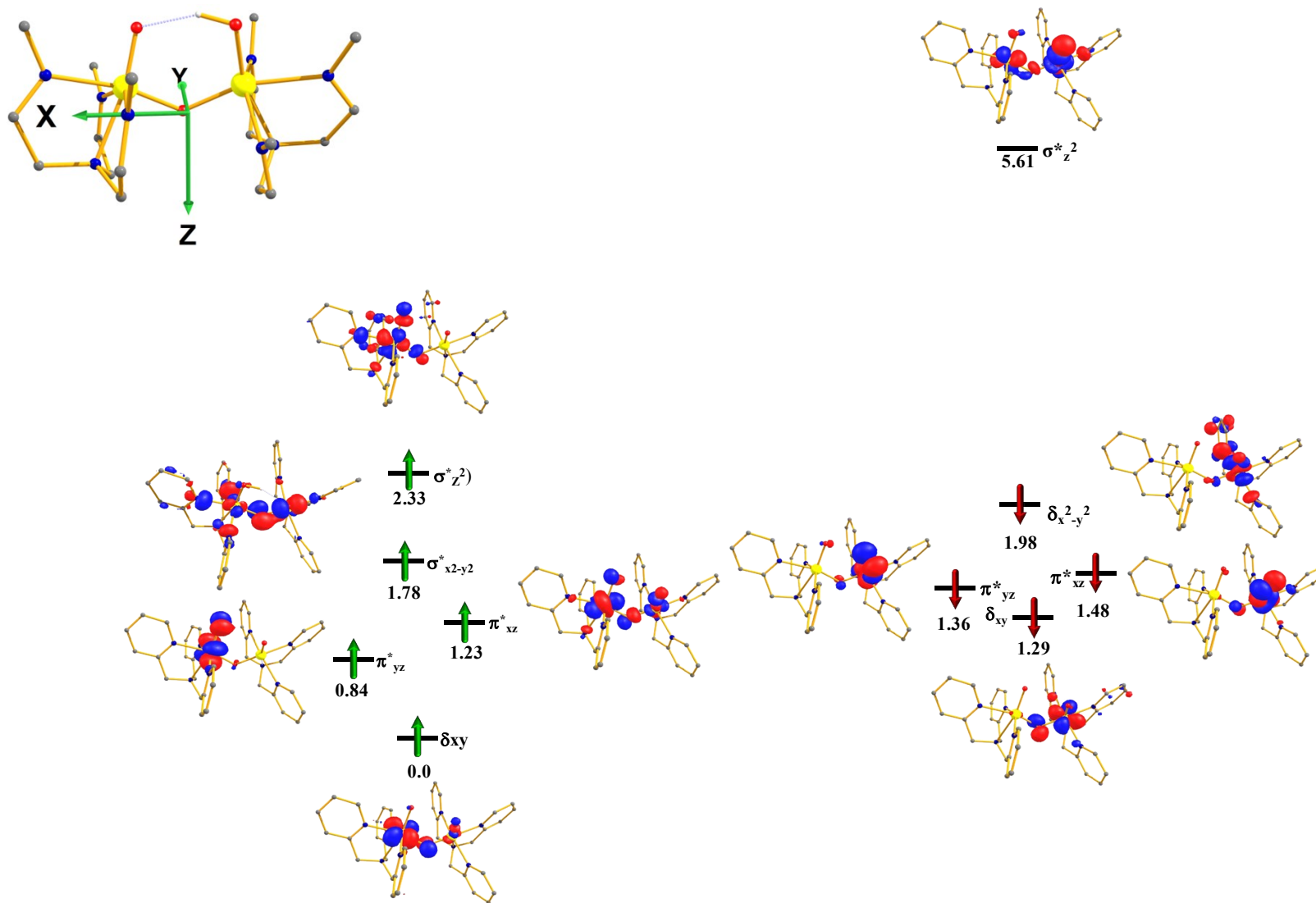


Figure S2. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state $^2\mathbf{1}_{\text{hs-hs}}$ of the complex **1** (energies are given in eV).

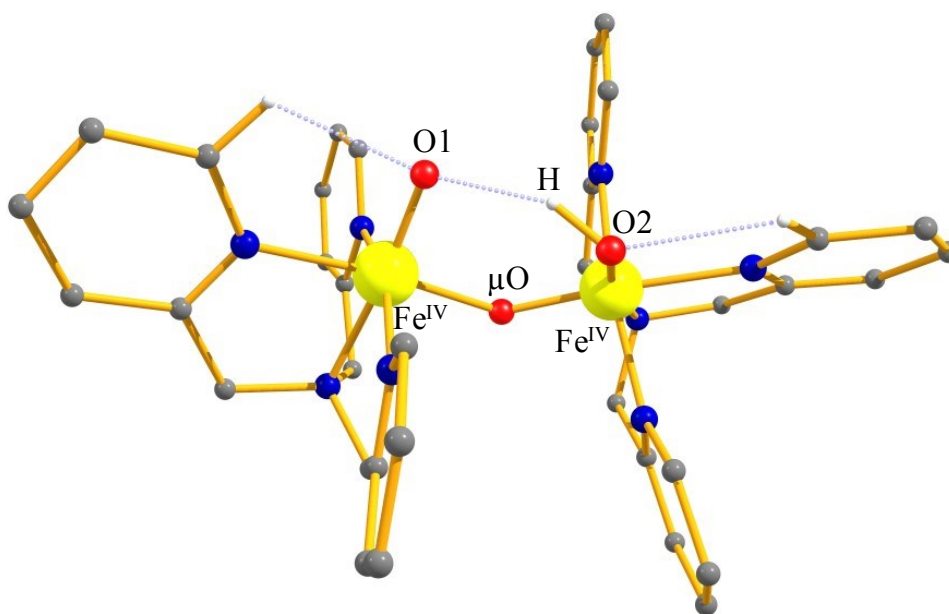


Figure S3. The optimized structure of the ground state of $[\text{HO}-(\text{L})\text{Fe}^{\text{IV}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{3+}$.

Table S2. Computed energy of possible spin states of $[\text{HO}-(\text{L})\text{Fe}^{\text{IV}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{3+}$ species.

Spin states	B3LYP-D3/def2-TZVP ($\Delta\text{E}+\text{GFE}$) (kJ/mol)
$[\text{HO}-(\text{L})\text{Fe}^{\text{IV}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L})]^{3+}$	
$^9\text{R}_{(\text{hs}, \text{hs})}$	35.8
$^1\text{R}_{(\text{hs}, \text{hs})}$	23.5
$^5\text{R}_{(\text{is}, \text{is})}$	0.0
$^1\text{R}_{(\text{is}, \text{is})}$	12.8

Table S3. SHAPE measures of six co-ordinates relative to structures of $^2\mathbf{1}_{\text{hs-hs}}$.

$^2\mathbf{1}_{\text{hs-hs}}$	Shape	Symmetry	Deviation
Fe^{IV}	Johnson pentagonal pyramid	C5v	30.017
	Trigonal prism	D3h	14.662
	Octahedron	Oh	1.336
	Pentagonal pyramid	C5v	26.616
	Hexagon	D6h	33.004
Fe^{III}	Johnson pentagonal pyramid	C5v	30.849
	Trigonal prism	D3h	14.056
	Octahedron	Oh	1.183
	Pentagonal pyramid	C5v	27.442
	Hexagon	D6h	33.674

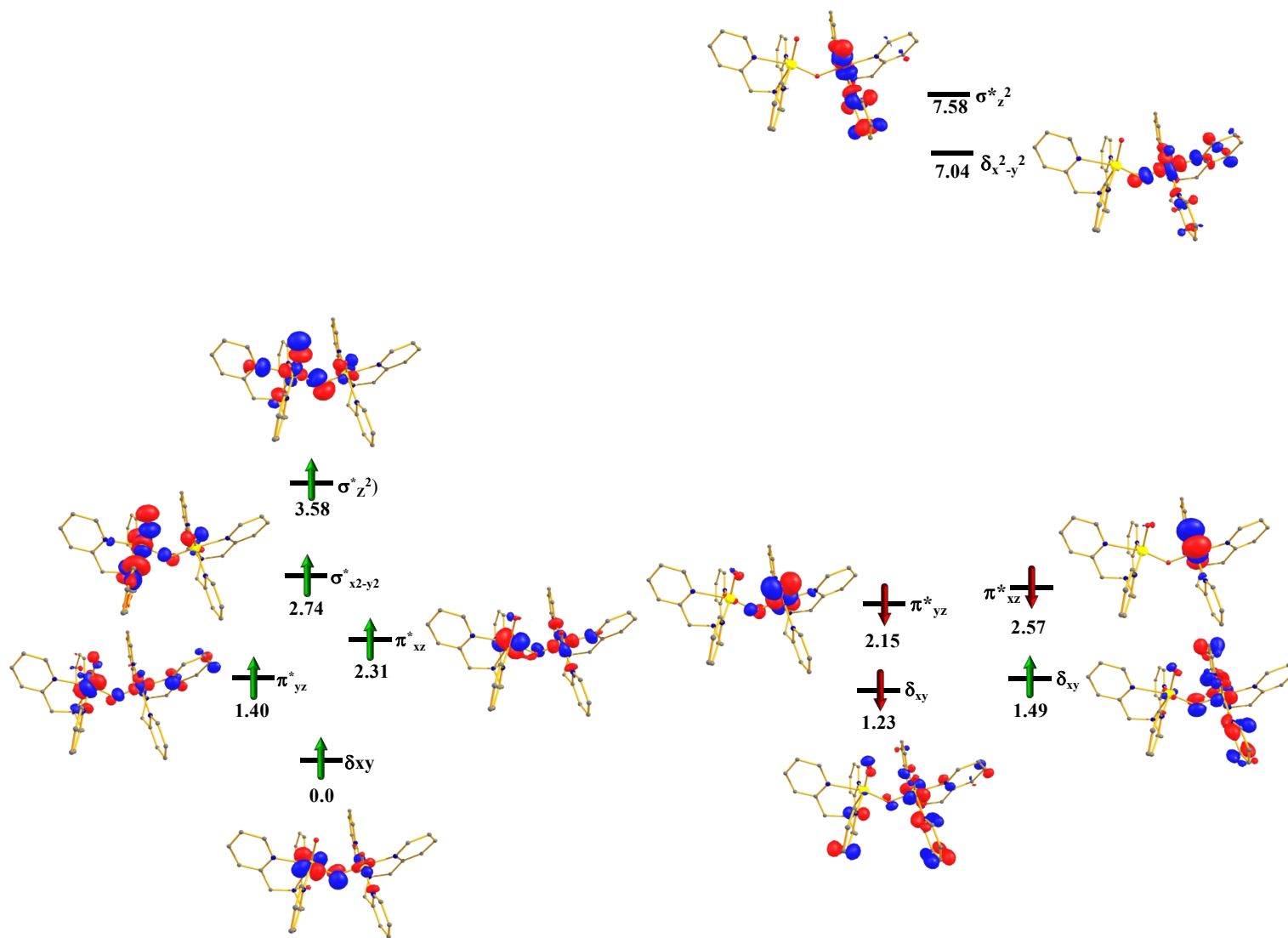


Figure S4. Computed eigenvalue plot incorporating energies computed for d-based orbitals for alpha and beta spin corresponding to the ground state $^4\mathbf{1}_{\text{hs-is}}$ of the complex **1** (energies are given in eV).

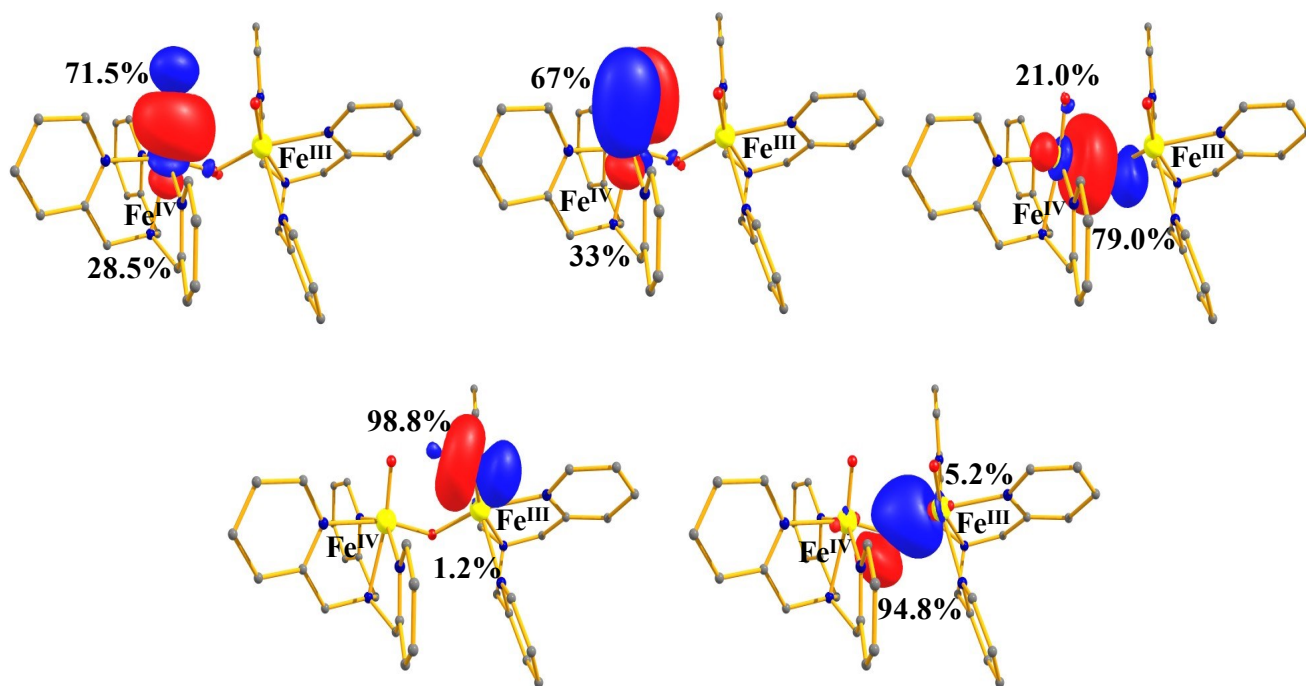
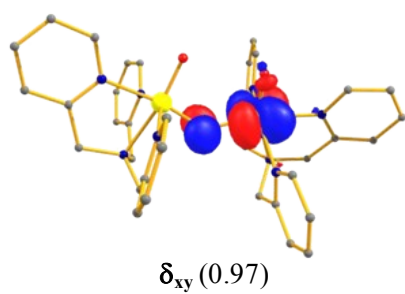
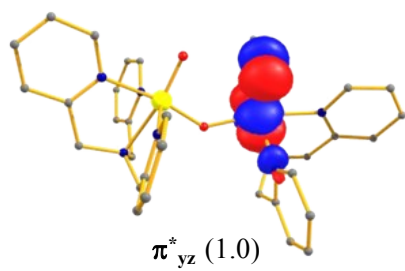
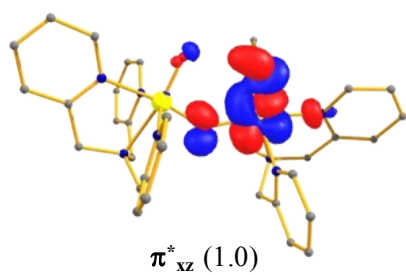
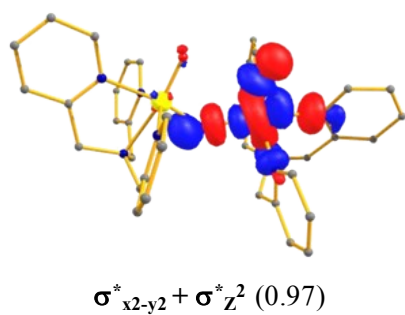
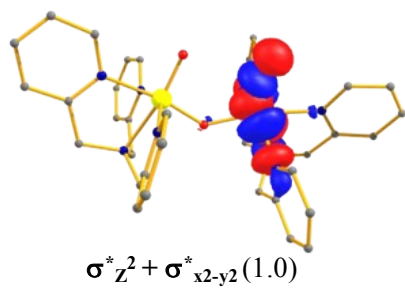
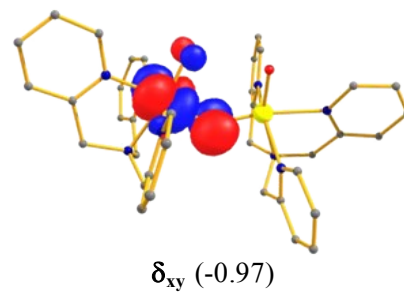
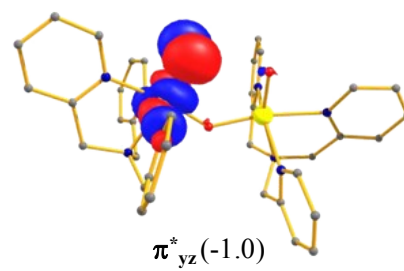
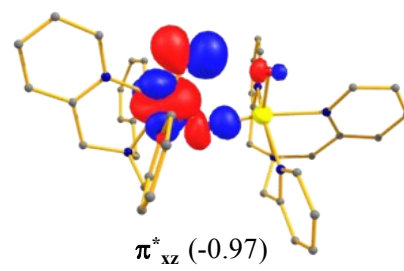
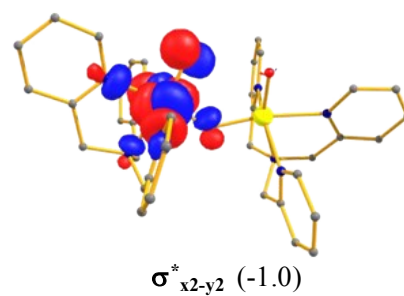
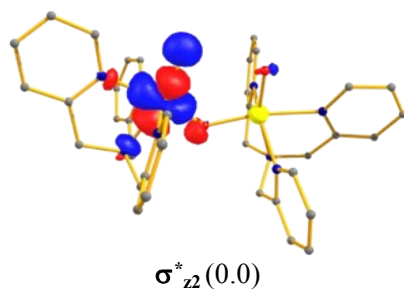


Figure S5. Computed natural bonding orbital (NBO) plots of 21_{hs-hs} .



Fe^{III}



Fe^{IV}

Figure S6. Spin nature orbitals and their occupations (noted in parenthesis) of $^2\mathbf{1}_{\text{hs-hs}}$.

Table S4a. Computed structural parameters of species **1**, and **RC**. All bond lengths are in Å.

Spin states	Fe ^{III} - μ O	Fe ^{IV} - μ O	Fe ^{III} - Fe ^{IV}	Fe ^{III} - N _{avg}	Fe ^{IV} - N _{avg}	Fe ^{III} - O2	Fe ^{IV} - -O1	H2- C2	O2- H2	O1- H1	C1- C2	C1- H1	O1- C1	$\angle$ Fe ^{III} - μ O- Fe ^{IV}	$\angle$ Fe ^{III} - -O2- H2	$\angle$ O2- -H2- C2	$\angle$ Fe ^{IV} - -O1- C1	$\angle$ Fe ^{IV} - -O1- H1	$\angle$ O1- H1- C1
1																			
¹⁰ 1 _(hs, hs)	1.901	1.778	3.187	2.233	2.209	1.834	1.642	-	-	-	-	-	-	120.0	-	-	-	-	-
² 1 _(hs, hs)	1.865	1.757	3.185	2.237	2.207	1.828	1.641	-	-	-	-	-	-	123.0	-	-	-	-	-
⁶ 1 _(is, is)	1.790	1.829	3.255	2.201	2.065	1.796	1.630	-	-	-	-	-	-	128.2	-	-	-	-	-
² 1 _(is, is)	1.784	1.828	3.252	2.199	2.068	1.794	1.631	-	-	-	-	-	-	128.4	-	-	-	-	-
⁴ 1 _(ls, is)	1.839	1.810	3.232	2.033	2.072	1.800	1.634	-	-	-	-	-	-	124.6	-	-	-	-	-
² 1 _(ls, is)	1.821	1.818	3.221	2.035	2.070	1.813	1.632	-	-	-	-	-	-	124.6	-	-	-	-	-
⁸ 1 _(hs, is)	1.834	1.831	3.242	2.257	2.058	1.844	1.628	-	-	-	-	-	-	124.3	-	-	-	-	-
⁴ 1 _(hs, is)	1.836	1.820	3.217	2.255	2.056	1.836	1.633	-	-	-	-	-	-	123.3	-	-	-	-	-
² 1 _(ls, ls)	1.840	1.797	3.220	2.034	2.067	1.799	1.647	-	-	-	-	-	-	124.5	-	-	-	-	-
RC																			
¹⁰ RC _(hs, hs)	1.896	1.780	3.238	2.239	2.205	1.830	1.639	-	2.784	2.561	1.546	1.097	3.261	123.5	114.8	163.4	128.6	112.2	120.7
² RC _(hs, hs)	1.867	1.757	3.215	2.243	2.204	1.825	1.639	-	2.726	2.576	1.546	1.097	3.275	125.0	117.1	161.9	128.4	112.1	120.7
⁶ RC _(is, is)	1.793	1.830	3.264	2.205	2.063	1.796	1.628	-	2.662	2.562	1.540	1.097	3.292	128.5	128.5	152.6	136.2	126.4	119.1
² RC _(is, is)	1.786	1.831	3.261	2.203	2.067	1.795	1.629	-	2.661	2.546	1.540	1.097	3.287	128.7	128.2	153.4	135.7	127.1	119.6
⁴ RC _(ls, is)	1.835	1.815	3.227	2.033	2.069	1.805	1.632	-	2.637	2.508	1.538	1.097	3.360	124.3	138.8	162.8	176.4	163.2	133.5
² RC _(ls, is)	1.820	1.821	3.217	2.035	2.069	1.815	1.631	-	2.648	2.503	1.536	1.099	3.357	124.2	139.5	164.6	176.7	164.8	133.7
⁸ RC _(hs, is)	1.834	1.832	3.251	2.262	2.057	1.846	1.626	-	2.631	2.579	1.558	1.095	3.317	124.9	125.1	151.1	136.6	158.1	110.6
⁴ RC _(hs, is)	1.835	1.822	3.228	2.261	2.056	1.839	1.630	-	2.639	2.578	1.543	1.097	3.320	123.8	126.8	150.7	137.4	121.9	124.1
² RC _(ls, ls)	1.852	1.791	3.227	2.032	2.065	1.792	1.652	-	2.601	2.522	1.538	1.098	3.374	124.7	138.9	159.8	176.0	162.2	133.6

Table S4b. Computed structural parameters of species **I-TS_H** and **I-Int1**. All bond lengths are in Å.

Spin states	Fe ^{III} - μ O	Fe ^{IV} - μ O	Fe ^{III} - Fe ^{IV}	Fe ^{III} - N _{avg}	Fe ^{IV} - N _{avg}	Fe ^{III} - O2	Fe ^{IV} - O1	H2- C2	O2- H2	O1- H1	C1- C2	C1- H1	O1- C1	$\angle$ Fe ^{III} - μ O- Fe ^{IV}	$\angle$ Fe ^{III} - -O2- H2	$\angle$ O2- H2- C2	$\angle$ Fe ^{IV} - -O1- C1	$\angle$ Fe ^{IV} - -O1- H1	$\angle$ O1- H1- C1
I-TS_H																			
I-¹⁰TS_H _(hs, hs)	1.869	1.843	3.277	2.252	2.244	1.834	1.751	1.096	2.586	1.299	1.524	1.234	2.522	124.0	124.1	145.4	155.2	155.9	169.3
I-²TS_H _(hs, hs)	1.826	1.805	3.252	2.255	2.243	1.835	1.753	1.096	2.555	1.304	1.524	1.231	2.524	127.1	125.0	145.4	155.3	156.6	169.9
I-⁶TS_H _(is, is)	1.797	1.802	3.257	2.199	2.192	1.798	1.737	1.097	2.649	1.385	1.537	1.192	2.550	129.6	126.0	145.1	133.4	126.6	163.2
I-²TS_H _(is, is)	1.785	1.817	3.272	2.210	2.058	1.795	1.766	1.098	2.494	1.237	1.532	1.302	2.516	130.5	125.7	150.9	132.1	124.2	164.3
I-⁴TS_H _(ls, is)	1.855	1.789	3.210	2.034	2.162	1.792	1.788	1.096	4.285	1.238	1.522	1.284	2.522	123.5	109.0	123.0	146.0	146.4	177.2
I-²TS_H _(ls, is)	1.824	1.803	3.189	2.034	2.164	1.812	1.783	1.096	4.487	1.244	1.525	1.282	2.524	123.1	106.1	151.8	142.1	143.3	175.9
I-⁸TS_H _(hs, is)	1.832	1.814	3.266	2.262	2.140	1.840	1.766	1.096	2.555	1.218	1.519	1.291	2.508	127.2	122.6	143.5	160.0	160.6	175.8
I-⁴TS_H _(hs, is)	1.838	1.810	3.226	2.263	2.133	1.833	1.773	1.096	2.656	1.206	1.519	1.301	2.504	124.3	123.7	142.3	161.2	161.2	173.9
I-²TS_H _(ls, ls)	1.843	1.786	3.251	2.041	2.062	1.792	1.819	1.096	4.544	1.264	1.525	1.293	2.531	127.2	103.7	122.5	128.5	123.9	163.4
I-Int1																			
I-¹²Int1 _(hs, hs)	1.881	1.846	3.268	2.253	2.257	1.828	1.863	1.098	2.603	0.976	1.503	2.055	3.008	122.5	117.4	158.0	139.6	131.6	165.0
I-¹⁰Int1 _(hs, hs)	1.875	1.850	3.268	2.254	2.258	1.831	1.849	1.098	2.565	0.986	1.503	1.912	2.880	122.7	119.9	155.3	142.1	135.5	166.6
I-²Int1 _(hs, hs)	1.825	1.806	3.215	2.248	2.261	1.836	1.854	1.098	2.558	0.981	1.502	2.012	2.977	124.6	140.9	106.4	136.0	129.3	167.2
I-¹⁰Int1 _(hs, is)	1.849	1.802	3.296	2.265	2.197	1.832	1.850	1.097	2.594	0.977	1.500	2.146	3.092	128.9	96.3	165.1	130.7	118.6	162.3
I-⁸Int1 _(hs, is)	1.844	1.799	3.311	2.264	2.196	1.834	1.842	1.097	2.505	0.983	1.501	2.006	2.953	130.7	101.2	161.2	134.2	121.6	161.1
I-⁴Int1 _(hs, is)	1.862	1.743	3.236	2.257	2.218	1.818	1.841	1.096	2.747	0.976	1.500	2.257	3.180	127.6	96.5	167.3	129.9	114.3	157.2
I-²Int1 _(hs, is)	1.866	1.754	3.183	2.253	2.207	1.829	1.842	1.099	4.392	0.971	1.502	2.595	3.453	123.1	83.1	120.7	86.2	110.1	147.3
I-⁸Int1 _(is, is)	1.817	1.781	3.215	2.202	2.197	1.793	1.837	1.099	3.962	0.972	1.497	3.350	3.849	126.7	97.0	146.8	133.6	108.1	113.9
I-⁶Int1 _(is, is)	1.817	1.781	3.215	2.202	2.197	1.794	1.837	1.099	3.951	0.972	1.497	3.334	3.830	126.6	97.0	147.1	133.7	108.0	113.7
I-²Int1 _(is, is)	1.800	1.786	3.176	2.209	2.213	1.803	1.835	1.096	4.858	0.980	1.499	2.225	3.094	124.6	65.9	105.8	134.4	113.8	147.1
I-⁴Int1 _(ls, ls)	1.842	1.784	3.254	2.039	2.045	1.787	1.865	1.101	6.107	0.970	1.504	2.454	3.216	127.6	78.4	95.1	131.3	111.6	135.2
I-²Int1 _(ls, ls)	1.842	1.785	3.255	2.039	2.045	1.787	1.865	1.101	6.112	0.970	1.504	2.453	3.217	127.5	78.4	94.9	131.3	111.6	135.3
I-²Int1 _(ls, ls)	1.847	1.779	3.253	2.038	2.047	1.788	1.867	1.098	4.138	0.970	1.502	2.478	3.258	127.5	110.3	130.8	130.3	113.7	137.3
I-⁶Int1 _(ls, is)	1.804	1.820	3.265	2.218	2.047	1.788	1.829	1.098	3.287	0.971	1.502	2.412	3.396	128.5	96.6	166.8	130.3	112.8	149.5
I-⁴Int1 _(ls, is)	1.804	1.821	3.265	2.217	2.046	1.788	1.829	1.098	3.406	0.970	1.502	2.421	3.293	128.5	96.5	162.9	130.2	112.8	149.1

Table S4c. Computed structural parameters of species **I-Int1**, and **Ia-TS_{Reb}**. All bond lengths are in Å.

Spin states	Fe ^{III} - μ O	Fe ^{IV} - μ O	Fe ^{III} - Fe ^{IV}	Fe ^{III} - N _{avg}	Fe ^{IV} - N _{avg}	Fe ^{III} - O2	Fe ^{IV} - O1	H2- C2	O2- H2	O1- H1	C1- C2	C1- H1	O1- C1	$\angle$ Fe ^{III} - μ O- Fe ^{IV}	$\angle$ Fe ^{III} - -O2- H2	$\angle$ O2- -H2- C2	$\angle$ Fe ^{IV} - -O1- C1	$\angle$ Fe ^{IV} - -O1- H1	$\angle$ O1- -H1- C1
I-Int1																			
I-⁴Int1 _(ls, is)	1.790	1.806	3.270	2.213	2.044	1.794	1.833	2.523	2.523	0.978	1.506	2.083	2.986	130.8	120.3	157.8	132.2	113.5	152.5
I-²Int1 _(ls, is)	1.795	1.807	3.255	2.215	2.047	1.789	1.840	3.511	4.574	0.970	0.970	2.472	3.322	129.3	95.8	163.2	129.6	112.4	146.1
Ia-TS_{Reb}																			
Ia-¹²TS_{Reb} _(hs, hs)	1.878	1.837	3.228	2.238	2.217	1.908	1.918	1.107	3.075	0.967	1.500	2.405	1.971	120.6	114.7	108.3	145.3	143.2	103.5
Ia-¹⁰TS_{Reb} _(hs, hs)	1.847	1.877	3.170	2.249	2.252	1.854	1.915	1.105	4.185	0.969	1.497	2.606	2.610	116.6	100.9	86.2	151.1	111.3	79.0
Ia-²TS_{Reb} _(hs, hs)	1.784	1.852	3.213	2.255	2.256	1.889	1.852	1.095	2.430	0.986	1.495	2.694	2.649	124.1	154.6	136.6	139.0	106.3	76.8
Ia-¹⁰TS_{Reb} _(hs, is)	1.801	1.944	3.306	2.246	2.284	1.858	2.114	1.103	2.426	0.971	1.491	2.384	2.241	123.9	141.5	156.3	165.8	99.7	86.3
Ia-⁸TS_{Reb} _(hs, is)	1.836	1.792	3.276	2.259	2.179	1.841	1.882	1.101	2.606	0.968	1.494	2.696	2.476	129.1	127.2	148.5	137.2	118.3	92.4
Ia-⁴TS_{Reb} _(hs, is)	1.836	1.794	3.298	2.272	2.199	1.882	1.790	1.098	3.579	0.990	1.495	2.797	2.460	130.5	83.4	102.7	130.3	110.8	99.2
Ia-²TS_{Reb} _(hs, is)	1.836	1.794	3.298	2.272	2.199	1.882	1.790	1.098	3.579	0.990	1.495	2.797	2.460	130.5	83.4	102.7	130.3	110.8	99.2
Ia-⁸TS_{Reb} _(is, is)	1.721	1.867	3.316	2.234	2.199	1.868	1.775	1.097	2.830	0.996	1.495	2.828	2.506	134.9	95.8	118.5	134.1	106.5	98.3
Ia-⁶TS_{Reb} _(is, is)	1.721	1.867	3.316	2.234	2.199	1.868	1.775	1.097	2.830	0.996	1.495	2.828	2.506	134.9	95.8	118.5	134.1	106.5	98.3
Ia-²TS_{Reb} _(is, is)	1.807	1.729	3.208	2.268	2.209	1.923	1.785	1.096	2.967	1.000	1.489	2.843	2.488	130.2	88.9	117.6	132.0	106.7	84.9
Ia-⁴TS_{Reb} _(ls, ls)	1.828	1.809	3.285	2.042	2.072	1.805	1.977	1.098	4.536	0.970	1.508	2.420	2.210	129.1	99.4	79.2	164.6	102.7	90.4
Ia-²TS_{Reb} _(ls, ls)	1.765	1.877	3.347	2.046	2.041	1.926	1.812	1.097	4.007	1.006	1.492	2.866	2.413	133.5	93.4	93.6	142.9	103.5	106.7
Ia-²TS_{Reb} _(ls, ls)	1.827	1.823	3.291	2.057	2.045	1.807	1.948	1.101	2.541	0.969	1.503	2.436	2.224	128.8	137.8	147.9	159.3	109.5	90.6
Ia-⁶TS_{Reb} _(ls, is)	1.777	1.846	3.274	2.209	2.059	1.811	1.925	1.103	4.419	0.972	1.505	2.412	2.286	129.3	96.4	83.4	169.2	101.5	85.4
Ia-⁴TS_{Reb} _(ls, is)	1.773	1.838	3.278	2.214	2.049	1.809	1.876	1.099	2.388	0.970	1.498	2.642	2.417	130.3	142.1	143.9	153.8	112.7	92.4
Ia-⁴TS_{Reb} _(ls, is)	1.770	1.838	3.271	2.218	2.049	1.809	1.875	1.096	2.342	0.971	1.493	2.668	2.406	130.0	136.8	142.4	148.3	114.7	94.7
Ia-²TS_{Reb} _(ls, is)	1.772	1.824	3.259	2.209	2.072	1.806	1.919	1.100	2.513	0.972	1.501	2.508	2.324	130.0	140.8	149.3	160.0	109.9	89.3

Table S4d. Computed structural parameters of species **Ib-TS_{2H}**. All bond lengths are in Å.

Spin states	Fe ^{III} - μ O	Fe ^{IV} - μ O	Fe ^{III} - Fe ^{IV}	Fe ^{III} - N _{avg}	Fe ^{IV} - N _{avg}	Fe ^{III} - O2	Fe ^{IV} - O1	H2- C2	O2- H2	O1- H1	C1- C2	C1- H1	O1- C1	$\angle$ Fe ^{III} - μ O- Fe ^{IV}	$\angle$ Fe ^{III} - -O2- H2	$\angle$ O2- -H2- C2	$\angle$ Fe ^{IV} - -O1- C1	$\angle$ Fe ^{IV} - -O1- H1	$\angle$ O1- -H1- C1
Ib-TS_{2H}																			
Ib-¹²TS_{2H}(hs, hs)	1.837	1.860	3.257	2.221	2.227	1.929	1.898	1.400	1.229	0.969	1.403	4.325	4.388	123.4	146.8	173.2	129.2	117.3	79.9
Ib-¹⁰TS_{2H}(hs, hs)	1.835	1.826	3.289	2.229	2.268	1.823	1.903	1.130	1.869	0.968	1.465	4.496	4.696	127.8	157.8	148.4	121.9	118.9	72.2
Ib-²TS_{2H}(hs, hs)	1.770	1.899	3.252	2.254	2.269	2.112	1.940	1.292	1.337	0.970	1.412	2.535	2.268	124.8	156.6	166.3	158.3	106.0	83.8
Ib-¹⁰TS_{2H}(hs, is)	1.835	1.826	3.289	2.229	2.268	1.823	1.903	1.131	1.869	0.968	1.465	4.494	4.695	127.9	157.9	148.4	122.0	118.9	95.9
Ib-⁸TS_{2H}(hs, is)	1.715	1.970	3.269	2.226	2.265	1.839	1.914	1.164	1.672	0.968	1.444	4.668	4.845	124.8	138.4	160.7	97.3	118.8	94.7
Ib-⁴TS_{2H}(hs, is)	1.829	1.807	3.318	2.218	2.282	1.934	1.845	1.210	1.512	0.985	1.422	4.291	4.913	131.7	131.9	167.2	98.9	106.2	124.2
Ib-²TS_{2H}(hs, is)	1.816	1.806	3.169	2.218	2.251	1.875	1.902	1.136	1.808	0.971	1.463	4.821	4.375	122.0	163.3	153.5	113.3	111.5	57.4
Ib-⁸TS_{2H}(is, is)	1.843	1.787	3.212	2.249	2.208	1.967	1.814	1.164	1.674	0.984	1.443	4.884	5.842	124.4	149.3	163.4	121.3	109.3	165.5
Ib-⁶TS_{2H}(is, is)	1.835	1.773	3.164	2.209	2.237	1.935	1.829	1.197	1.564	0.979	1.426	4.504	5.333	122.5	128.7	177.0	95.7	108.9	144.5
Ib-²TS_{2H}(is, is)	1.841	1.760	3.258	2.096	2.218	2.018	1.812	1.216	1.504	0.982	1.424	3.924	4.572	129.6	147.1	165.5	120.8	105.4	126.1
Ib-⁴TS_{2H}(ls, ls)	1.831	1.784	3.269	2.100	2.036	2.078	1.842	1.241	1.475	0.978	1.417	3.409	3.871	129.4	170.5	159.8	124.8	104.3	111.1
Ib-²TS_{2H}(ls, ls)	1.879	1.785	3.315	2.039	2.049	1.974	1.812	1.243	1.460	0.980	1.418	4.284	5.144	129.5	130.3	163.1	103.0	102.5	148.2
Ib-²TS_{2H}(ls, ls)	1.881	1.775	3.332	2.032	2.036	1.921	1.888	1.198	1.558	0.973	1.428	4.488	5.253	131.3	142.4	161.3	128.1	103.8	138.1
Ib-⁶TS_{2H}(is, ls)	1.871	1.773	3.285	2.102	2.242	1.999	1.811	1.201	1.554	0.981	1.428	4.496	5.368	128.6	146.7	162.5	105.7	105.8	149.9
Ib-⁴TS_{2H}(is, ls)	1.878	1.763	3.323	2.043	2.239	1.932	1.816	1.181	1.603	0.977	1.432	3.906	4.512	131.6	142.8	169.5	126.1	104.7	122.8
Ib-⁴TS_{2H}(is, ls)	1.878	1.757	3.305	2.039	2.234	1.934	1.819	1.191	1.575	0.978	1.430	4.183	4.947	130.8	139.2	173.4	116.2	103.9	137.3
Ib-²TS_{2H}(is, ls)	1.844	1.761	3.274	2.099	2.220	2.032	1.816	1.213	1.524	0.982	1.422	3.292	3.718	130.4	159.6	162.1	125.7	106.6	108.2

Table S4e. Computed structural parameters of species **Ia-P_{Reb}**, and **Ib-P_{2H}**. All bond lengths are in Å.

Spin states	Fe ^{III} - μ O	Fe ^{IV} - μ O	Fe ^{III} - Fe ^{IV}	Fe ^{III} - N _{avg}	Fe ^{IV} - N _{avg}	Fe ^{III} - O2	Fe ^{IV} - O1	H2- C2	O2- H2	O1- H1	C1- C2	C1- H1	O1- C1	$\angle$ Fe ^{III} - μ O- Fe ^{IV}	$\angle$ Fe ^{III} - -O2- H2	$\angle$ O2- -H2- C2	$\angle$ Fe ^{IV} - -O1- C1	$\angle$ Fe ^{IV} - -O1- H1	$\angle$ O1- -H1- C1
Ia-P_{Reb}																			
Ia-¹⁰P_{Reb}(hs, hs)	1.803	1.935	3.396	2.271	2.266	1.940	2.067	1.096	4.403	1.037	1.531	2.044	1.451	130.5	123.7	62.0	126.6	108.0	109.3
Ia-²P_{Reb}(hs, hs)	1.769	1.876	3.296	2.275	2.287	1.923	2.159	1.094	2.608	1.010	1.537	2.026	1.444	129.4	110.6	131.0	139.7	101.6	109.9
Ia-⁸P_{Reb}(hs, is)	2.066	1.666	3.412	2.281	2.168	1.948	2.139	1.095	4.224	1.037	1.532	2.053	1.438	131.9	137.4	67.4	124.5	103.8	111.0
Ia-⁴P_{Reb}(hs, is)	1.771	1.897	3.333	2.281	2.105	1.921	2.201	1.095	4.269	1.016	1.533	2.022	1.437	130.5	139.2	66.5	131.8	100.4	109.8
Ia-⁶P_{Reb}(is, is)	1.685	1.898	3.365	2.222	2.151	1.931	2.051	1.093	2.652	1.031	1.544	2.051	1.441	139.7	148.2	108.8	141.1	104.8	111.0
Ia-²P_{Reb}(is, is)	1.685	1.898	3.365	2.222	2.151	1.931	2.051	1.093	2.652	1.031	1.544	2.051	1.441	139.7	148.2	108.8	141.1	104.8	111.0
Ia-⁴P_{Reb}(is, ls)	1.769	1.861	3.375	2.041	2.289	1.895	2.164	1.093	1.569	0.970	1.543	2.420	1.445	136.7	98.9	108.4	142.5	130.9	108.4
Ia-⁴P_{Reb}(is, ls)	1.769	1.861	3.375	2.041	2.289	1.895	2.164	1.093	1.569	0.970	1.543	2.420	1.445	136.7	98.9	108.4	142.5	130.9	108.4
Ia-²P_{Reb}(ls, ls)	1.761	1.907	3.381	2.033	2.044	1.937	2.067	1.094	4.096	1.039	1.536	2.088	1.436	134.3	127.8	72.1	135.2	103.1	114.0
Ib-P_{2H}																			
Ib-¹⁰P_{2H}(hs, hs)	1.959	1.782	3.314	2.273	2.273	2.130	1.923	2.231	0.974	0.968	1.341	4.808	4.828	124.5	131.6	155.5	117.7	118.3	83.1
Ib-²P_{2H}(hs, hs)	1.879	1.769	3.233	2.256	2.272	2.163	1.928	2.583	0.978	0.968	1.341	4.497	4.446	124.7	114.4	176.3	104.4	118.8	86.7
Ib-⁸P_{2H}(hs, is)	1.666	2.076	3.331	2.155	2.261	2.145	1.950	2.385	0.972	0.968	1.339	4.519	4.695	125.4	132.0	145.6	122.4	118.2	73.6
Ib-⁴P_{2H}(hs, is)	1.897	1.773	3.257	2.091	2.276	2.210	1.928	2.218	0.975	0.968	1.341	5.352	5.237	125.1	117.1	146.7	95.2	117.5	91.5
Ib-⁶P_{2H}(is, is)	1.893	1.691	3.334	2.172	2.234	2.059	1.925	2.375	0.973	0.972	1.340	3.933	4.282	136.9	134.0	169.7	130.6	106.1	62.7
Ib-²P_{2H}(is, is)	1.893	1.691	3.334	2.172	2.234	2.059	1.925	2.375	0.973	0.972	1.340	3.933	4.282	136.9	134.0	169.7	130.6	106.1	62.7
Ib-⁴P_{2H}(is, ls)	1.934	1.678	3.308	2.005	2.209	2.011	1.982	2.309	0.975	0.972	1.340	4.214	4.173	132.5	117.1	24.0	144.6	108.1	85.8
Ib-²P_{2H}(ls, ls)	1.879	1.772	3.334	2.014	2.034	2.002	1.959	2.413	0.974	0.969	1.340	3.797	3.869	131.7	114.7	14.2	148.8	108.5	78.5

Table S5a. Computed spin densities of species **1**, **RC**, **I-TS_H**, and **I-Int** as obtained from optimized geometries in Gaussian 09.

Spin states	Fe ^{III} (<i>S_a</i>)	Fe ^{IV/III} (<i>S_b</i>)	μ -O	O1	O2	C1	C2
1							
¹⁰ 1 _(hs, hs)	4.04	3.05	0.42	0.39	0.56	0.00	0.00
² 1 _(hs, hs)	3.99	-3.03	0.06	0.37	-0.49	0.00	0.00
⁸ 1 _(hs, is)	3.98	1.36	0.35	0.36	0.71	0.00	0.00
⁴ 1 _(hs, is)	3.97	-1.29	0.36	0.34	-0.69	0.00	0.00
⁶ 1 _(hs, ls)	3.96	-0.23	0.28	0.35	0.35	0.00	0.00
⁸ 1 _(is, hs)	2.84	3.13	0.19	0.11	0.48	0.00	0.00
⁴ 1 _(is, hs)	-2.72	3.08	0.09	-0.07	0.55	0.00	0.00
⁶ 1 _(is, is)	2.73	1.35	0.05	0.09	0.69	0.00	0.00
² 1 _(is, is)	2.71	-1.41	0.15	0.07	-0.67	0.00	0.00
⁴ 1 _(is, ls)	2.72	0.06	0.12	0.07	-0.08	0.00	0.00
⁶ 1 _(ls, hs)	0.96	3.00	0.24	0.15	0.52	0.00	0.00
⁴ 1 _(ls, hs)	-0.89	3.00	0.25	-0.12	0.52	0.00	0.00
⁴ 1 _(ls, is)	0.95	1.41	-0.03	0.10	0.64	0.00	0.00
² 1 _(ls, is)	-0.91	1.39	-0.10	-0.05	0.66	0.00	0.00
² 1 _(ls, ls)	0.93	-0.21	-0.09	0.08	0.32	0.00	0.00
RC							
¹⁰ RC _(hs, hs)	4.03	3.05	0.43	0.41	0.55	0.00	0.00
² RC _(hs, hs)	3.99	-3.03	0.05	0.38	-0.48	0.00	0.00
⁶ RC _(is, is)	2.73	1.35	0.05	0.09	0.68	0.00	0.00
² RC _(is, is)	2.71	-1.42	0.15	0.07	-0.67	0.00	0.00
⁴ RC _(ls, is)	0.95	1.42	-0.02	0.09	0.64	0.00	0.00
² RC _(ls, is)	-0.91	1.41	-0.11	-0.05	0.65	0.00	0.00
⁸ RC _(hs, is)	3.98	1.36	0.35	0.36	0.70	0.00	0.00
⁴ RC _(hs, is)	3.97	-1.29	0.37	0.34	-0.69	0.00	0.00
² RC _(ls, ls)	0.95	0.25	0.12	0.12	-0.36	0.00	0.00
I-TS_H							
I-¹⁰TS_H _(hs, hs)	4.00	3.82	0.62	0.39	-0.00	0.39	0.01
I-²TS_H _(hs, hs)	3.97	-3.78	0.00	0.38	0.02	0.39	-0.01
I-⁶TS_H _(is, is)	2.70	2.66	-0.03	0.08	-0.27	-0.34	0.01
I-²TS_H _(is, is)	2.73	-1.02	0.06	0.07	-0.53	-0.51	0.02
I-⁴TS_H _(ls, is)	0.95	2.57	-0.08	0.11	-0.08	-0.46	0.02
I-²TS_H _(ls, is)	-0.94	2.61	-0.15	-0.07	-0.08	-0.46	0.02
I-⁸TS_H _(hs, is)	3.95	2.54	0.32	0.37	0.01	-0.47	0.02
I-⁴TS_H _(hs, is)	3.97	-2.44	0.38	0.36	-0.01	0.48	-0.02
I-²TS_H _(ls, ls)	0.95	-0.79	-0.17	0.12	0.47	0.48	-0.00
I-Int1							
I-¹²Int1 _(hs, hs)	4.00	4.03	0.69	0.40	0.28	0.96	-0.07
I-¹⁰Int1 _(hs, hs)	4.00	4.01	0.69	0.39	0.22	-0.91	0.07
I-²Int1 _(hs, hs)	3.96	-3.97	-0.07	0.38	-0.25	0.93	-0.07
I-¹⁰Int1 _(hs, is)	3.96	2.89	0.28	0.39	0.15	0.96	-0.07
I-⁸Int1 _(hs, is)	3.95	2.80	0.43	0.15	0.23	-0.93	0.07
I-⁴Int1 _(hs, is)	3.98	-2.71	0.09	0.41	0.05	0.98	-0.07

Table S5b. Computed spin densities of species **I-Int**, **Ia-TS_{Reb}**, and **Ib-TS_{2H}** as obtained from optimized geometries in Gaussian 09.

Spin states	Fe ^{III} (S_a)	Fe ^{IV/III} (S_b)	μ -O	O1	O2	C1	C2
I-Int1							
I-²Int1 _(hs, is)	3.98	-2.75	0.10	0.41	0.05	-0.95	0.08
I-⁸Int1 _(is, is)	2.78	2.75	0.09	0.11	0.05	1.01	-0.08
I-⁶Int1 _(is, is)	2.78	2.74	0.09	0.11	0.04	-1.01	0.08
I-²Int1 _(is, is)	2.80	-2.83	0.03	0.07	-0.07	1.01	-0.08
I-⁴Int1 _(ls, ls)	0.94	0.85	0.17	0.12	0.03	0.98	-0.08
I-²Int1 _(ls, ls)	0.94	0.84	0.17	0.11	0.01	-0.98	0.08
I-²Int1 _(ls, ls)	0.95	-0.82	-0.21	0.11	-0.01	0.98	-0.07
I-⁶Int1 _(is, is)	2.75	0.92	0.11	0.07	0.09	0.97	-0.08
I-⁴Int1 _(is, is)	2.75	0.92	0.11	0.09	0.05	-0.98	0.08
I-⁴Int1 _(is, is)	2.75	-0.95	0.01	0.08	-0.01	0.96	-0.08
I-²Int1 _(is, is)	2.75	-0.95	-0.01	0.08	-0.05	0.98	0.08
Ia-TS_{Reb}							
Ia-¹²TS_{Reb} _(hs, hs)	4.04	4.06	0.73	0.24	0.21	0.37	-0.03
Ia-¹⁰TS_{Reb} _(hs, hs)	3.99	3.95	0.67	0.33	0.27	-0.76	0.06
Ia-²TS_{Reb} _(hs, hs)	3.96	-3.93	0.22	0.23	-0.37	0.85	-0.07
Ia-¹⁰TS_{Reb} _(hs, is)	3.29	3.01	0.13	0.09	0.08	0.71	0.01
Ia-⁸TS_{Reb} _(hs, is)	3.94	2.63	0.34	0.36	0.19	-0.82	0.06
Ia-⁴TS_{Reb} _(hs, is)	3.96	-2.49	0.48	0.24	-0.16	0.83	-0.07
Ia-²TS_{Reb} _(hs, is)	3.94	-3.18	0.48	0.21	0.03	-0.65	0.05
Ia-⁸TS_{Reb} _(is, is)	2.99	2.17	0.14	0.07	0.11	0.75	0.01
Ia-⁶TS_{Reb} _(is, is)	2.71	2.60	0.17	0.17	-0.01	-0.85	0.07
Ia-²TS_{Reb} _(is, is)	3.46	-2.62	-0.33	0.09	-0.17	0.58	-0.05
Ia-⁴TS_{Reb} _(ls, ls)	0.96	1.43	0.09	0.08	-0.12	0.66	-0.05
Ia-²TS_{Reb} _(ls, ls)	0.67	0.55	0.35	-0.02	0.24	-0.74	0.06
Ia-²TS_{Reb} _(ls, ls)	0.98	-0.40	-0.16	0.07	-0.10	0.64	-0.05
Ia-⁶TS_{Reb} _(is, ls)	2.73	1.46	0.09	0.06	-0.10	0.70	-0.06
Ia-⁴TS_{Reb} _(is, ls)	2.71	0.59	0.16	0.07	0.12	-0.74	0.06
Ia-⁴TS_{Reb} _(is, ls)	2.75	-0.58	0.04	0.06	-0.12	0.73	-0.06
Ia-²TS_{Reb} _(is, ls)	2.75	-1.39	0.06	0.07	0.09	-0.73	0.06
Ib-TS_{2H}							
Ib-¹²TS_{2H} _(hs, hs)	4.04	4.04	0.74	0.17	0.24	0.41	-0.01
Ib-¹⁰TS_{2H} _(hs, hs)	3.29	3.90	0.53	0.02	0.20	0.75	-0.09
Ib-²TS_{2H} _(hs, hs)	3.94	-3.65	0.42	0.15	-0.02	0.02	-0.01
Ib-¹⁰TS_{2H} _(hs, is)	3.29	3.90	0.53	0.02	0.20	0.75	-0.09
Ib-⁸TS_{2H} _(hs, is)	2.73	3.83	0.41	0.14	0.17	-0.57	0.09
Ib-⁴TS_{2H} _(hs, is)	3.95	-2.21	0.39	0.35	-0.10	0.48	-0.10
Ib-²TS_{2H} _(hs, is)	-3.14	3.98	0.31	0.14	0.24	-0.74	0.10
Ib-⁸TS_{2H} _(is, is)	3.85	2.77	0.31	0.19	0.08	-0.56	0.09
Ib-⁶TS_{2H} _(is, is)	2.35	2.70	0.05	0.14	0.05	-0.51	0.09
Ib-²TS_{2H} _(is, is)	2.74	-1.69	0.09	0.06	0.09	-0.53	0.11
Ib-⁴TS_{2H} _(ls, ls)	1.73	0.87	0.14	0.11	0.03	-0.12	0.01
Ib-²TS_{2H} _(ls, ls)	0.23	0.95	0.18	0.06	0.06	-0.44	0.07
Ib-²TS_{2H} _(ls, ls)	-0.35	0.79	0.23	-0.09	-0.03	0.49	-0.09

Table S5c. Computed spin densities of species **Ib-TS_{2H}**, **Ia-P_{Reb}**, and **Ib-P_{2H}** as obtained from optimized geometries in Gaussian 09.

Spin states	Fe ^{III} (<i>S_a</i>)	Fe ^{IV/II} (<i>S_b</i>)	μ -O	O1	O2	C1	C2
Ib-TS_{2H}							
Ib-⁶TS_{2H}(is, ls)	1.67	2.74	0.11	-0.09	0.05	0.53	-0.11
Ib-⁴TS_{2H}(is, ls)	0.34	2.72	0.16	0.11	0.06	-0.51	0.09
Ib-⁴TS_{2H}(is, ls)	-0.33	2.74	0.07	-0.10	0.05	0.50	-0.09
Ib-²TS_{2H}(is, ls)	-1.69	2.76	0.08	0.10	0.07	-0.51	0.11
Ia-P_{Reb}							
Ia-¹⁰P_{Reb}(hs, hs)	3.89	3.77	0.74	0.15	0.05	0.00	0.00
Ia-²P_{Reb}(hs, hs)	3.96	-3.66	0.41	0.18	-0.03	-0.00	0.00
Ia-⁸P_{Reb}(hs, is)	3.74	2.61	0.34	0.10	0.05	0.00	0.00
Ia-⁴P_{Reb}(hs, is)	3.94	-1.91	0.56	0.17	-0.03	-0.00	0.00
Ia-⁶P_{Reb}(is, is)	2.66	1.99	0.19	0.00	0.04	0.00	0.00
Ia-²P_{Reb}(is, is)	2.76	-1.99	0.21	0.01	-0.03	-0.00	0.00
Ia-⁴P_{Reb}(is, ls)	0.55	1.99	0.09	0.00	0.03	0.01	0.00
Ia-²P_{Reb}(is, ls)	-0.77	1.99	-0.31	0.01	0.00	0.00	0.00
Ia-²P_{Reb}(ls, ls)	0.63	0.04	0.39	-0.01	0.00	-0.00	0.00
Ib-P_{2H}							
Ib-¹⁰P_{2H}(hs, hs)	3.70	3.95	0.69	0.03	0.18	0.00	0.00
Ib-²P_{2H}(hs, hs)	-3.65	3.95	0.41	-0.03	0.18	0.00	0.00
Ib-⁸P_{2H}(is, hs)	2.60	3.74	0.35	0.03	0.11	0.00	0.00
Ib-⁴P_{2H}(is, hs)	-1.92	3.94	0.56	-0.03	0.17	0.00	0.00
Ib-⁶P_{2H}(is, is)	2.00	2.68	0.18	0.03	-0.00	0.00	0.00
Ib-²P_{2H}(is, is)	-2.03	2.84	0.13	-0.02	0.00	0.00	0.00
Ib-⁴P_{2H}(ls, is)	0.00	2.72	0.19	0.00	0.01	0.00	0.00
Ib-²P_{2H}(ls, ls)	0.11	0.59	0.39	0.00	-0.00	0.00	0.00

Table S6. Computed overlap integral values of d orbitals of two Fe ions of complex $^2\mathbf{1}_{\text{hs-hs}}$. The values are given a mod($\text{Fe}^{\text{III}}\text{Fe}^{\text{IV}}$). Overlap integral between the d-orbitals is computed using the methodology described in this paper (*J. Comput. Chem.*, 1999, 20, 1391-1400)

$\text{Fe}^{\text{III}}/\text{Fe}^{\text{IV}}$	$\mathbf{d}_{\text{xy}}$	$\mathbf{d}_{\text{yz}}$	$\mathbf{d}_{\text{xz}}$	$\mathbf{d}_{\text{x}^2-\text{y}^2}$	$\mathbf{d}_{\text{z}}^2$
$\mathbf{d}_{\text{xy}}$	0.119	0.033	0.095	0.052	0.064
$\mathbf{d}_{\text{yz}}$	0.136	0.048	0.240	0.044	0.019
$\mathbf{d}_{\text{xz}}$	0.138	0.391	0.075	0.111	0.144
$\mathbf{d}_{\text{x}^2-\text{y}^2}$	0.350	0.006	0.102	0.070	0.026
$\mathbf{d}_{\text{z}}^2$	0.236	0.040	0.134	0.080	0.022

Table S7. Computed overlap integral values of d orbitals of two Fe ions of complex $^4\mathbf{1}_{\text{hs-is}}$. The values are given a mod($\text{Fe}^{\text{III}}\text{Fe}^{\text{IV}}$).

$\text{Fe}^{\text{III}}/\text{Fe}^{\text{IV}}$	$\mathbf{d}_{\text{xy}}$	$\mathbf{d}_{\text{yz}}$	$\mathbf{d}_{\text{xz}}$	$\mathbf{d}_{\text{x}^2-\text{y}^2}$	$\mathbf{d}_{\text{z}}^2$
$\mathbf{d}_{\text{xy}}$	0.085	0.035	0.030	0.055	0.104
$\mathbf{d}_{\text{yz}}$	0.203	0.126	0.096	0.124	0.096
$\mathbf{d}_{\text{xz}}$	0.001	0.214	0.064	0.072	0.096
$\mathbf{d}_{\text{x}^2-\text{y}^2}$	0.097	0.072	0.044	0.011	0.137
$\mathbf{d}_{\text{z}}^2$	0.095	0.043	0.007	0.061	0.114

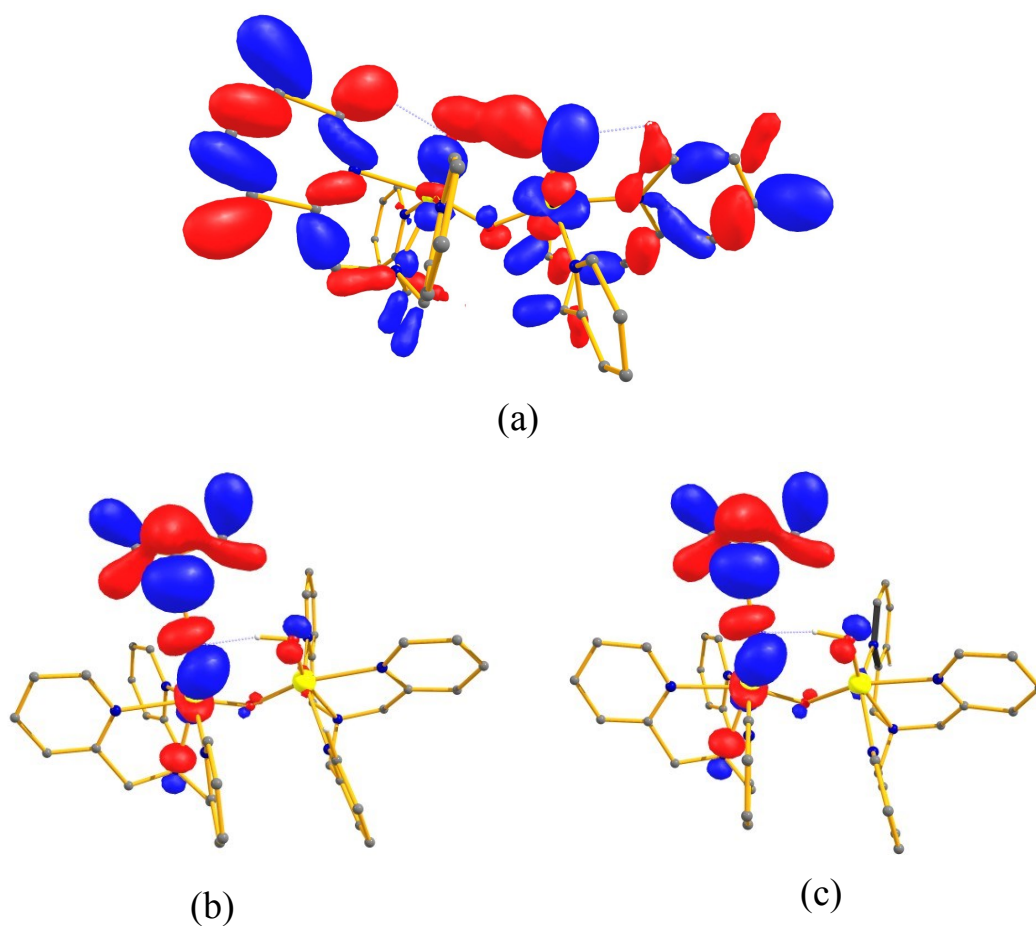


Figure S7. DFT computed a) frontier molecular bonding orbitals between $\text{Fe}^{\text{IV}}\sigma_z^{*2}$ with $\text{Fe}^{\text{III}}\pi_{xz}^*$ of ${}^2\mathbf{I}_{\text{hs-hs}}$ b) α -HOMO-1 of $\mathbf{I}-{}^2\mathbf{TS}_{\text{Hhs-hs}}$ and b) β -HOMO of $\mathbf{I}-{}^{10}\mathbf{TS}_{\text{Hhs-hs}}$ transition states of the C-H bond activation.

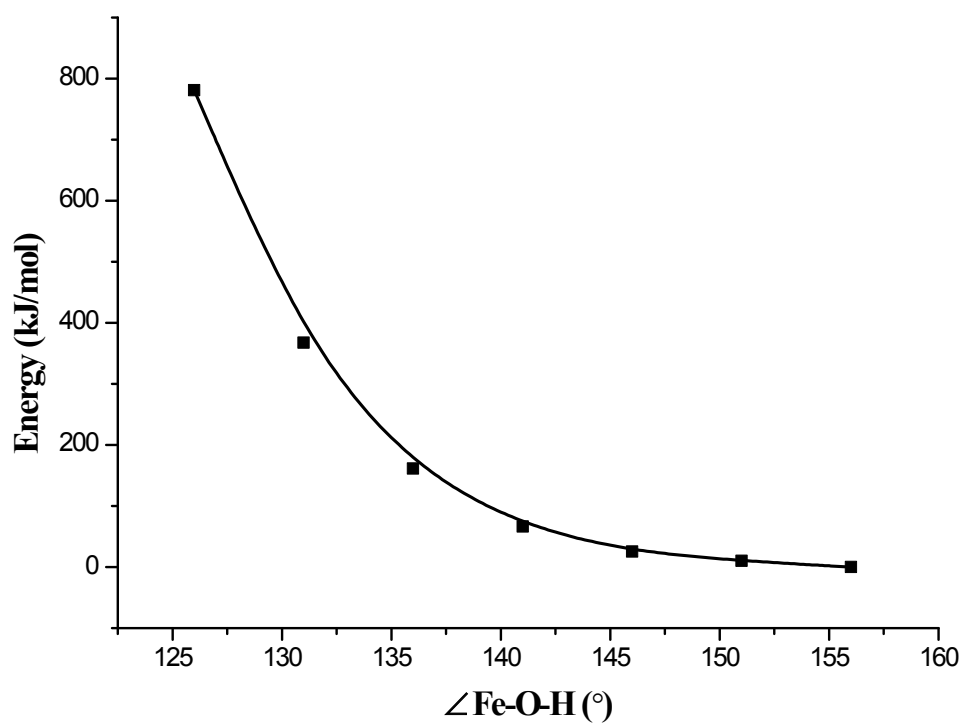


Figure S8. Rigid scan of the potential energy surface with changes of the $\text{Fe}^{\text{IV}}\text{-O(1)-H(1)}$ bond angle with a 5° interval for the species $\text{I-}^2\text{TS}_{\text{Hhs-hs}}$.

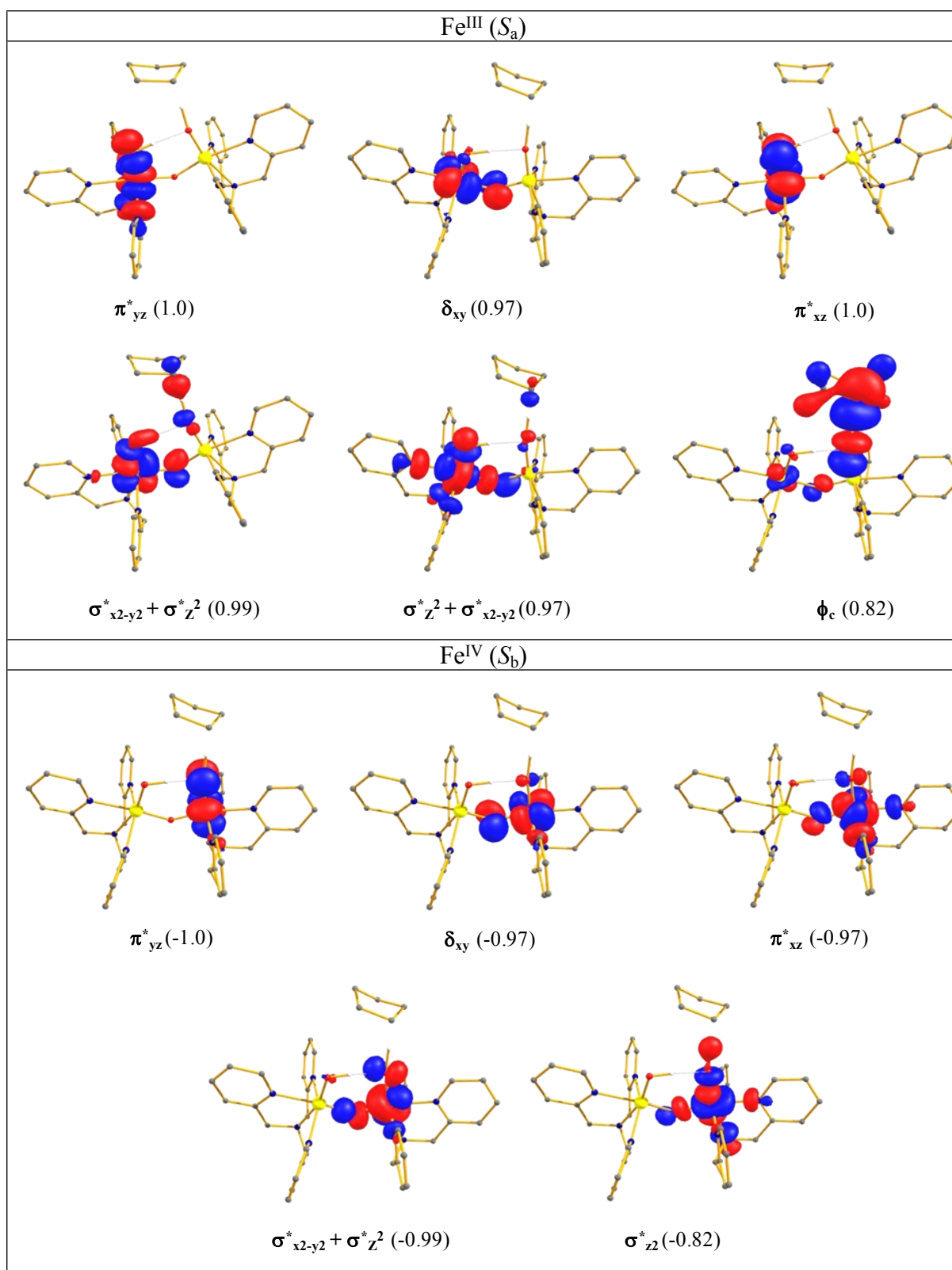


Figure S9. Spin natural orbitals and their occupations (noted in parenthesis) of $\text{I}^2\text{TS}_{\text{Hhs-hs}}$.

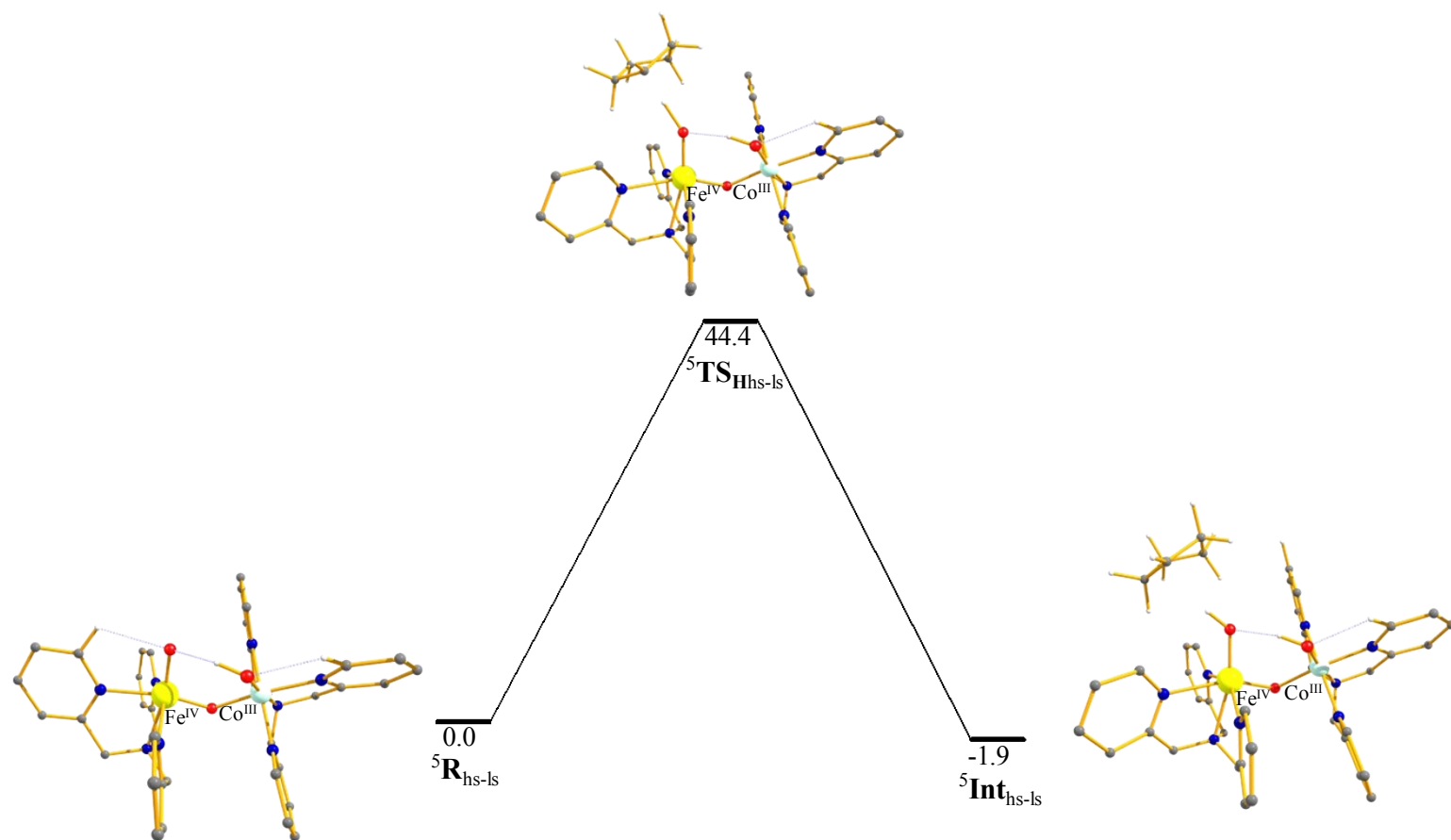


Figure S10. B3LYP-D3 computed energy for the C-H bond hydroxylation as well as desaturation of cyclopentane (CP) by $[(\text{HO}(\text{L})\text{Co}^{\text{III}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L}))^{2+}]$ complex (energies are in kJ/mol). The computed barrier height is shown with respect to the reactant (**R**).

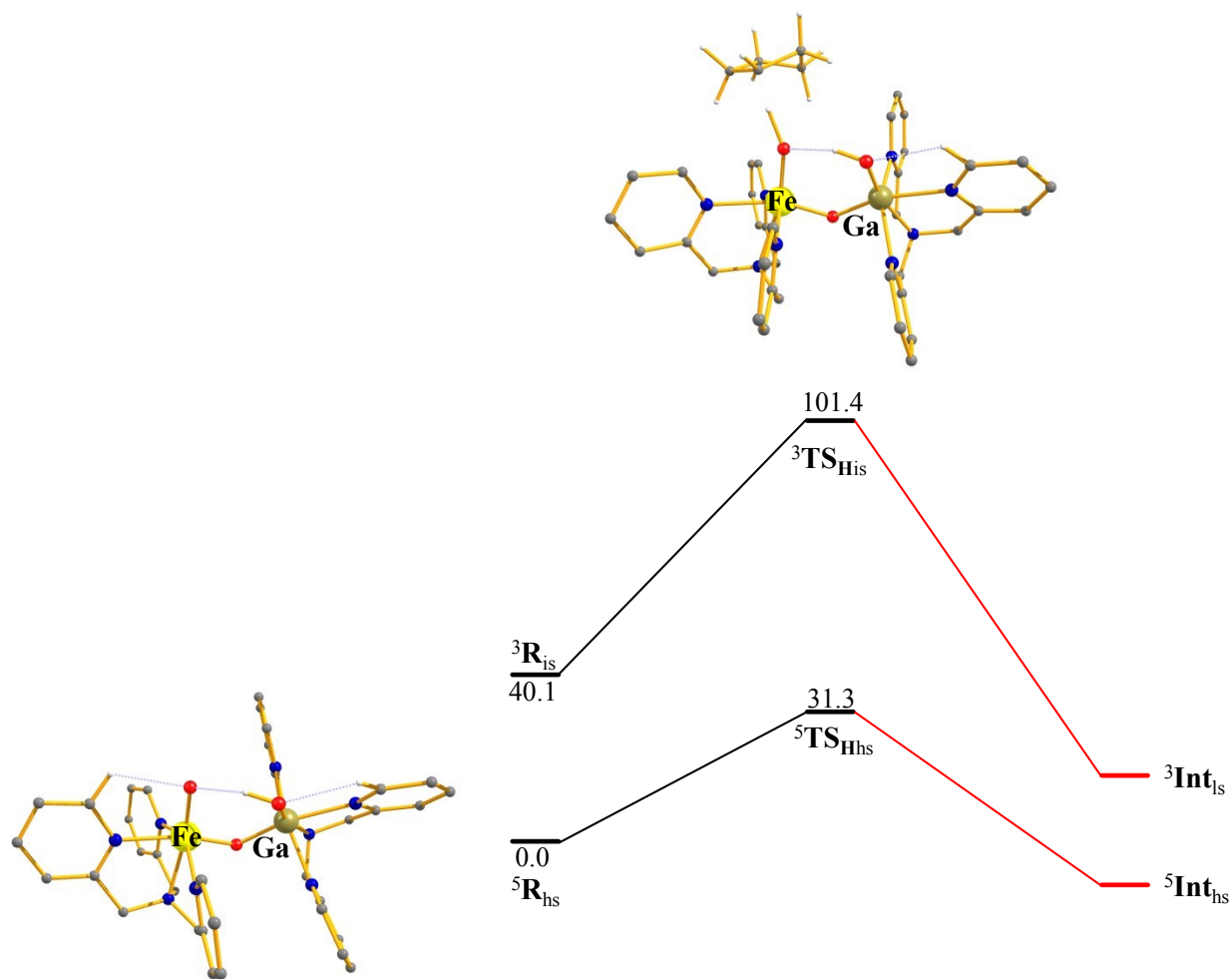


Figure S11. B3LYP-D3 computed energy for the C-H bond hydroxylation as well as desaturation of cyclopentane (CP) by $[(\text{HO}(\text{L})\text{Ga}^{\text{III}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L}))^{2+}]$ complex (energies are in kJ/mol). The red colour indicates approximate stabilisation as the corresponding intermediates were not computed. The computed barrier height is shown with respect to the reactant (**R**).

Table S8. Computed overlap integral values of d orbitals of two Fe ions of complex **I**-²**TS**_{Hhs-}. The values are given a mod(Fe^{III}Fe^{IV}).

Fe^{III}/Fe^{IV}	d_{xy}	d_{xz}	d_{yz}	d_{x²-y²}	d_z²
d_{xy}	-0.109	-0.074	-0.098	-0.016	0.044
d_{xz}	0.117	-0.191	0.407	-0.083	0.030
d_{yz}	0.216	-0.042	-0.053	-0.054	-0.047
d_{x²-y²}	-0.076	-0.222	0.039	-0.051	0.105
d_z²	-0.061	0.000	0.089	-0.071	0.054
Crad	0.110	0.050	-0.237	0.278	0.434

Table S9. Computed overlap integral values of d orbitals of two Fe ions of complex **I**-¹⁰**TS**_{Hhs-}. The values are given a mod(Fe^{III}Fe^{IV}).

Fe^{III}/Fe^{IV}	Crad				
d_{xy}	0.201	--	--	--	--
d_{yz}	-0.194	--	--	--	--
d_{xz}	0.113	--	--	--	--
d_{x²-y²}	0.259	--	--	--	--
d_z²	0.388	--	--	--	--

PCET vs. HAT

If the substrate undergoes C–H bond activation via metal-oxo species, the activation barriers $\Delta E^\ddagger$ values are close to the corresponding ΔE_{def} , $\Delta E_{\text{def}} \approx \Delta E^\ddagger$. In this case, the barrier height derives from the deformation energy (ΔE_{def}) required to establish the TS, and the interaction energy (ΔE_{int}) is not playing a very significant role. But in the second case, the barriers are significantly smaller than the deformation energies (ΔE_{def}), and it's revealing that the corresponding TSs have very large stabilizing interactions, which has a lower the barriers below the corresponding deformation energies, i.e., $\Delta E_{\text{int}} \ll 0$. The C-H activation exhibits the same large and negative ΔE_{int} quantity, even in the TS of the substrate. As such, the comparison of the differences $\Delta E_{\text{def}} - \Delta E^\ddagger = \Delta E_{\text{int}}$ for the reactions of the substrate and it has the normal HAT reactions for substrate and the very basic iron-oxo species with the substrate. By contrast, if the C–H bond activation undergoes via PCET for catalyst **1** with cyclopentane, the deformation energy in figure 4b is significantly smaller than the barriers and plotted between ΔE_{def} vs. $\Delta E^\ddagger$. Figure 4b clearly shows that these two criteria ($\Delta E_{\text{def}} < \Delta E^\ddagger$ and $\Delta E_{\text{int}} > 0$) should be followed for PCET.

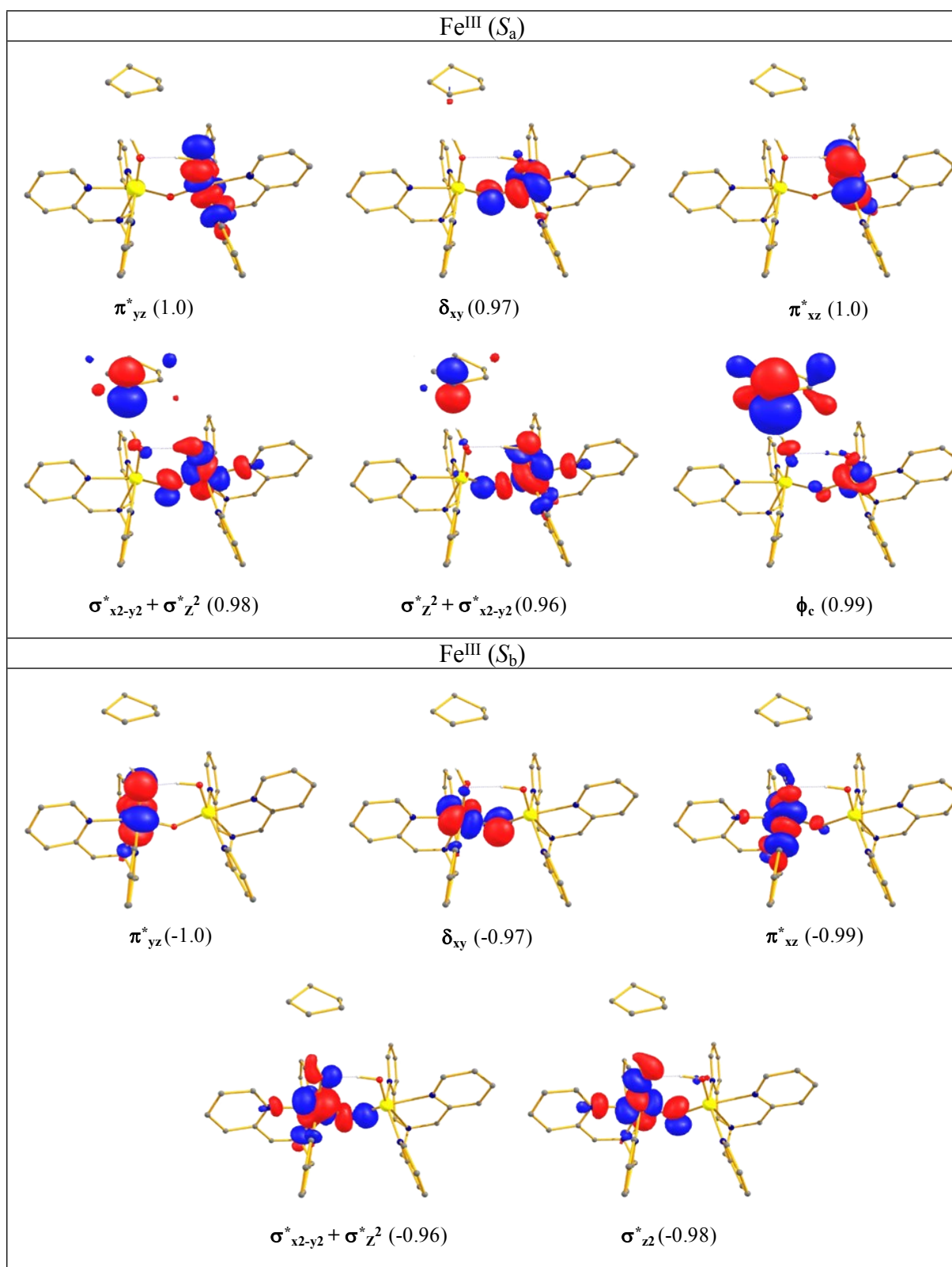


Figure S12. Spin nature orbitals and their occupations (noted in parenthesis) of **I-²Int_{hs-hs}**.

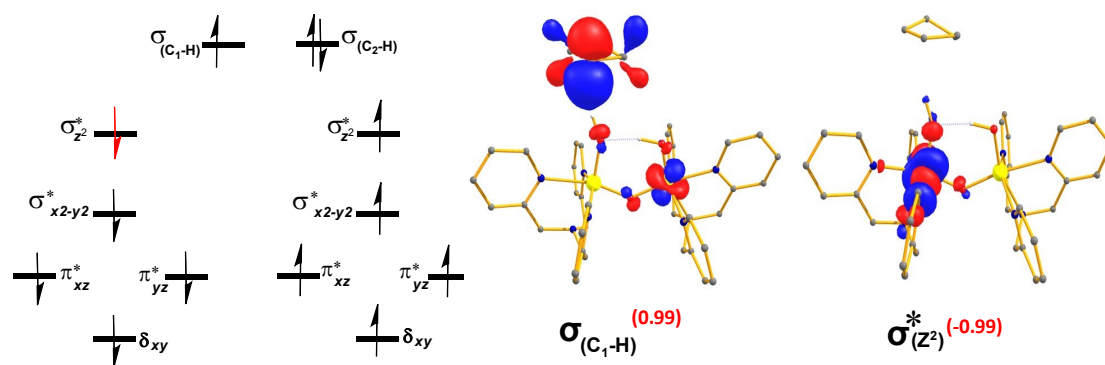
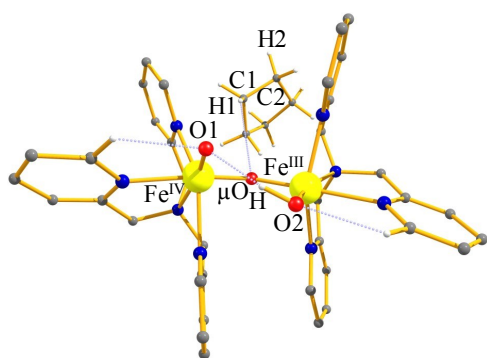
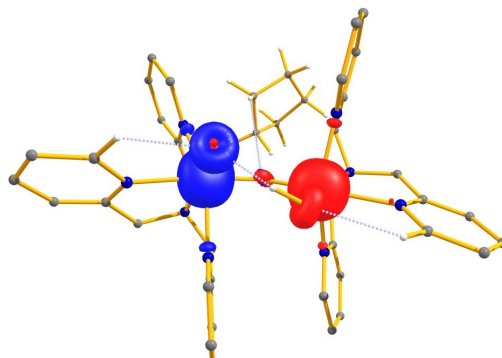


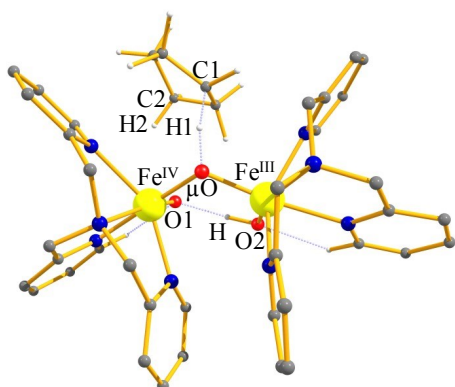
Figure S13. Electron shift diagrams of $\mathbf{I}^{-2}\mathbf{Int}_{\text{hs-hs}}$ for spin natural orbitals and their occupation (noted in parenthesis)



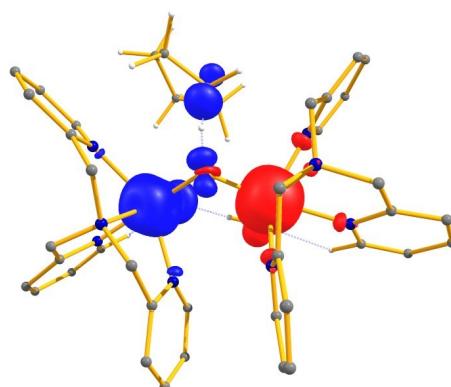
(a)



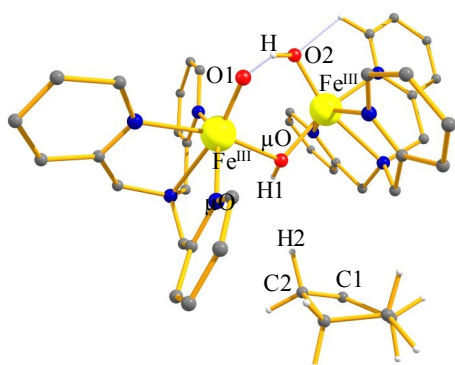
(b)



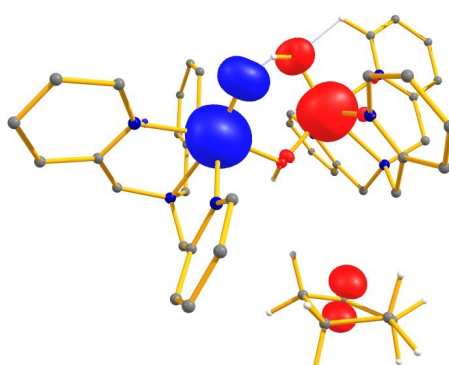
(c)



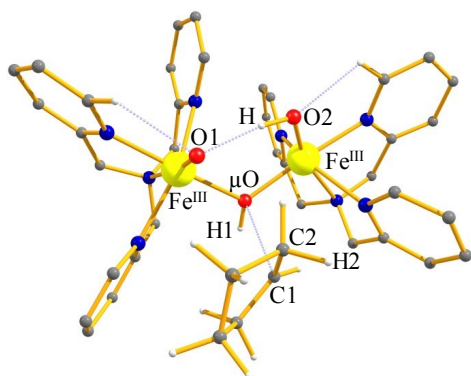
(d)



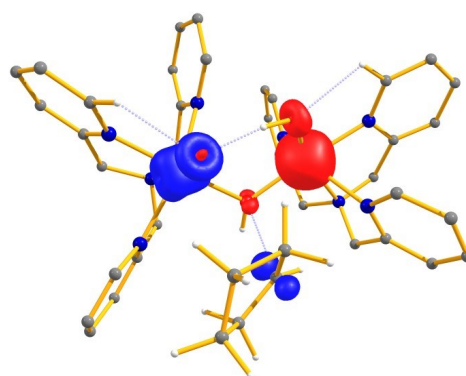
(e)



(f)



(g)



(h)

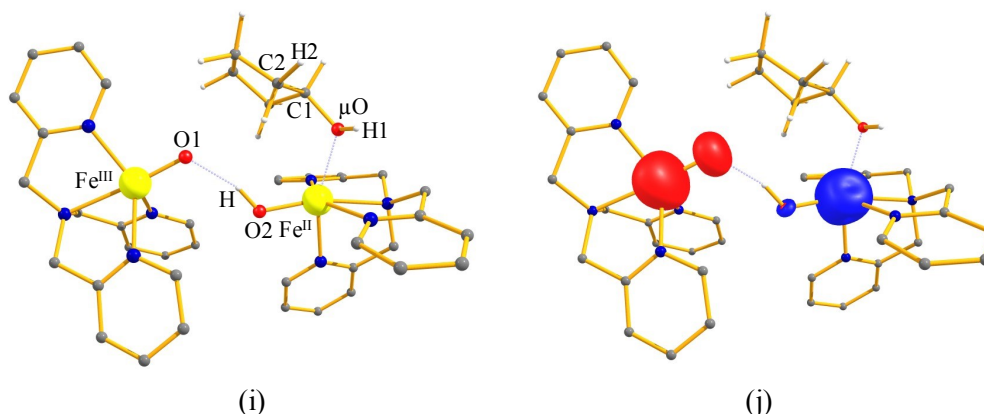


Figure S14. a-b) The optimized structure of $\text{II-}^2\text{RC}_{\text{hs-hs}}$ and its corresponding spin density plot, c-d) optimized structure of $\text{II-}^2\text{TS}_{\text{Hhs-hs}}$ and its corresponding spin density plot, e-f) optimized structure of $\text{II-}^2\text{Int}_{\text{hs-hs}}$ and its corresponding spin density plot, g-h) optimized structure of $\text{II-}^2\text{TS}_{\text{Rebhs-hs}}$ and its corresponding spin density plot, i-j) optimized structure of $\text{II-}^2\text{P}_{\text{Rebhs-hs}}$ and its corresponding spin density plot. Some important structural parameters computed for the spin states and spin density values are given below for pathway **II**. For spin state $\text{II-}^2\text{RC}_{\text{hs-hs}}$, $\text{Fe}^{\text{IV}}\text{-O1} = 1.642$, $\text{Fe}^{\text{III}}\text{-O2} = 1.832$, $\text{Fe}^{\text{IV}}\text{-}\mu\text{O} = 1.756$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O1} = 1.870$, $\mu\text{O-H1} = 3.454$, $\text{H1-C1} = 1.096$, $\angle\text{Fe}^{\text{IV}}\text{-}\mu\text{O-H1} = 120^\circ$, $\angle\mu\text{O-H1-C1} = 139^\circ$ and spin density $\text{Fe}^{\text{IV}} = -3.03$, $\text{Fe}^{\text{III}} = 3.99$, $\text{O1} = -0.49$, $\text{O2} = 0.37$, $\mu\text{O} = 0.05$, $\text{C1} = 0.00$. For spin state $\text{II-}^2\text{TS}_{\text{Hhs-hs}}$, $\text{Fe}^{\text{IV}}\text{-O1} = 1.639$, $\text{Fe}^{\text{III}}\text{-O2} = 1.810$, $\text{Fe}^{\text{IV}}\text{-}\mu\text{O} = 1.983$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O} = 1.940$, $\mu\text{O-H1} = 1.259$, $\text{H1-C1} = 1.335$, $\angle\text{Fe}^{\text{IV}}\text{-}\mu\text{O-H1} = 106^\circ$, $\angle\mu\text{O-H1-C1} = 167^\circ$ and spin density $\text{Fe}^{\text{IV}} = -2.64$, $\text{Fe}^{\text{III}} = 3.98$, $\text{O1} = -0.34$, $\text{O2} = 0.44$, $\mu\text{O} = -0.14$, $\text{C1} = -0.47$. For spin state $\text{II-}^2\text{Int}_{\text{hs-hs}}$, $\text{Fe}^{\text{III}}\text{-O1} = 1.723$, $\text{Fe}^{\text{III}}\text{-O2} = 1.802$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O} = 2.104$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O} = 2.010$, $\mu\text{O-H1} = 0.969$, $\text{H1-C1} = 4.001$, $\angle\text{Fe}^{\text{III}}\text{-}\mu\text{O-H1} = 110^\circ$, $\angle\mu\text{O-H1-C1} = 98^\circ$ and spin density $\text{Fe}^{\text{III}} = -3.88$, $\text{Fe}^{\text{III}} = 4.02$, $\text{O1} = -0.73$, $\text{O2} = 0.46$, $\mu\text{O} = 0.07$, $\text{C1} = 0.99$. For spin state $\text{II-}^2\text{TS}_{\text{Rebhs-hs}}$, $\text{Fe}^{\text{III}}\text{-O1} = 1.630$, $\text{Fe}^{\text{III}}\text{-O2} = 1.840$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O} = 2.130$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O} = 2.051$, $\mu\text{O-H1} = 0.968$, $\mu\text{O-C1} = 2.627$, $\angle\text{Fe}^{\text{III}}\text{-}\mu\text{O-H1} = 115^\circ$, $\angle\text{Fe}^{\text{III}}\text{-}\mu\text{O-C1} = 107^\circ$, $\angle\text{H1-}\mu\text{O-C1} = 77^\circ$ and spin density $\text{Fe}^{\text{III}} = -2.56$, $\text{Fe}^{\text{III}} = 3.86$, $\text{O1} = -0.35$, $\text{O2} = 0.30$, $\mu\text{O} = 0.13$, $\text{C1} = -0.50$. For spin state $\text{II-}^2\text{P}_{\text{Rebhs-hs}}$, $\text{Fe}^{\text{III}}\text{-O1} = 1.703$, $\text{Fe}^{\text{II}}\text{-O2} = 1.876$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O} = 4.556$, $\text{Fe}^{\text{II}}\text{-}\mu\text{O} = 2.243$, $\mu\text{O-H1} = 0.971$, $\mu\text{O-C1} = 1.455$, $\angle\text{Fe}^{\text{III}}\text{-}\mu\text{O-H1} = 162^\circ$, $\angle\text{Fe}^{\text{III}}\text{-}\mu\text{O-C1} = 162^\circ$, $\angle\text{H1-}\mu\text{O-C1} = 107^\circ$ and spin density $\text{Fe}^{\text{III}} = 3.81$, $\text{Fe}^{\text{II}} = -3.69$, $\text{O1} = 0.91$, $\text{O2} = -0.15$, $\mu\text{O} = -0.02$, $\text{C1} = -0.01$. All bond lengths are given in Å and angles are given in $^\circ$. All hydrogen atoms (except O2-H, C1-H1 and C2-H2) are omitted for clarity.

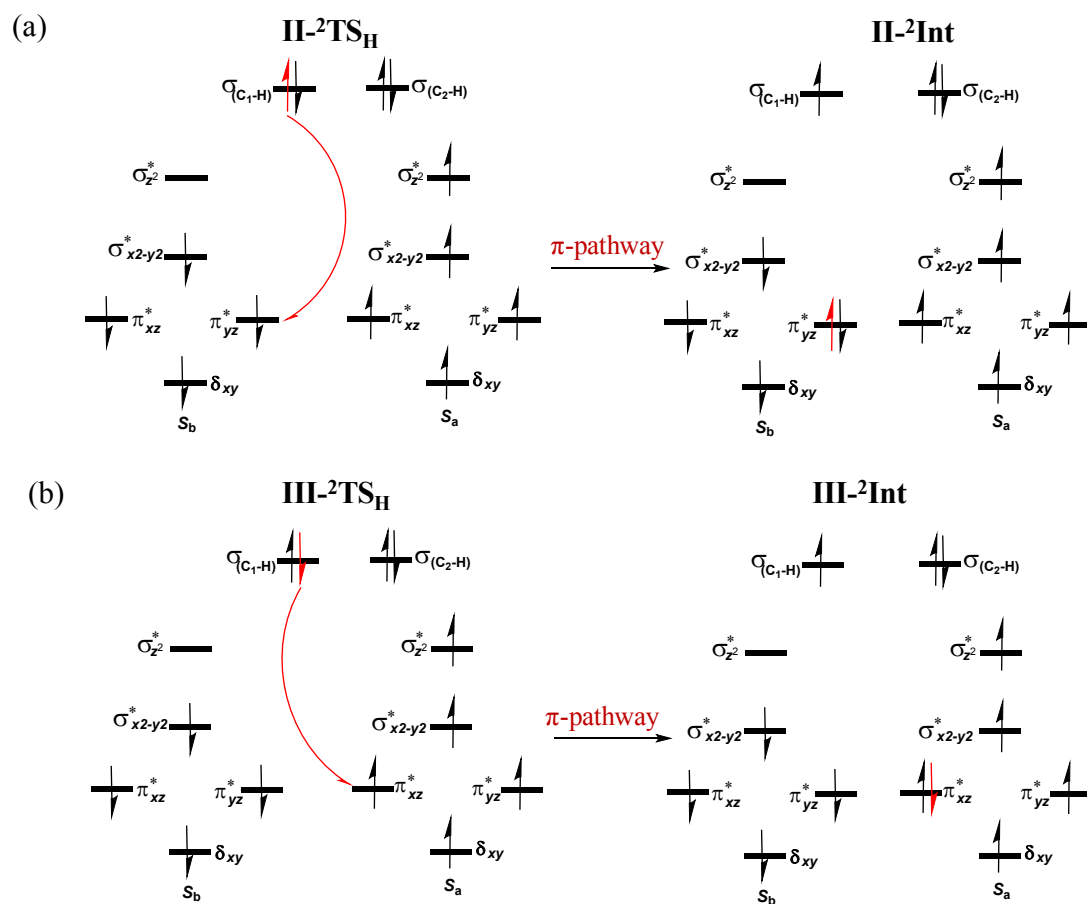
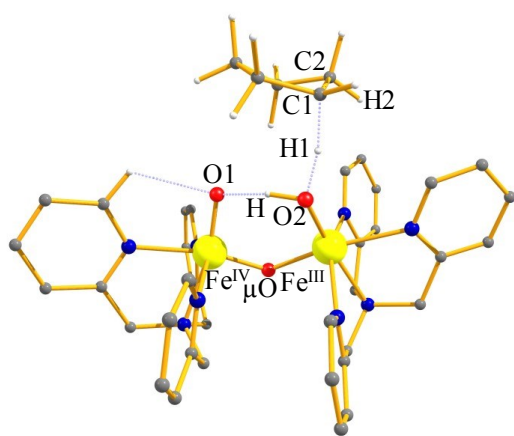
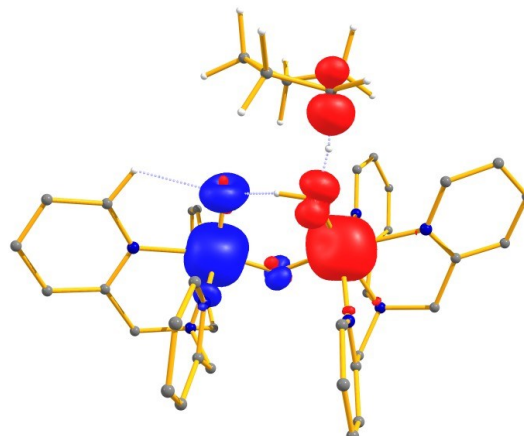


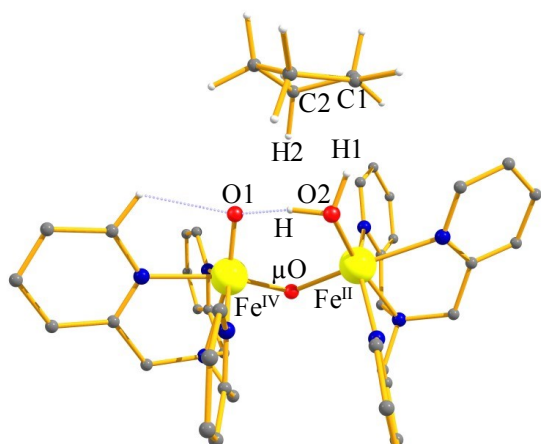
Figure S15. Electron shift diagrams of **TS_H** for both (a) **II-²TS_H_{hs-hs}** and (b) **III-²TS_H_{hs-hs}**.



(a)

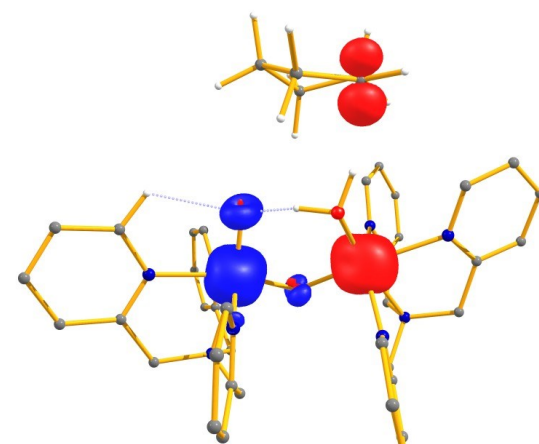


(b)



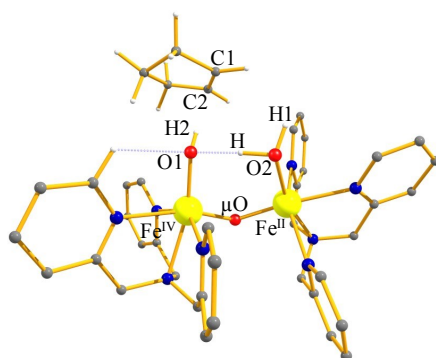
(c)

(e)

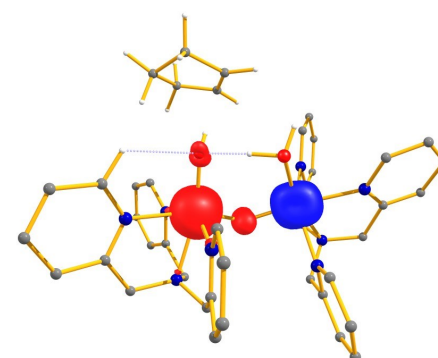


(d)

(f)



(g)



(h)

Figure S16. a-b) The optimized structure of **III**- $^2\text{TS}_{\text{Hhs-hs}}$ and its corresponding spin density plot, c-d) optimized structure of **III**- $^2\text{Int}_{\text{hs-hs}}$ and its corresponding spin density plot, e-f) optimized structure of **III**- $^2\text{TS}_{2\text{Hhs-hs}}$ and its corresponding spin density plot, g-h) optimized structure of **III**- $^2\text{P}_{2\text{Hhs-hs}}$ and its corresponding spin density plot. Some important structural parameters computed for the spin states and spin density values are given below for pathway **III**. For spin state **III**- $^2\text{TS}_{\text{Hhs-hs}}$, $\text{Fe}^{\text{IV}}\text{-O1}=1.663$, $\text{Fe}^{\text{III}}\text{-O2}=2.014$, $\text{Fe}^{\text{IV}}\text{-}\mu\text{O}=1.721$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O1}=1.929$, $\text{O2-H1}=1.235$, $\text{H1-C1}=1.329$, $\angle\text{Fe}^{\text{III}}\text{-O2-H1}=130^\circ$, $\angle\text{O2-H1-C1}=168^\circ$ and spin density $\text{Fe}^{\text{IV}}=-3.06$, $\text{Fe}^{\text{III}}=3.77$, $\text{O1}=-0.41$, $\text{O2}=0.36$, $\mu\text{O}=-0.16$, $\text{C1}=0.50$. For spin state **III**- $^2\text{Int}_{\text{hs-hs}}$, $\text{Fe}^{\text{IV}}\text{-O1}=1.672$, $\text{Fe}^{\text{II}}\text{-O2}=2.130$, $\text{Fe}^{\text{IV}}\text{-}\mu\text{O}=1.714$, $\text{Fe}^{\text{II}}\text{-}\mu\text{O1}=1.933$, $\text{O2-H1}=0.982$, $\text{H1-C1}=2.043$, $\angle\text{Fe}^{\text{II}}\text{-O2-H1}=123^\circ$, $\angle\text{O2-H1-C1}=164^\circ$ and spin density $\text{Fe}^{\text{IV}}=-3.08$, $\text{Fe}^{\text{II}}=3.69$, $\text{O1}=-0.39$, $\text{O2}=0.05$, $\mu\text{O}=-0.19$, $\text{C1}=0.93$. For spin state **III**- $^2\text{TS}_{2\text{Hhs-hs}}$, $\text{Fe}^{\text{IV}}\text{-O1}=1.729$, $\text{Fe}^{\text{II}}\text{-O2}=2.148$, $\text{Fe}^{\text{IV}}\text{-}\mu\text{O}=1.714$, $\text{Fe}^{\text{II}}\text{-}\mu\text{O1}=1.918$, $\text{O1-H2}=1.621$, $\text{H2-C2}=1.166$, $\angle\text{Fe}^{\text{IV}}\text{-O1-H2}=119^\circ$, $\angle\text{O1-H2-C2}=162^\circ$ and spin density $\text{Fe}^{\text{IV}}=-2.88$, $\text{Fe}^{\text{II}}=3.68$, $\text{O1}=-0.35$, $\text{O2}=0.02$, $\mu\text{O}=-0.15$, $\text{C2}=-0.14$. For spin state **III**- $^2\text{P}_{2\text{Hhs-hs}}$, $\text{Fe}^{\text{III}}\text{-O1}=1.931$, $\text{Fe}^{\text{II}}\text{-O2}=2.203$, $\text{Fe}^{\text{III}}\text{-}\mu\text{O}=1.779$, $\text{Fe}^{\text{II}}\text{-}\mu\text{O1}=1.868$, $\text{O1-H2}=0.976$, $\text{H2-C2}=2.251$, $\angle\text{Fe}^{\text{III}}\text{-O1-H2}=115^\circ$, $\angle\text{O1-H2-C2}=146^\circ$ and spin density $\text{Fe}^{\text{III}}=3.98$, $\text{Fe}^{\text{II}}=-3.65$, $\text{O1}=0.18$, $\text{O2}=-0.02$, $\mu\text{O}=0.37$, $\text{C2}=-0.01$. All bond lengths are given in Å and angles are given in $^\circ$. All hydrogen atoms (except O2-H, C1-H1 and C2-H2) are omitted for clarity.

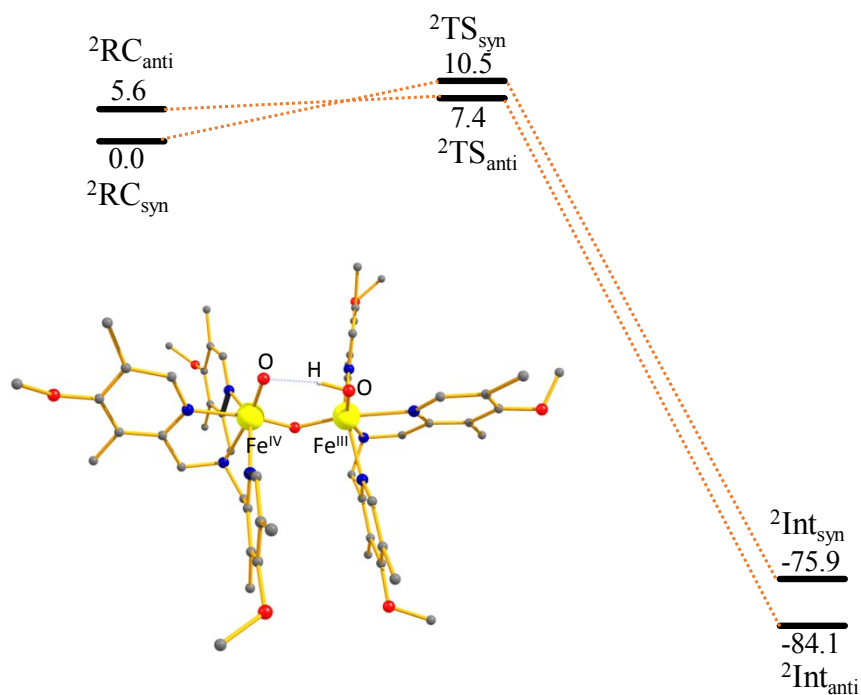


Figure S17a. B3LYP-D3 computed energy for the C-H bond activation of DHA by $[(\text{HO}(\text{L})\text{Fe}^{\text{III}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L}))]^{2+}$ complex (energies are in kJ/mol).

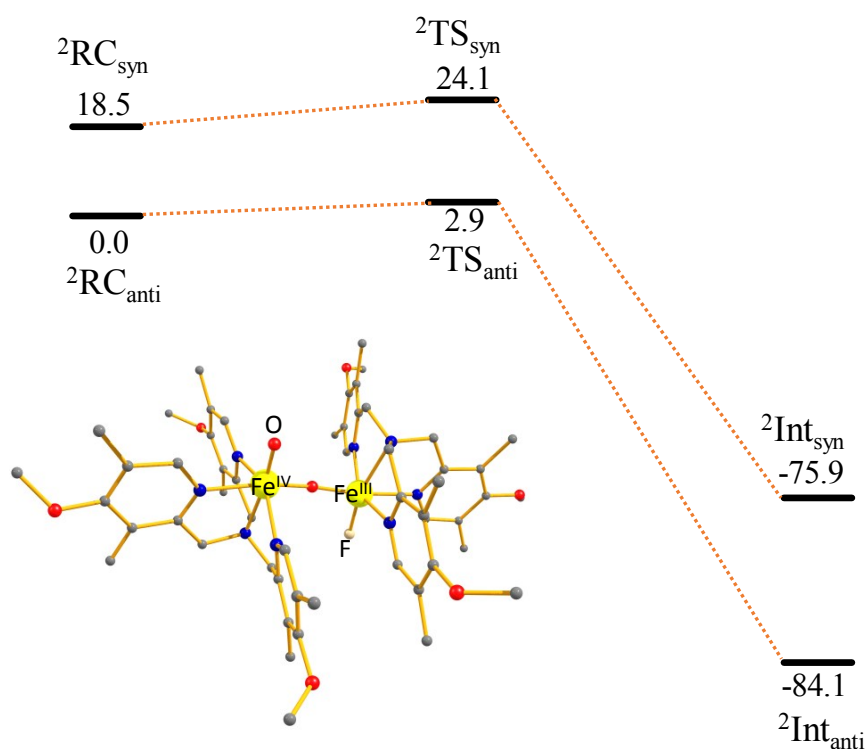


Figure S17b. B3LYP-D3 computed energy for the C-H bond activation of DHA by $[(\text{F}(\text{L})\text{Fe}^{\text{III}}-\text{O}-\text{Fe}^{\text{IV}}(\text{O})(\text{L}))]^{2+}$ complex (energies are in kJ/mol).

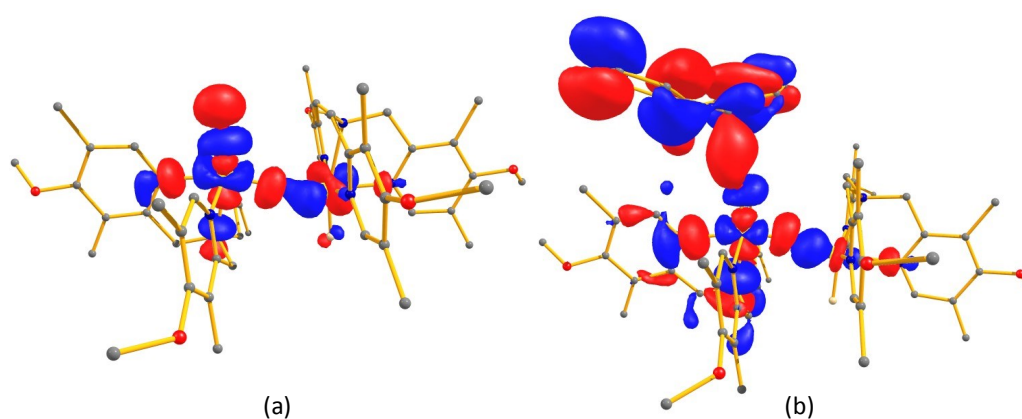


Figure17c. Computed orbital diagram corresponding to a) LUMO of the $^2\text{R}_{\text{hs-hs}}$, b) HOMO of the $^2\text{TS}_{\text{Hhs-hs}}$.

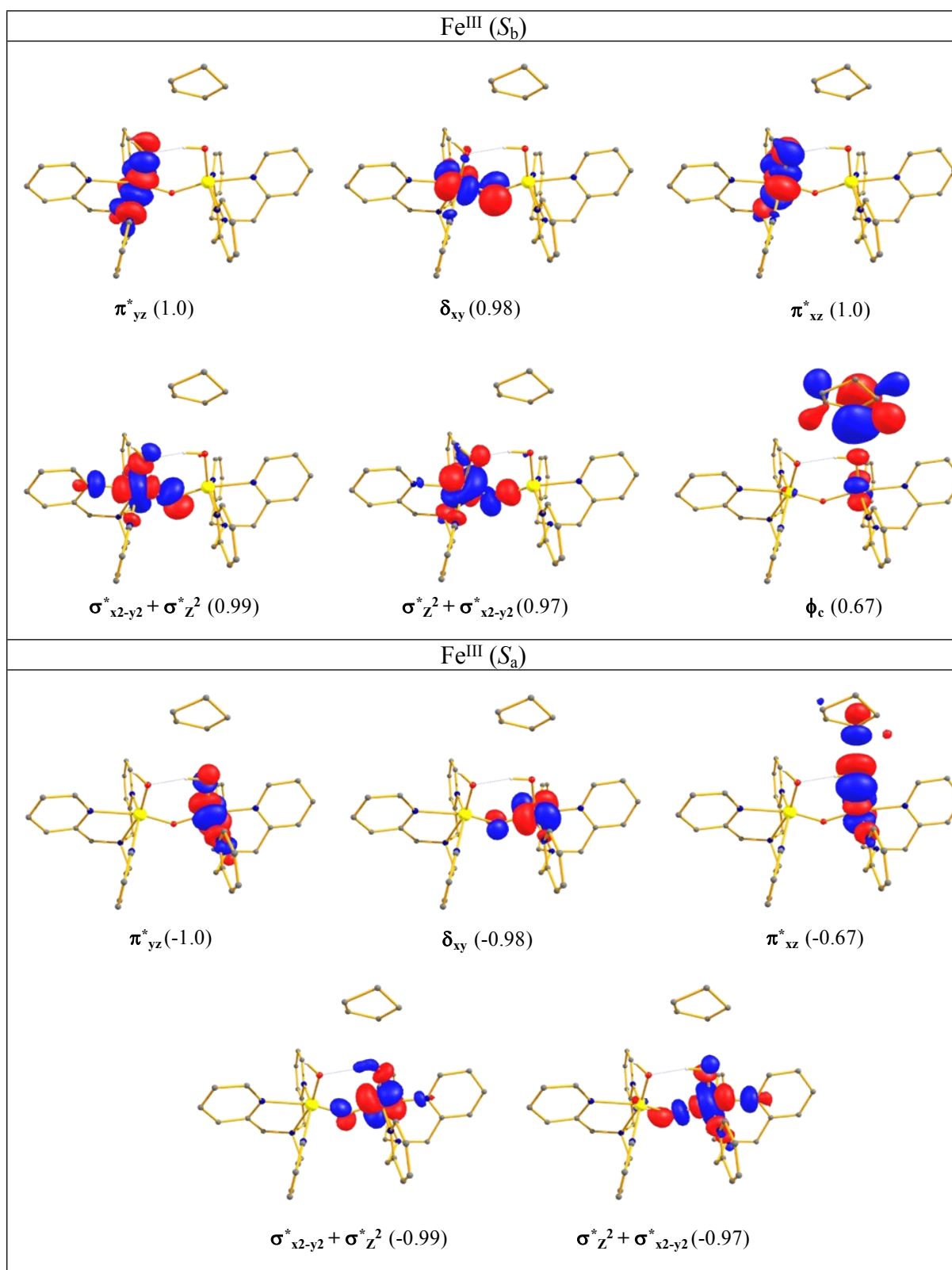


Figure S18. Spin nature orbitals and their occupations (noted in parenthesis) of $\text{Ia}^{-2}\text{TS}_{\text{rebhs-hs}}$.

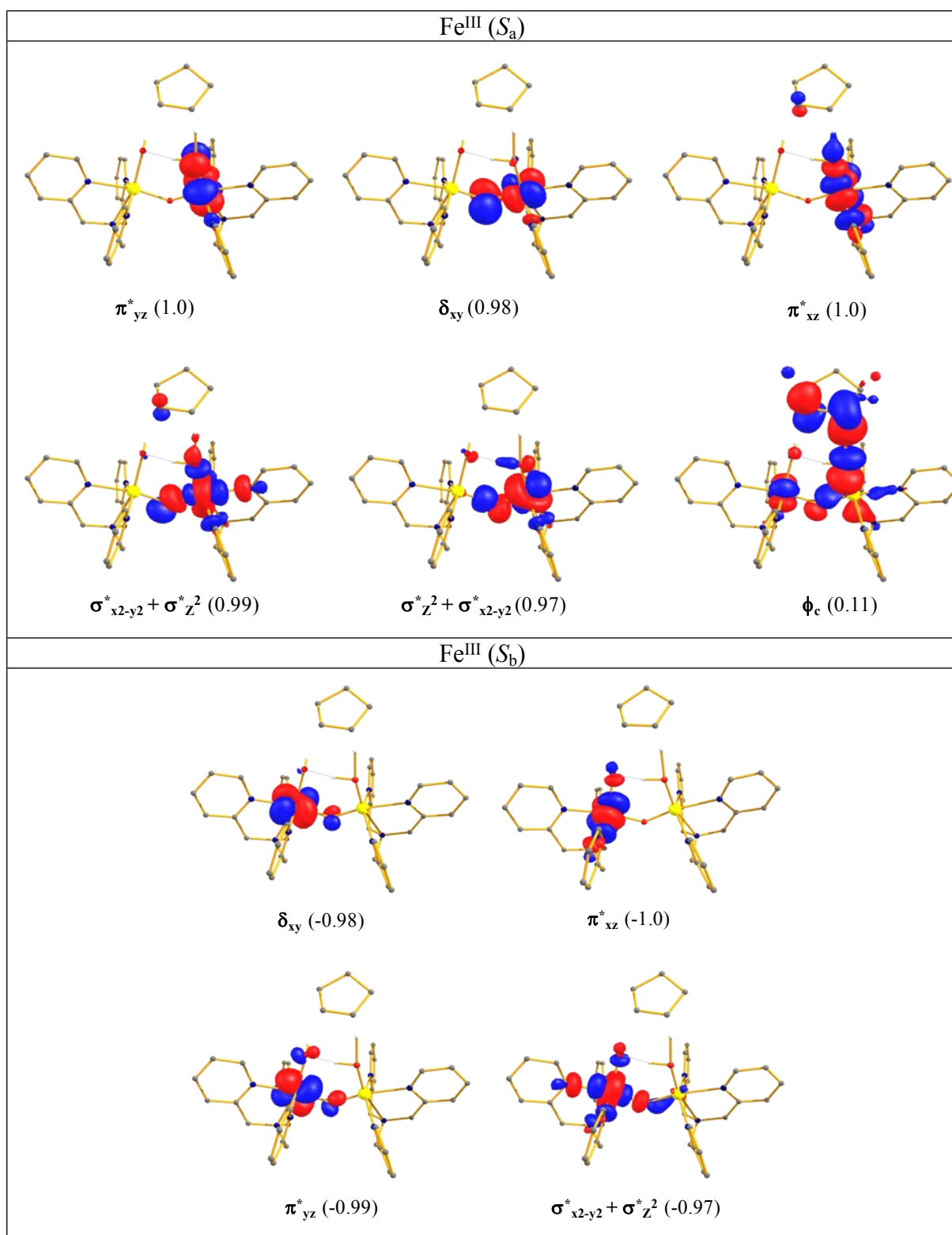


Figure S20. Spin nature orbitals and their occupations (noted in parenthesis) of **Ib**-²**TS**_{2Hhs-hs}.

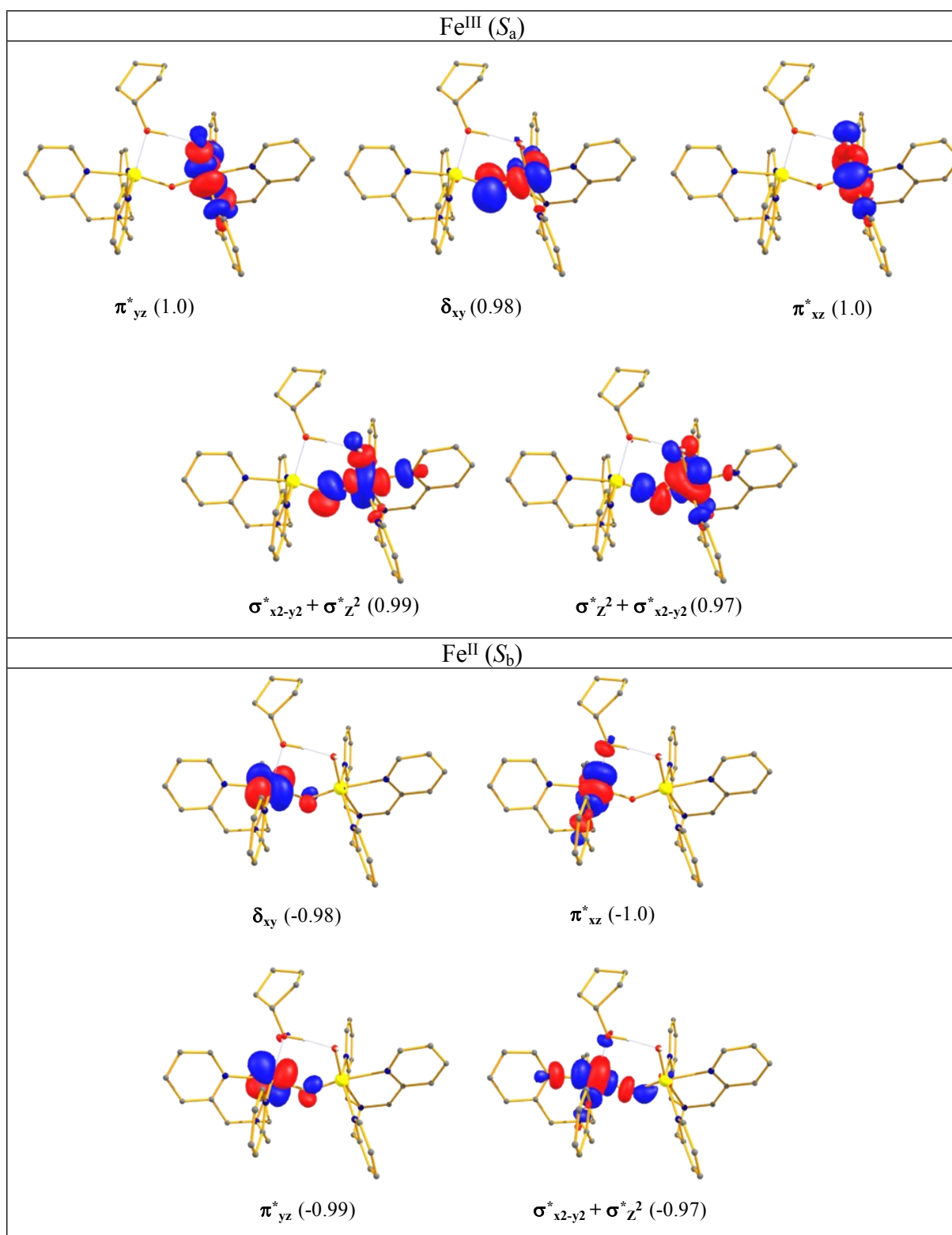


Figure S21. Spin nature orbitals and their occupations (noted in parenthesis) of **Ia**- $2\mathbf{P}_{\text{rebhs-hs}}$.

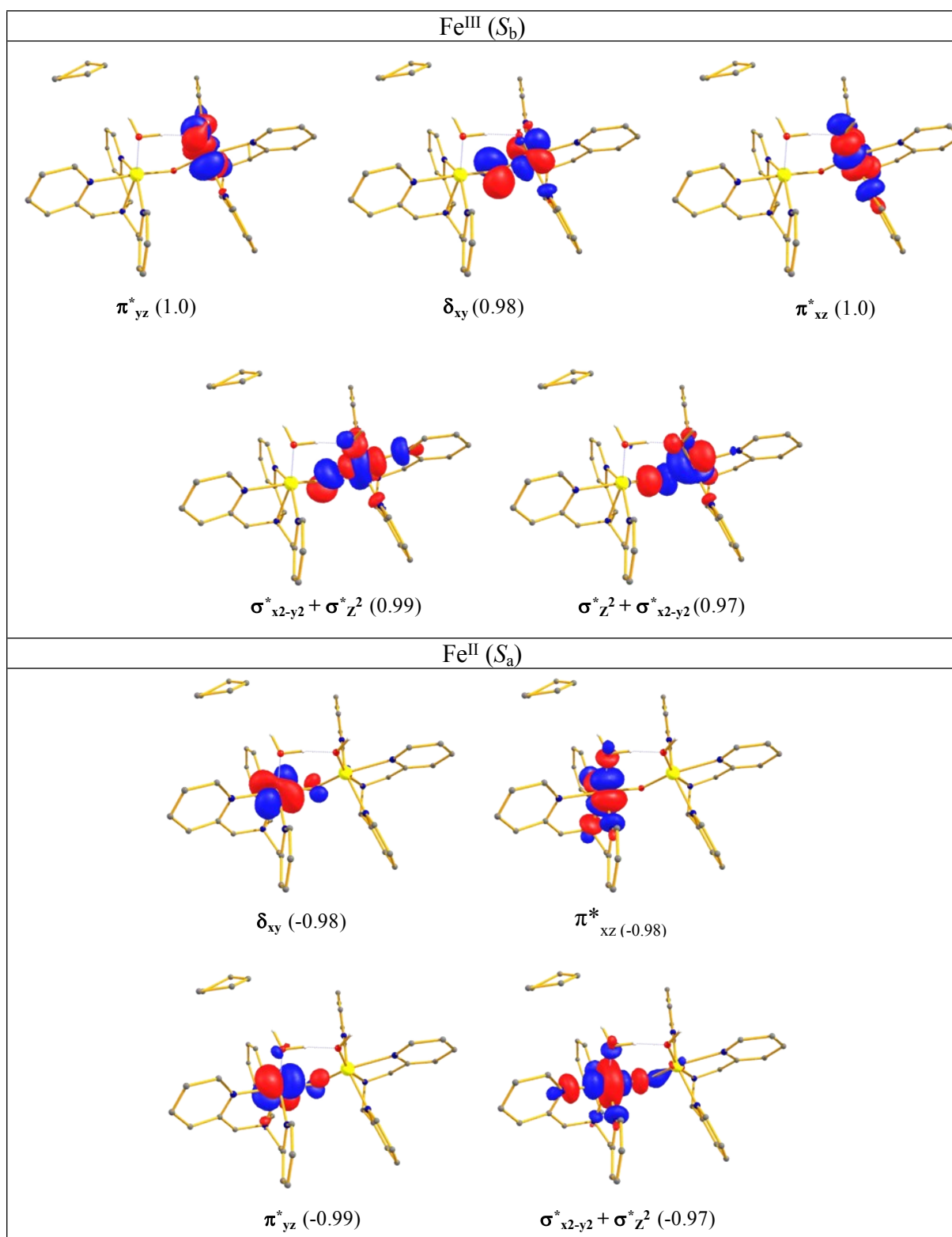


Figure S22. Spin nature orbitals and their occupations (noted in parenthesis) of **Ib**- $^2\text{P}_{2\text{Hhs-hs}}$.

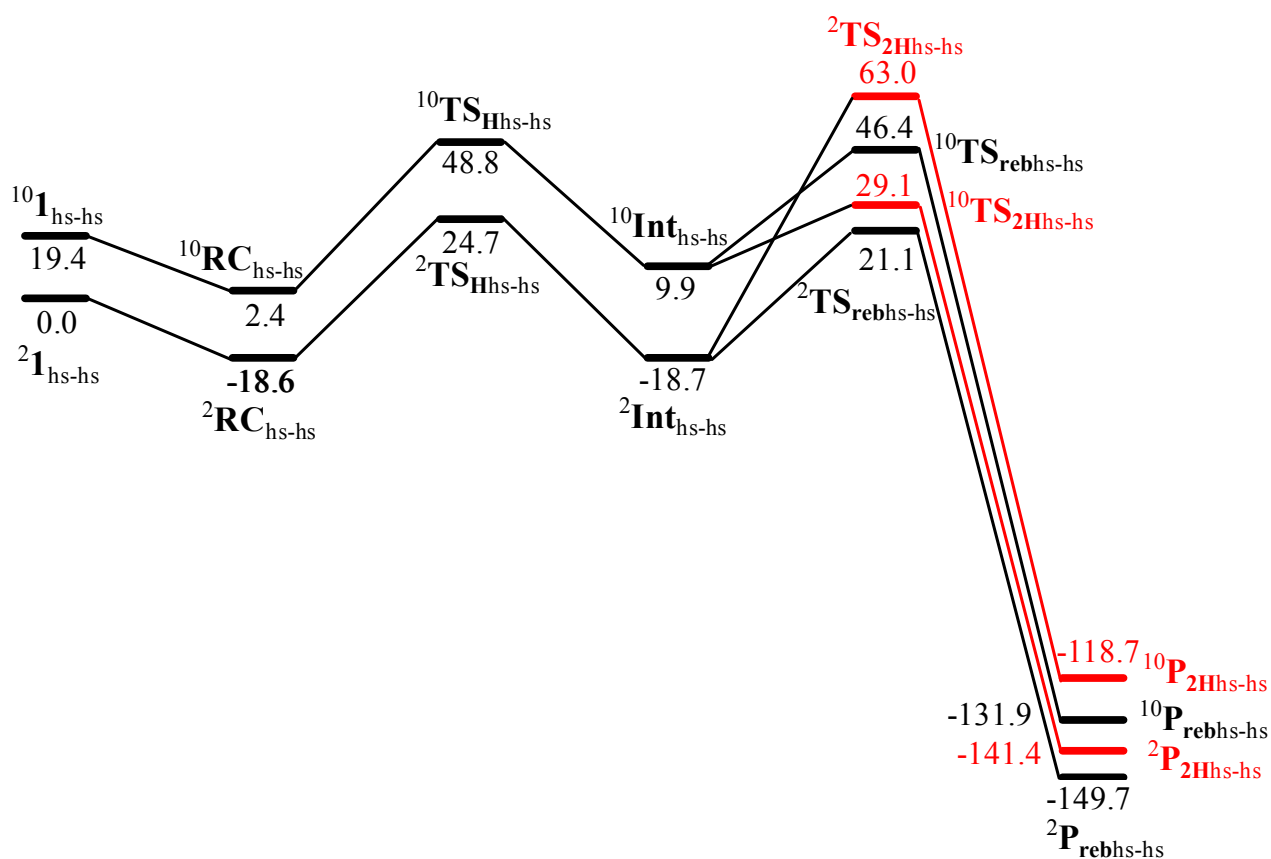


Figure S23. B3LYP-D3 computed potential energy surface for C-H bond activation of cyclohexane by complex **1** with adding of two perchloride counterions. All energies ($\Delta E_{\text{solv}} + \text{ZPE}$) are reported in kJ/mol.

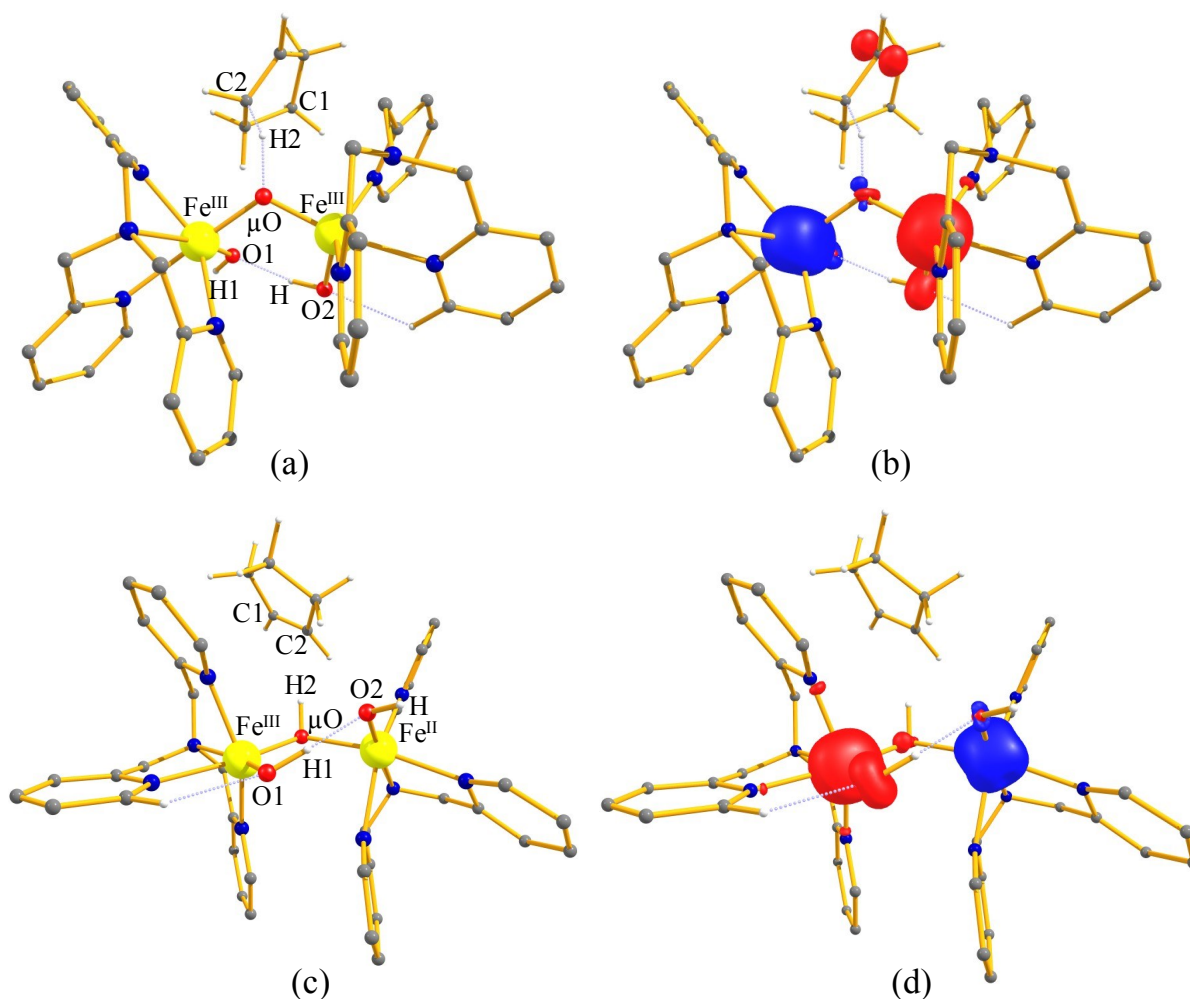


Figure S24. a-b) The optimized structure of **Ic-²TS_{2Hhs-hs}** and its corresponding spin density plot, c-d) optimized structure of **Ic-²P_{2Hhs-hs}** and its corresponding spin density plot. Some important structural parameters computed for the spin states and spin density values are given below for pathway **Ic**. For spin state **Ic-²TS_{2Hhs-hs}**, Fe^{III}-O1= 1.836, Fe^{III}-O2= 1.897, Fe^{III}-μO= 1.842, Fe^{III}-μO1= 1.958, μO-H2= 1.625, H2-C2= 1.188, ∠Fe^{III}-μO-H2= 116°, ∠O2-H1-C1= 159° and spin density Fe^{IV}= 3.96, Fe^{III}= -3.83, O1= 0.38, O2= -0.18, μO= 0.03, C1= 0.58, C2= -0.11. For spin state **Ic-²P_{2Hhs-hs}**, Fe^{III}-O1= 1.808, Fe^{II}-O2= 1.916, Fe^{III}-μO= 1.956, Fe^{II}-μO1= 2.179, μO-H2= 0.973, H2-C2= 2.424, ∠Fe^{III}-μO-H2= 112°, ∠μO-H2-C2= 166° and spin density Fe^{III}= 4.02, Fe^{II}= -3.71, O1= 0.47, O2= -0.12, μO= 0.14, C1= 0.0 C2= 0.0. All bond lengths are given in Å and angles are given in °. All hydrogen atoms (except O2-H, C1-H1 and C2-H2) are omitted for clarity.

Table S10. Comparative energy barrier for the activation of C-H bond of DHA by various mono/dinuclear Fe^{IV}=O species reported in the literature along with the theoretical level that are reported.

Complex name	Barrier height (kJ/mol)	Level of theory	References
$[\text{OH}-\text{Fe}^{\text{III}}-\text{O}-\text{Fe}^{\text{IV}}=\text{O}]^{2+}$	13.8	UB3LYP/def2-TZVPP	Inorg. Chem. 2013, 52, 3976–3984.
$[(6\text{-PhTPA})\text{Fe}^{\text{IV}}\text{QO}]^{2+}$	54.6	UB3LYP/TZVP	Chem. Commun., 2017, 53, 3193–3196.
$[(\text{TMC})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$	70.6□	UB3LYP/lacv3p-(d,p)	J. Phys. Chem. C, Vol. 111, No. 33, 2007.
$[(\text{TMC})\text{Fe}^{\text{IV}}(\text{O})(\text{CF}_3\text{CO}_2^-)]^+$	60.61	UB3LYP/lacv3p-(d,p)	J. Phys. Chem. C, Vol. 111, No. 33, 2007 .
$[(\text{H}_3\text{buea})\text{Fe}^{\text{IV}}(\text{O})]^-$	109.1	UB3LYP/LACV 3P+*(Fe,K)/6-311+G*	J. Am. Chem. Soc. 2013, 135, 17090–17104.
$[(\text{H1}^{\text{cyp}})\text{Fe}^{\text{IV}}(\text{O})]^-$	88.2	UB3LYP/LACV 3P+*(Fe,K)/6-311+G*	J. Am. Chem. Soc. 2013, 135, 17090–17104.
$[(\text{H}_3\text{buea})\text{Fe}^{\text{III}}(\text{O})]^{2-}$	99.9	UB3LYP/LACV 3P+*(Fe,K)/6-311+G*	J. Am. Chem. Soc. 2013, 135, 17090–17104.
$[(\text{N4Py})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$	36.8	UB3LYP/LACV 3P+*(Fe,K)/6-311+G*	J. Am. Chem. Soc. 2013, 135, 17090–17104.
$[(\text{TMC})\text{Fe}^{\text{IV}}(\text{O})(\text{CH}_3\text{CN})]^{2+}$	108.3	UB3LYP/LACV 3P+*(Fe)/def2-tzvpp	J. Am. Chem. Soc. 2015, 137, 722–733.
$[(\text{TMC})\text{Fe}^{\text{IV}}(\text{O})(\text{CH}_2\text{S})]^+$	110.4	UB3LYP/LACV 3P+*(Fe)/def2-tzvpp	J. Am. Chem. Soc. 2015, 137, 722–733.
$[(\text{TMC})\text{Fe}^{\text{IV}}(\text{O})(\text{N}_3)]^+$	106.2	UB3LYP/LACV 3P+*(Fe)/def2-tzvpp	J. Am. Chem. Soc. 2015, 137, 722–733.
$[(\text{Bn-TPEN})\text{Fe}^{\text{IV}}\text{O}]^{2+}$	60.2	UB3LYP/Def2-TZVPP//LACVP*(Fe)/6-31G*(rest)	J. Am. Chem. Soc. 2016, 138, 2094–209.
$[(14\text{-TMC})\text{Fe}(\text{OO})]^+$	77.7	UB3LYP/TZVP	Angew. Chem.2015,127, 574 –578.
Cpd-I of HRP	59.4*	UB3LYP/LACV P**	Chem. Eur. J.2014,20, 14437 – 14450.
Cpd-II of HRP	68.6*	UB3LYP/LACV P**	Chem. Eur. J.2014,20,

			14437 – 14450.
$[(\text{TPFPP})\text{Fe}^{\text{IV}}=\text{(O)}]^{2+}$	73.6*	UB3LYP/def2-TZVP//LACVP*	J. Am. Chem. Soc. 2017, 139, 11451–11459.
$[(\text{TMP})\text{Fe}^{\text{IV}}=\text{(O)}]^{2+}$	84.9*	UB3LYP/def2-TZVP//LACVP*	J. Am. Chem. Soc. 2017, 139, 11451–11459.
$[(\text{TMG3tren})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$	60.2	UB3LYP-D3/def2-SVP(Fe: def2-TZVP)	Chem. Commun., 2016, 52, 10509—10512.
$[\text{TMG}_2\text{dien}(\text{MeCN})\text{Fe}^{\text{IV}}(\text{O})]^{2+}$	45.6□	UB3LYP-D3/def2-SVP(Fe: def2-TZVP)	Chem. Commun., 2016, 52, 10509—10512.
Cpd I	38.9	UB3LYP/Def2-TZVPP	Chem.Eur.J.2015,21,9083–9092.

Note- * represents a zero-point energy correction

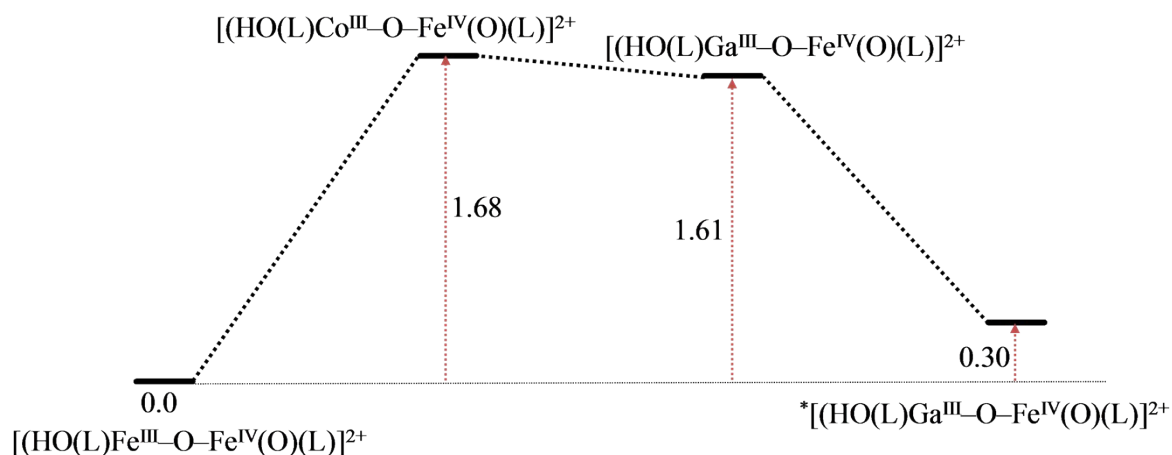


Figure S25. We computed relative energies of σ_z^{*2} orbital of all four species. Here, we have plotted the difference of difference in energy between the $\delta_{xy}-\sigma_z^{*2}$ gap. i.e $\Delta\Delta E(E(\delta_{xy})-E(\sigma_z^{*2}))$ using $[HO-(L)Fe^{III}-O-Fe^{IV}(O)(L)]^{2+}$ as a reference. This figure suggests that the σ_z^{*2} is getting destabilized when Co^{III}/Ga^{III} are the presence in the place of Fe^{III} ion. Here, $*[HO-(L)Ga^{III}-O-Fe^{IV}(O)(L)]^{2+}$ correspond to single-point calculations performed by substituting Fe^{III} by Ga^{III} ion in **1**.

Table S11. Computed relative deformation energies in each fragment with respect to the pre-reacting complex and interaction energy in the reorganization TSs are values for the **I**- $^2TS_{Hhs-hs}$, **II**- $^2TS_{Hhs-hs}$, and **III**- $^2TS_{Hhs-hs}$. All energies are in kJ/mol.

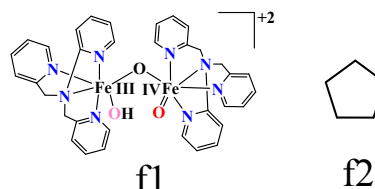
TSs	E _{def}	E _{int}	E _{act}
I - ² TS _{H_{hs}-hs}	29.9	23.6	54.9
II - ² TS _{H_{hs}-hs}	118.1	59.4	177.5
III - ² TS _{H_{hs}-hs}	71.9	72.7	144.7

Where, E_{def}, E_{int}, and E_{act} are a deformation, interaction and activation strain energy, respectively.

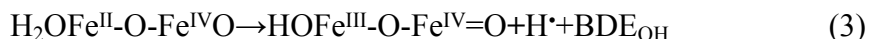
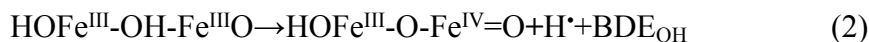
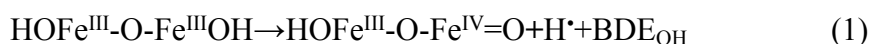
$$E_{\text{act}} = E_{\text{def}} + E_{\text{int}}$$

$$E_{\text{dis}} = [\{E_{\text{f1(TS)}} + E_{\text{f2(TS)}}\} - \{E_{\text{f1}} + E_{\text{f2}}\}]$$

$$E_{\text{int}} = [E_{\text{(TS)}} - \{E_{\text{f1}} + E_{\text{f2}}\}]$$



Thermochemistry. The estimation of the bond dissociation energies (BDE_{OH} and BDE_{CH}) of diiron-hydroxo and diiron-aqua complexes of the O–H and the substrate (C₅H₉-H) of the C–H was determined from the relative energy (E_{solv}+ ZPE) for the following three equations:



For calculating the reorganization energy of the cyclopentyl radical (RE_{Alk•}), the energy difference of the cyclopentyl radical (Alk•) moiety in its geometry in cyclopentane (Alk-H) relative to its final optimized geometry. The combination of BDE_{CH} and RE_{Alk•} in eq.5 defines the bond strength (*D*_{CH}), which is a more accurate measure of the interaction between the bonded cyclopentyl and H moieties of the cyclopentane (Ref- *J. Am. Chem. Soc.* 2004, 126, 27, 8362–8363).

$$D_{\text{CH}} = \text{BDE}_{\text{CH}} + \text{RE}_{\text{Alk}^{\bullet}} \quad (5)$$

Table S12. The percentage of the bond breaking of the C-H bond (% BB_{CH}) and bond formation of the O-H bond (% FB_{OH}) are values for the **I**-²**TS**_{H_{hs}-hs}, **II**-²**TS**_{H_{hs}-hs}, and **III**-²**TS**_{H_{hs}-hs}.

TSs	(%BB _{C-H})	(%FB _{O-H})
I - ² TS _{H_{hs}-hs}	89	74

II-²TS_{Hhs-hs}	82	77
III-²TS_{Hhs-hs}	83	78
*⁵TS_{Hhs-ls}	86	78
**⁵TS_{Hhs-ls}	87	-

* and ** represents a where Fe^{III} centre replaced by Co^{III} and Ga^{III} metal ion (low spin)

The percentages of the bond breaking of the C-H bond (% BB_{CH}) is defined as the ratio of the C-H bond in a reactant divided by the elongation of the C-H in the transition state. Similarly, the percentages of bond formation of the O-H bond (% BF_{OH}) is defined as the ratio of the O-H bond in an intermediate divided by the elongation of the O-H in the transition state.

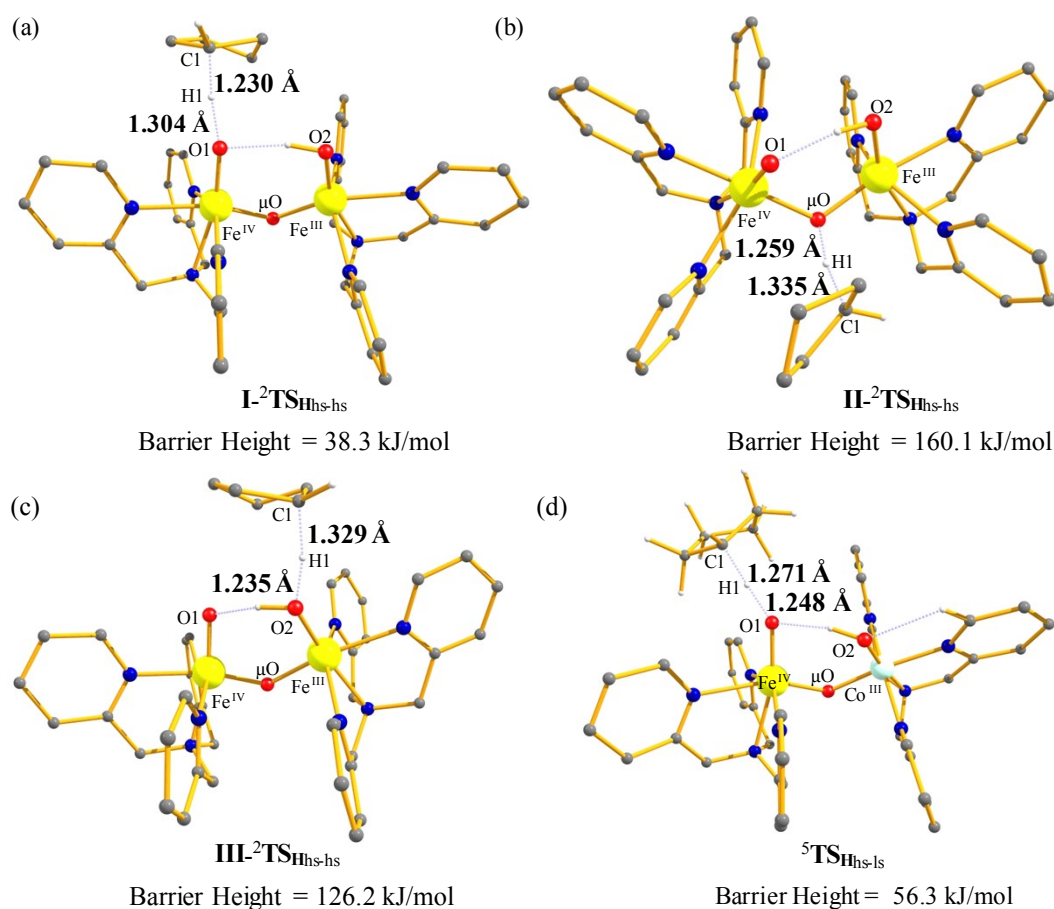


Figure S26. The optimized structure and its corresponding bond length of the C-H and O-H for a) **I-²TS_{Hhs-hs}**, b) **II-²TS_{Hhs-hs}**, c) **III-²TS_{Hhs-hs}** and d) **⁵TS_{Hhs-ls}**. All computed barrier heights are shown with respect to the reactant complex (**RC**).

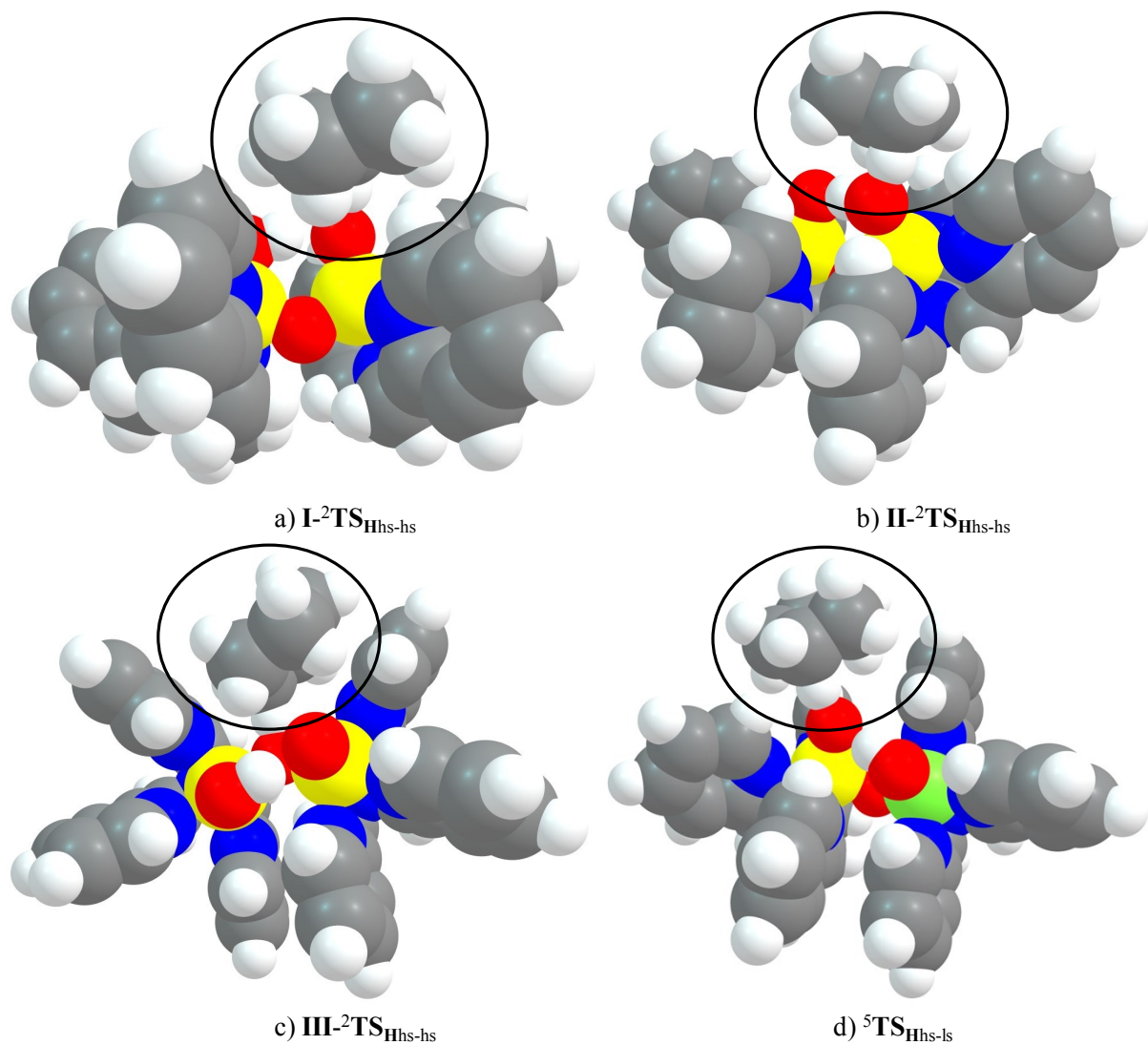


Figure S27. Space-filling models of a) $\text{I-}^2\text{TS}_{\text{Hhs-hs}}$ b) $\text{II-}^2\text{TS}_{\text{Hhs-hs}}$ c) $\text{III-}^2\text{TS}_{\text{Hhs-hs}}$ and d) $^5\text{TS}_{\text{Hhs-ls}}$. Atom color scheme: C, grey; H, white; N, blue; O, red; Fe, yellow; Co, pale green.

Table S13. The percentage of the bond interaction of the O-C/O-H bond ($\% \text{BI}_{\text{OC/O-H}}$) and bond formation of the O-C/O-H bond ($\% \text{BF}_{\text{OC/O-H}}$) are values for the **Ia**- $^2\text{TS}_{\text{Rebhs-hs}}$ and **Ib**- $^2\text{TS}_{\text{Hhs-hs}}$.

TSS	($\% \text{BB}_{\text{C-H/O-H}}$)	($\% \text{FB}_{\text{O-C/O-H}}$)
Ia - $^2\text{TS}_{\text{Rebhs-hs}}$ / Ib - $^2\text{TS}_{\text{Hhs-hs}}$	89 / 54	54 / 60

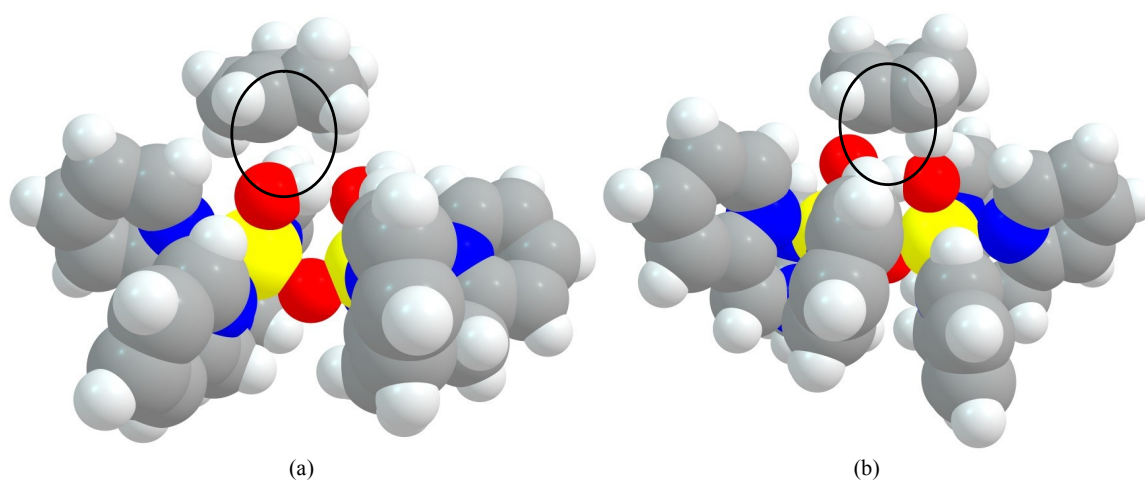
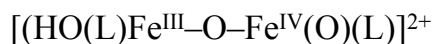


Figure S28. Space-filling models of (a) rebound transition state (**Ia**- $^2\text{TS}_{\text{Rebhs-hs}}$) and (b) second hydrogen abstraction transition states (**Ib**- $^2\text{TS}_{\text{Hhs-hs}}$) for complex **1**. Atom colour scheme: C, gray; H, white; N, blue; O, red; Fe, yellow.

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.



$2^1_{\text{hs-hs}}$

Fe	1.653095000	0.267296000	-0.444585000
O	1.311258000	0.738616000	-1.979278000
Fe	-1.529935000	0.169138000	-0.512238000
O	-1.170560000	-0.433080000	-2.200894000
H	-0.277886000	-0.098885000	-2.447599000
O	0.097386000	0.477057000	0.346039000
N	1.363451000	-1.963426000	-0.559661000
N	2.600274000	2.021950000	0.495557000
N	3.628457000	-0.310653000	-1.004608000
C	1.510981000	-2.591880000	0.618718000
C	1.467528000	-3.980532000	0.718859000
H	1.602461000	-4.463482000	1.681869000
C	1.251257000	-4.728711000	-0.442411000
H	1.221659000	-5.813456000	-0.396740000
C	1.082580000	-4.065741000	-1.659785000
H	0.914313000	-4.612037000	-2.582017000
C	1.151814000	-2.671620000	-1.674399000
H	1.026878000	-2.096581000	-2.585442000
C	2.802451000	1.903699000	1.821519000
C	3.420340000	2.909786000	2.559578000
H	3.585686000	2.783100000	3.625223000
C	3.823309000	4.074613000	1.898590000
H	4.310246000	4.874284000	2.448700000
C	3.602388000	4.191748000	0.524965000
H	3.906411000	5.078333000	-0.021392000
C	2.987323000	3.133114000	-0.144015000
H	2.792141000	3.153880000	-1.211960000
C	4.411539000	-0.883336000	-0.074709000
C	5.649417000	-1.435586000	-0.402026000
H	6.257934000	-1.898397000	0.369194000
C	6.087107000	-1.375547000	-1.725274000
H	7.048438000	-1.796820000	-2.003680000
C	5.271160000	-0.768970000	-2.683876000
H	5.573971000	-0.701518000	-3.723298000
C	4.042453000	-0.254404000	-2.282973000
H	3.343343000	0.211055000	-2.970017000
C	1.650867000	-1.679389000	1.817216000
H	2.051818000	-2.220965000	2.684935000
C	2.281582000	0.620712000	2.434072000
H	1.200748000	0.716259000	2.577728000
H	2.755838000	0.421372000	3.404670000
C	3.927686000	-0.848404000	1.356883000
H	4.131265000	-1.808979000	1.846493000
H	4.516680000	-0.094575000	1.893008000
N	2.484421000	-0.500827000	1.485179000
H	0.653825000	-1.299898000	2.061233000
H	-2.901280000	-4.635925000	2.881490000
C	-2.605436000	-3.791747000	2.265669000
C	-2.616008000	-2.497170000	2.794327000
C	-2.221943000	-3.982043000	0.936952000
C	-2.240704000	-1.433621000	1.976518000
H	-2.917052000	-2.312917000	3.821068000
H	-2.206522000	-4.970013000	0.489332000
C	-1.869057000	-2.865792000	0.180150000
N	-1.876077000	-1.629346000	0.695014000
C	-2.158703000	-0.003311000	2.473600000
H	-1.570568000	-2.937499000	-0.860693000
H	-1.106984000	0.219846000	2.686231000
H	-2.730475000	0.111184000	3.406147000
N	-2.598311000	0.945982000	1.437529000
N	-3.719528000	-0.135440000	-0.868159000
N	-1.888342000	2.277510000	-0.837492000

C	-2.020774000	2.299922000	1.581428000
C	-4.069350000	0.980530000	1.274196000
C	-4.580771000	0.136008000	0.123566000
C	-4.148546000	-0.790742000	-1.961186000
C	-2.099523000	3.033440000	0.257336000
C	-1.887205000	2.839181000	-2.054920000
H	-2.511094000	2.878950000	2.376940000
H	-0.962957000	2.171587000	1.833573000
H	-4.365515000	2.017354000	1.072822000
H	-4.569654000	0.689055000	2.207832000
C	-5.916909000	-0.260050000	0.065194000
C	-5.470798000	-1.203865000	-2.104355000
H	-3.389851000	-0.974498000	-2.715161000
C	-2.339200000	4.401193000	0.158828000
C	-2.105460000	4.204650000	-2.233610000
H	-1.708815000	2.160185000	-2.882535000
H	-6.588927000	-0.031337000	0.887200000
C	-6.368701000	-0.939252000	-1.067225000
H	-5.784091000	-1.724025000	-3.003384000
H	-2.525103000	4.986714000	1.054033000
C	-2.338149000	4.995635000	-1.107064000
H	-2.101235000	4.630012000	-3.231488000
H	-7.405239000	-1.255169000	-1.138871000
H	-2.524923000	6.060398000	-1.210515000

$10^1_{\text{hs-hs}}$

Fe	1.635247000	0.040246000	-0.430926000
O	1.266923000	0.670483000	-1.901875000
Fe	-1.545582000	0.246158000	-0.480467000
O	-1.269543000	-0.419278000	-2.167109000
H	-0.358100000	-0.166375000	-2.426923000
O	0.112506000	0.302361000	0.448671000
N	1.171798000	-2.144607000	-0.712507000
N	2.748853000	1.645467000	0.639171000
N	3.604661000	-0.456111000	-1.040941000
C	1.164532000	-2.850679000	0.431575000
C	0.872487000	-4.212781000	0.451333000
H	0.891944000	-4.761563000	1.387981000
C	0.560955000	-4.848286000	-0.754223000
H	0.337421000	-5.911022000	-0.770995000
C	0.552889000	-4.103616000	-1.935371000
H	0.320729000	-4.561835000	-2.890996000
C	0.870328000	-2.746301000	-1.869139000
H	0.883514000	-2.116139000	-2.751518000
C	3.079324000	1.336269000	1.905938000
C	3.891902000	2.166327000	2.674200000
H	4.152002000	1.888065000	3.690949000
C	4.359995000	3.356245000	2.107920000
H	4.996485000	4.022024000	2.683120000
C	4.006230000	3.672610000	0.794806000
H	4.353704000	4.584973000	0.321578000
C	3.199269000	2.779598000	0.089095000
H	2.900198000	2.956153000	-0.939915000
C	4.414925000	-1.049036000	-0.146547000
C	5.768701000	-1.251080000	-0.412224000
H	6.401992000	-1.726702000	0.330676000
C	6.285183000	-0.839539000	-1.641161000
H	7.336209000	-0.987719000	-1.870347000
C	5.432954000	-0.235004000	-2.568989000

H	5.794476000	0.097320000	-3.536191000
C	4.096830000	-0.054916000	-2.226529000
H	3.376435000	0.421796000	-2.883145000
C	1.442735000	-2.047686000	1.682874000
H	1.775708000	-2.694935000	2.505860000
C	2.453800000	0.064572000	2.435976000
H	1.408389000	0.278404000	2.681271000
H	2.967884000	-0.283374000	3.342330000
C	3.786143000	-1.552686000	1.132513000
H	3.695515000	-2.642702000	1.054474000
H	4.450640000	-1.354180000	1.982820000
N	2.433404000	-0.984296000	1.390147000
H	0.516092000	-1.541523000	1.969492000
H	-3.646164000	-4.399670000	2.730605000
C	-3.218530000	-3.588790000	2.148331000
C	-3.065715000	-2.319929000	2.716840000
C	-2.825202000	-3.796691000	0.825075000
C	-2.523078000	-1.297470000	1.942106000
H	-3.367005000	-2.124882000	3.741514000
H	-2.932969000	-4.765770000	0.349606000
C	-2.300641000	-2.720473000	0.110654000
N	-2.155895000	-1.509166000	0.663703000
C	-2.245079000	0.091581000	2.483658000
H	-1.986270000	-2.800886000	-0.925370000
H	-1.176008000	0.149416000	2.716069000
H	-2.812199000	0.263415000	3.410023000
N	-2.518724000	1.126557000	1.470665000
N	-3.752502000	0.270770000	-0.867890000
N	-1.559585000	2.385807000	-0.756567000
C	-1.744506000	2.372482000	1.660357000
C	-3.963493000	1.389878000	1.290225000
C	-4.578351000	0.648972000	0.119809000
C	-4.258252000	-0.302308000	-1.974552000
C	-1.676992000	3.138824000	0.354584000
C	-1.432389000	2.969044000	-1.957071000
H	-2.160482000	3.001888000	2.459845000
H	-0.724947000	2.077835000	1.928299000
H	-4.093799000	2.462709000	1.102024000
H	-4.517263000	1.165834000	2.212276000
C	-5.956560000	0.449717000	0.041594000
C	-5.624298000	-0.519568000	-2.136664000
H	-3.525838000	-0.586346000	-2.723066000
C	-1.692557000	4.529317000	0.288393000
C	-1.427194000	4.355454000	-2.102710000
H	-1.337053000	2.291729000	-2.799388000
H	-6.598467000	0.760548000	0.860661000
C	-6.487639000	-0.142088000	-1.105329000
H	-5.997607000	-0.978466000	-3.046071000
H	-1.806108000	5.115238000	1.195325000
C	-1.563689000	5.146087000	-0.960120000
H	-1.328138000	4.798402000	-3.087939000
H	-7.557806000	-0.305133000	-1.191998000
H	-1.577667000	6.229178000	-1.038078000

⁴¹_{hs-is}

Fe	1.782423000	0.158695000	-0.383911000
O	1.496738000	0.575967000	-1.937008000
Fe	-1.432026000	0.107329000	-0.502055000
O	-1.073750000	-0.365669000	-2.240067000
H	-0.168334000	-0.047203000	-2.446419000
O	0.149788000	0.341049000	0.399502000
N	1.470238000	-1.804042000	-0.542332000
N	2.266480000	1.954253000	0.309916000
N	3.774269000	-0.264928000	-0.813670000
C	1.579995000	-2.487218000	0.618008000
C	1.496141000	-3.875554000	0.646027000
H	1.600222000	-4.403612000	1.588570000
C	1.280919000	-4.565639000	-0.550217000
H	1.221570000	-5.649938000	-0.553055000
C	1.152474000	-3.844797000	-1.737982000
H	0.986184000	-4.341786000	-2.687731000
C	1.258150000	-2.455687000	-1.694521000
H	1.171466000	-1.833467000	-2.575983000
C	2.442230000	2.025225000	1.648777000

C	2.828212000	3.213781000	2.260423000
H	2.982289000	3.243648000	3.334619000
C	3.013976000	4.353196000	1.471585000
H	3.317893000	5.290385000	1.927973000
C	2.813668000	4.267199000	0.093130000
H	2.950740000	5.127836000	-0.552672000
C	2.442936000	3.040919000	-0.455719000
H	2.276391000	2.890606000	-1.516578000
C	4.549988000	-0.723544000	0.182707000
C	5.846168000	-1.183387000	-0.046232000
H	6.444029000	-1.554087000	0.781007000
C	6.353153000	-1.150292000	-1.344987000
H	7.360086000	-1.501147000	-1.549824000
C	5.545522000	-0.660762000	-2.374815000
H	5.900684000	-0.616140000	-3.398780000
C	4.257534000	-2.069526000	-2.069526000
H	3.565682000	0.138582000	-2.816950000
C	1.719093000	-1.643902000	1.865802000
H	2.159279000	-2.221511000	2.688661000
C	2.140835000	0.755356000	2.415399000
H	1.062245000	0.712143000	2.580309000
H	2.657887000	0.740389000	3.383243000
C	3.972656000	-0.651896000	1.576166000
H	4.213812000	-1.561323000	2.140087000
H	4.456719000	0.179550000	2.102455000
N	2.502199000	-0.416272000	1.576279000
H	0.713765000	-1.323266000	2.149195000
H	-2.993412000	-4.884886000	2.557930000
C	-2.669255000	-4.011951000	1.999058000
C	-2.641263000	-2.754754000	2.610436000
C	-2.292002000	-4.125562000	0.659956000
C	-2.231510000	-1.652026000	1.863673000
H	-2.942447000	-2.628125000	3.645890000
H	-2.312669000	-5.081388000	0.147006000
C	-1.902372000	-2.972609000	-0.021245000
N	-1.867519000	-1.773537000	0.572982000
C	-2.125878000	-0.257404000	2.451389000
H	-1.611383000	-2.986118000	-1.066928000
H	-1.070885000	-0.058633000	2.670199000
H	-2.691591000	-0.197465000	3.393239000
N	-2.558400000	0.759188000	1.480477000
N	-3.642518000	-0.138899000	-0.921582000
N	-1.822843000	2.240390000	-0.694464000
C	-1.985029000	2.100312000	1.715576000
C	-4.026760000	0.796931000	1.303108000
C	-4.521658000	0.066168000	0.068695000
C	-4.058204000	-0.694180000	-2.073087000
C	-2.063384000	2.919384000	0.442657000
C	-1.833305000	2.876611000	-1.873781000
H	-2.476576000	2.625636000	2.547316000
H	-0.926716000	1.955427000	1.955969000
H	-4.333871000	1.845745000	1.207383000
H	-4.533492000	0.407036000	2.196693000
C	-5.863742000	-0.297081000	-0.050687000
C	-5.383758000	-1.068998000	-2.279334000
H	-3.284982000	-0.829503000	-2.822717000
C	-2.336688000	4.284854000	0.429469000
C	-2.085739000	4.245040000	-1.968737000
H	-1.638178000	2.252471000	-2.740502000
H	-6.550543000	-0.123510000	0.772774000
C	-6.301415000	-0.872089000	-1.244282000
H	-5.684935000	-1.508030000	-3.224675000
H	-2.545794000	4.807077000	1.358205000
C	-2.343283000	4.958055000	-0.796319000
H	-2.091650000	4.731847000	-2.938272000
H	-7.341523000	-1.160485000	-1.364322000
H	-2.558283000	6.021905000	-0.834253000

⁸¹_{hs-is}

Fe	1.798563000	0.186215000	-0.392951000
O	1.516559000	0.610499000	-1.939652000
Fe	-1.440722000	0.127770000	-0.498921000
O	-1.087598000	-0.359401000	-2.242536000
H	-0.187324000	-0.039526000	-2.455969000

C	-2.076088000	2.917183000	0.455312000
C	-1.857140000	2.884494000	-1.862370000
H	-2.479009000	2.611609000	2.560306000
H	-0.928402000	1.951834000	1.960131000
H	-4.336979000	1.830335000	1.219895000
H	-4.527931000	0.387592000	2.205000000
C	-5.861749000	-0.314792000	-0.041051000
C	-5.384708000	-1.076329000	-2.273958000
H	-3.288488000	-0.825422000	-2.822416000
C	-2.358458000	4.280817000	0.448766000
C	-2.119307000	4.251554000	-1.950848000
H	-1.662627000	2.264330000	-2.732121000
H	-6.546998000	-0.147231000	0.784942000
C	-6.300258000	-0.887287000	-1.235572000
H	-5.686673000	-1.513105000	-3.220093000
H	-2.566571000	4.798116000	1.380478000
C	-2.375494000	4.958536000	-0.774460000
H	-2.133552000	4.741905000	-2.918511000
H	-7.339437000	-1.179765000	-1.353765000
H	-2.597626000	6.021085000	-0.807311000

⁸¹_{is-hs}

Fe	1.644307000	0.118237000	-0.506174000
O	1.374682000	0.698165000	-2.019179000
Fe	-1.620456000	0.248308000	-0.464537000
O	-1.181645000	-0.235593000	-2.116948000
H	-0.262660000	0.082059000	-2.298532000
O	0.061630000	0.352445000	0.234883000
N	1.220921000	-2.077172000	-0.750163000
N	2.667150000	1.757692000	0.591050000
N	3.632147000	-0.423141000	-0.998739000
C	1.222308000	-2.773822000	0.398142000
C	1.008793000	-4.150362000	0.420971000
H	1.033693000	-4.691771000	1.361810000
C	0.762822000	-4.809131000	-0.787548000
H	0.601327000	-5.883088000	-0.802667000
C	0.733870000	-4.071497000	-1.972988000
H	0.545117000	-4.547323000	-2.929642000
C	0.975512000	-2.697779000	-1.909065000
H	0.972914000	-2.067429000	-2.792127000
C	2.892685000	1.504793000	1.893219000
C	3.625939000	2.377493000	2.692996000
H	3.804440000	2.143013000	3.738050000
C	4.124362000	3.552022000	2.119865000
H	4.701838000	4.249995000	2.718697000
C	3.878708000	3.810646000	0.770132000
H	4.253024000	4.709254000	0.291115000
C	3.145996000	2.877597000	0.035384000
H	2.930173000	3.009217000	-1.020800000
C	4.396254000	-1.003026000	-0.058287000
C	5.736768000	-1.309068000	-0.294211000
H	6.331318000	-1.775319000	0.485934000
C	6.290348000	-1.010013000	-1.538444000
H	7.331451000	-1.239931000	-1.744301000
C	5.486631000	-0.411716000	-2.512877000
H	5.877025000	-0.163891000	-3.494098000
C	4.160751000	-0.131440000	-2.201846000
H	3.474986000	0.337391000	-2.899679000
C	1.396223000	-1.941925000	1.649387000
H	1.704991000	-2.562859000	2.501756000
C	2.251422000	0.236090000	2.413070000
H	1.182087000	0.424969000	2.556456000
H	2.690719000	-0.066317000	3.373723000
C	3.750336000	-1.346037000	1.266525000
H	3.746905000	-2.437217000	1.377112000
H	4.368579000	-0.954831000	2.084015000
N	2.355446000	-0.840874000	1.402366000
H	0.430947000	-1.477346000	1.870988000
H	-3.392252000	-4.423701000	3.017775000
C	-3.002527000	-3.630761000	2.386323000
C	-2.89522000	-2.326266000	2.880295000
C	-2.610010000	-3.897595000	1.073421000
C	-2.399769000	-1.334828000	2.036956000
H	-3.193657000	-2.083999000	3.895934000

H	-2.680281000	-4.896781000	0.656531000
C	-2.133520000	-2.843105000	0.293172000
N	-2.033597000	-1.598010000	0.770822000
C	-2.162583000	0.092739000	2.481561000
H	-1.818443000	-2.982137000	-0.736920000
H	-1.095945000	0.206268000	2.705241000
H	-2.731671000	0.324005000	3.392355000
N	-2.472773000	1.050871000	1.396161000
N	-3.616117000	0.021582000	-0.902465000
N	-1.766601000	2.440166000	-0.799506000
C	-1.800076000	2.359345000	1.606516000
C	-3.943810000	1.217178000	1.200660000
C	-4.491290000	0.408151000	0.045946000
C	-4.053794000	-0.609575000	-2.005851000
C	-1.832994000	3.168303000	0.327325000
C	-1.723500000	3.052508000	-1.988924000
H	-2.250434000	2.912198000	2.442301000
H	-0.754593000	2.136343000	1.843558000
H	-4.139259000	2.273607000	0.983359000
H	-4.482542000	0.978698000	2.126379000
C	-5.854676000	0.147489000	-0.076410000
C	-5.402765000	-0.888212000	-2.204073000
H	-3.278409000	-0.873523000	-2.717561000
C	-1.884673000	4.559527000	0.303411000
C	-1.756103000	4.442998000	-2.102599000
H	-1.659588000	2.396653000	-2.851901000
H	-6.539835000	0.463294000	0.704430000
C	-6.317086000	-0.509625000	-1.217970000
H	-5.724601000	-1.393257000	-3.108481000
H	-1.956685000	5.122478000	1.229209000
C	-1.842289000	5.205894000	-0.936292000
H	-1.722153000	4.911038000	-3.080742000
H	-7.375892000	-0.719655000	-1.336216000
H	-1.882572000	6.289847000	-0.988675000

²¹_{is-hs}

Fe	1.631456000	0.029875000	-0.540626000
O	1.385926000	0.591048000	-2.068179000
Fe	-1.615454000	0.291586000	-0.455584000
O	-1.224583000	-0.219728000	-2.116500000
H	-0.292284000	0.041609000	-2.303207000
O	0.071892000	0.327918000	0.221951000
N	1.178390000	-2.147245000	-0.758423000
N	2.668417000	1.674669000	0.550245000
N	3.656741000	-0.479324000	-0.990716000
C	1.133873000	-2.831835000	0.396990000
C	0.856286000	-4.196507000	0.429212000
H	0.846597000	-4.729759000	1.374946000
C	0.593650000	-4.854512000	-0.776196000
H	0.382948000	-5.919989000	-0.783253000
C	0.612904000	-4.128296000	-1.968818000
H	0.413844000	-4.604414000	-2.923202000
C	0.916369000	-2.766783000	-1.915033000
H	0.953594000	-2.144715000	-2.803234000
C	2.933366000	1.409347000	1.842134000
C	3.706037000	2.265923000	2.622220000
H	3.914530000	2.022326000	3.659596000
C	4.204016000	3.436205000	2.040073000
H	4.811714000	4.121286000	2.623705000
C	3.917927000	3.707214000	0.700831000
H	4.290335000	4.602792000	0.214654000
C	3.147004000	2.789793000	-0.014391000
H	2.901003000	2.930226000	-1.062868000
C	4.413152000	-1.029142000	-0.025775000
C	5.783485000	-1.225048000	-0.194520000
H	6.370981000	-1.665917000	0.605328000
C	6.375215000	-0.853093000	-1.401911000
H	7.440210000	-0.997514000	-1.557143000
C	5.579141000	-0.293360000	-2.404587000
H	5.999278000	0.006983000	-3.358506000
C	4.221849000	-0.116609000	-2.156029000
H	3.540816000	0.326253000	-2.875489000
C	1.343004000	-1.999877000	1.643786000
H	1.635709000	-2.627751000	2.496862000
C	2.284416000	0.152541000	2.381847000

H	1.223838000	0.365384000	2.553895000
H	2.742458000	-0.151811000	3.333217000
C	3.707477000	-1.495757000	1.227494000
H	3.630660000	-2.588701000	1.180429000
H	4.315575000	-1.263834000	2.111200000
N	2.337581000	-0.934867000	1.380372000
H	0.396446000	-1.501216000	1.871089000
H	-3.594667000	-4.417121000	2.843179000
C	-3.162703000	-3.625247000	2.238419000
C	-2.977432000	-2.348197000	2.779581000
C	-2.794628000	-3.864903000	0.913626000
C	-2.429338000	-1.356290000	1.970274000
H	-3.256674000	-2.127418000	3.805443000
H	-2.927066000	-4.841658000	0.460224000
C	-2.259730000	-2.811634000	0.169762000
N	-2.083684000	-1.593673000	0.692173000
C	-2.118207000	0.041138000	2.463472000
H	-1.960471000	-2.928222000	-0.867689000
H	-1.042691000	0.103363000	2.662273000
H	-2.655351000	0.260617000	3.396244000
N	-2.413958000	1.053198000	1.422740000
N	-3.629250000	0.165398000	-0.899951000
N	-1.692735000	2.482287000	-0.733641000
C	-1.700000000	2.333110000	1.670655000
C	-3.883629000	1.272206000	1.259287000
C	-4.476110000	0.528702000	0.082940000
C	-4.103595000	-0.402631000	-2.021841000
C	-1.721203000	3.179731000	0.415034000
C	-1.646411000	3.123687000	-1.907872000
H	-2.126152000	2.873660000	2.526758000
H	-0.659666000	2.071293000	1.889965000
H	-4.047979000	2.342272000	1.087620000
H	-4.413613000	1.014507000	2.184795000
C	-5.847683000	0.309007000	-0.022939000
C	-5.463316000	-0.638330000	-2.205227000
H	-3.346731000	-0.658664000	-2.756311000
C	-1.728492000	4.571902000	0.427885000
C	-1.636396000	4.516826000	-1.982922000
H	-1.615178000	2.489143000	-2.788270000
H	-6.509999000	0.605140000	0.784865000
C	-6.348169000	-0.283030000	-1.184453000
H	-5.815693000	-1.094038000	-3.124367000
H	-1.771030000	5.112112000	1.368894000
C	-1.682612000	5.249502000	-0.794920000
H	-1.600930000	5.010490000	-2.948310000
H	-7.414088000	-0.461417000	-1.290441000
H	-1.689812000	6.335201000	-0.817738000

⁶¹_{is-is}

Fe	1.760441000	0.201568000	-0.421231000
O	1.561033000	0.696765000	-1.961455000
Fe	-1.494244000	0.125810000	-0.444383000
O	-0.983698000	-0.285075000	-2.116589000
H	-0.110528000	0.136495000	-2.276098000
O	0.099933000	0.435555000	0.309234000
N	1.416014000	-1.747818000	-0.659972000
N	2.278876000	1.957920000	0.363214000
N	3.770808000	-0.281137000	-0.787722000
C	1.498906000	-2.477127000	0.474112000
C	1.433151000	-3.866424000	0.444229000
H	1.515743000	-4.430070000	1.367986000
C	1.260010000	-4.509509000	-0.784648000
H	1.216462000	-5.593480000	-0.834219000
C	1.148675000	-3.741361000	-1.944291000
H	1.011741000	-4.201111000	-2.917160000
C	1.237811000	-2.353684000	-1.842485000
H	1.171320000	-1.696508000	-2.699443000
C	2.402375000	1.975178000	1.709516000
C	2.802535000	3.126222000	2.380650000
H	2.913899000	3.111508000	3.460452000
C	3.058964000	4.286234000	1.643193000
H	3.375468000	5.195032000	2.146097000
C	2.912378000	4.256876000	0.255865000
H	3.104348000	5.134871000	-0.351458000
C	2.522757000	3.064900000	-0.352994000

H	2.394000000	2.960243000	-1.424609000
C	4.485668000	-0.803842000	0.221773000
C	5.764082000	-1.324965000	0.026765000
H	6.312121000	-1.747494000	0.863626000
C	6.318979000	-1.283645000	-1.252310000
H	7.313623000	-1.680571000	-1.431601000
C	5.576026000	-0.725364000	-2.295662000
H	5.971123000	-0.671505000	-3.304473000
C	4.300276000	-0.241293000	-2.023755000
H	3.655974000	0.185073000	-2.784918000
C	1.581873000	-1.680249000	1.755873000
H	1.966268000	-2.292550000	2.581874000
C	2.031089000	0.687951000	2.414346000
H	0.945527000	0.669078000	2.526723000
H	2.501355000	0.623691000	3.403932000
C	3.862714000	-0.726347000	1.594970000
H	4.066245000	-1.640882000	2.165690000
H	4.344056000	0.095732000	2.138232000
N	2.398415000	-0.459766000	1.548090000
H	0.566547000	-1.350767000	1.990025000
H	-3.108836000	-4.693877000	2.933941000
C	-2.734983000	-3.874841000	2.326678000
C	-2.723604000	-2.570663000	2.832496000
C	-2.271692000	-4.105994000	1.030321000
C	-2.246574000	-1.544354000	2.019991000
H	-3.084296000	-2.353859000	3.833518000
H	-2.273120000	-5.102637000	0.601188000
C	-1.816700000	-3.018560000	0.282777000
N	-1.802071000	-1.774500000	0.772046000
C	-2.144272000	-0.104370000	2.479353000
H	-1.452491000	-3.129674000	-0.734401000
H	-1.098186000	0.108206000	2.724002000
H	-2.749197000	0.062287000	3.381827000
N	-2.523471000	0.824161000	1.394946000
N	-3.461685000	-0.299325000	-0.958794000
N	-1.941414000	2.283351000	-0.784446000
C	-2.008216000	2.195594000	1.621519000
C	-3.994536000	0.817587000	1.149045000
C	-4.406891000	-0.020960000	-0.041916000
C	-3.793180000	-0.951721000	-2.086396000
C	-2.110817000	2.997444000	0.340327000
C	-1.960717000	2.893435000	-1.975141000
H	-2.529450000	2.696848000	2.449223000
H	-0.947490000	2.088160000	1.871523000
H	-4.312373000	1.848028000	0.951524000
H	-4.532006000	0.490312000	2.048506000
C	-5.732108000	-0.414734000	-0.220478000
C	-5.097992000	-1.364043000	-2.341009000
H	-2.968156000	-1.120764000	-2.770829000
C	-2.328420000	4.372874000	0.311320000
C	-2.158088000	4.269868000	-2.093364000
H	-1.811958000	2.244445000	-2.833197000
H	-6.474662000	-0.181927000	0.536859000
C	-6.082736000	-1.096420000	-1.386901000
H	-5.332603000	-1.884186000	-3.263613000
H	-2.482283000	4.923972000	1.234323000
C	-2.347772000	5.018134000	-0.929414000
H	-2.171947000	4.737798000	-3.072147000
H	-7.109656000	-1.410144000	-1.549007000
H	-2.517975000	6.089295000	-0.985136000

²¹_{is-is}

Fe	1.756679000	0.222453000	-0.427592000
O	1.569118000	0.705959000	-1.974178000
Fe	-1.494350000	0.114471000	-0.438155000
O	-0.981280000	-0.292605000	-2.109111000
H	-0.103253000	0.121241000	-2.261166000
O	0.094314000	0.457640000	0.297398000
N	1.419895000	-1.732896000	-0.654788000
N	2.268825000	1.984277000	0.348660000
N	3.775851000	-0.275924000	-0.788155000
C	1.513570000	-2.454776000	0.483146000
C	1.464926000	-3.844974000	0.461270000
H	1.555382000	-4.402270000	1.388145000

C	1.299706000	-4.497241000	-0.763816000
H	1.269881000	-5.581942000	-0.807165000
C	1.179054000	-3.737158000	-1.927897000
H	1.048719000	-4.204162000	-2.898225000
C	1.250210000	-2.347923000	-1.833760000
H	1.176438000	-1.696587000	-2.694703000
C	2.386696000	2.010626000	1.695407000
C	2.779157000	3.167560000	2.360891000
H	2.886511000	3.160059000	3.441180000
C	3.033727000	4.323996000	1.617121000
H	3.344288000	5.237299000	2.115553000
C	2.893408000	4.285117000	0.229411000
H	3.084580000	5.159950000	-0.382708000
C	2.511293000	3.087677000	-0.373550000
H	2.387763000	2.975241000	-1.445011000
C	4.485414000	-0.791348000	0.228418000
C	5.757196000	-1.330896000	0.040914000
H	6.301294000	-1.747025000	0.883533000
C	6.310986000	-1.315447000	-1.239493000
H	7.300615000	-1.726929000	-1.413711000
C	5.573883000	-0.763952000	-2.290501000
H	5.968951000	-0.729865000	-3.300205000
C	4.303913000	-0.260785000	-2.024625000
H	3.663355000	0.161925000	-2.791215000
C	1.591174000	-1.650333000	1.760828000
H	1.981149000	-2.256016000	2.589145000
C	2.020796000	0.725274000	2.406853000
H	0.935149000	0.700063000	2.517205000
H	2.489177000	0.669600000	3.397876000
C	3.864078000	-0.678733000	1.599864000
H	4.075949000	-1.573130000	2.198890000
H	4.338569000	0.164719000	2.115689000
N	2.397789000	-0.424320000	1.547483000
H	0.573533000	-1.328495000	1.995510000
H	-3.069181000	-4.723063000	2.928386000
C	-2.702241000	-3.899696000	2.322774000
C	-2.698821000	-2.596945000	2.832424000
C	-2.240047000	-4.123853000	1.024821000
C	-2.230562000	-1.565039000	2.022049000
H	-3.058951000	-2.385559000	3.834794000
H	-2.235476000	-5.119208000	0.592760000
C	-1.793718000	-3.031309000	0.279581000
N	-1.786672000	-1.788442000	0.772455000
C	-2.138858000	-0.125443000	2.484617000
H	-1.430152000	-3.137100000	-0.738358000
H	-1.094512000	0.095833000	2.729269000
H	-2.744332000	0.034603000	3.387885000
N	-2.526940000	0.801207000	1.401652000
N	-3.459551000	-0.310334000	-0.961990000
N	-1.954327000	2.266471000	-0.775449000
C	-2.025014000	2.177668000	1.630084000
C	-3.998822000	0.782518000	1.157540000
C	-4.406257000	-0.044942000	-0.042766000
C	-3.788165000	-0.952246000	-2.096529000
C	-2.133327000	2.978755000	0.348945000
C	-1.976703000	2.875558000	-1.966581000
H	-2.552960000	2.673004000	2.457016000
H	-0.963875000	2.081052000	1.882348000
H	-4.327821000	1.812143000	0.974479000
H	-4.530859000	0.438338000	2.053835000
C	-5.729970000	-0.441489000	-0.226235000
C	-5.091457000	-1.366218000	-2.356259000
H	-2.961847000	-1.112130000	-2.781604000
C	-2.364689000	4.351859000	0.319026000
C	-2.187418000	4.249964000	-2.085292000
H	-1.819276000	2.227643000	-2.823788000
H	-6.473810000	-0.219234000	0.533018000
C	-6.077632000	-1.112021000	-1.399991000
H	-5.323679000	-1.877613000	-3.284339000
H	-2.526198000	4.901684000	1.241471000
C	-2.387490000	4.996506000	-0.921990000
H	-2.203347000	4.717578000	-3.064185000
H	-7.103360000	-1.427639000	-1.565905000
H	-2.568233000	6.065893000	-0.978411000

41_{is-ls}

Fe	1.756251000	0.197440000	-0.420300000
O	1.567081000	0.694016000	-1.963724000
Fe	-1.491490000	0.122484000	-0.441461000
O	-0.977874000	-0.296434000	-2.112551000
H	-0.103309000	0.118173000	-2.276005000
O	0.101370000	0.427194000	0.310886000
N	1.412329000	-1.753481000	-0.656218000
N	2.276257000	1.958994000	0.357571000
N	3.759432000	-0.293680000	-0.784990000
C	1.493388000	-2.477546000	0.481158000
C	1.427478000	-3.867063000	0.457320000
H	1.508185000	-4.426903000	1.383578000
C	1.257310000	-4.515537000	-0.769166000
H	1.213514000	-5.599714000	-0.813931000
C	1.150235000	-3.752676000	-1.932762000
H	1.016816000	-4.216986000	-2.903974000
C	1.239066000	-2.364580000	-1.836446000
H	1.176835000	-1.710664000	-2.696381000
C	2.396015000	1.980653000	1.703994000
C	2.793064000	3.134080000	2.373028000
H	2.901634000	3.122788000	3.453175000
C	3.050274000	4.292181000	1.632768000
H	3.364591000	5.202773000	2.133822000
C	2.907015000	4.258665000	0.245172000
H	3.099368000	5.135252000	-0.364093000
C	2.520038000	3.064344000	-0.360896000
H	2.392003000	2.956331000	-1.432375000
C	4.476306000	-0.808811000	0.227077000
C	5.753852000	-1.332672000	0.033891000
H	6.302716000	-1.748429000	0.873576000
C	6.306431000	-1.303321000	-1.246352000
H	7.300355000	-1.702692000	-1.424157000
C	5.561466000	-0.753862000	-2.292896000
H	5.954027000	-0.709463000	-3.303156000
C	4.286954000	-0.266016000	-2.022890000
H	3.642304000	0.153174000	-2.787509000
C	1.576405000	-1.676149000	1.760727000
H	1.961669000	-2.286377000	2.587923000
C	2.024456000	0.695171000	2.412881000
H	0.938994000	0.676147000	2.525975000
H	2.494830000	0.634441000	3.402687000
C	3.855860000	-0.720300000	1.600181000
H	4.060965000	-1.629712000	2.178532000
H	4.337137000	0.107061000	2.135421000
N	2.392154000	-0.455198000	1.550619000
H	0.561125000	-1.346873000	1.995096000
H	-3.139332000	-4.693258000	2.922970000
C	-2.759066000	-3.875354000	2.318172000
C	-2.743646000	-2.571793000	2.825522000
C	-2.291183000	-4.107348000	1.023642000
C	-2.258272000	-1.546860000	2.016286000
H	-3.107341000	-2.354496000	3.825352000
H	-2.295264000	-5.103540000	0.593492000
C	-1.827865000	-3.021271000	0.279215000
N	-1.809721000	-1.777741000	0.769844000
C	-2.149978000	-0.108189000	2.478730000
H	-1.459584000	-3.133022000	-0.736436000
H	-1.103778000	0.098028000	2.728356000
H	-2.757620000	0.060041000	3.379061000
N	-2.519660000	0.825146000	1.394891000
N	-3.459749000	-0.284629000	-0.964530000
N	-1.917659000	2.282485000	-0.780886000
C	-1.995964000	2.192835000	1.625225000
C	-3.990188000	0.829773000	1.145039000
C	-4.405287000	-0.003000000	-0.048839000
C	-3.793008000	-0.931639000	-2.094829000
C	-2.086112000	2.996497000	0.344159000
C	-1.925944000	2.894245000	-1.970932000
H	-2.518176000	2.697115000	2.450442000
H	-0.937401000	2.078420000	1.880971000
H	-4.299844000	1.862974000	0.948885000
H	-4.532355000	0.504512000	2.042373000
C	-5.732573000	-0.387590000	-0.231547000
C	-5.099981000	-1.334436000	-2.353613000

H	-2.967492000	-1.104940000	-2.777566000
C	-2.291552000	4.373805000	0.315837000
C	-2.110874000	4.272444000	-2.088140000
H	-1.778806000	2.245391000	-2.829303000
H	-6.475256000	-0.152325000	0.524897000
C	-6.085080000	-1.063289000	-1.400921000
H	-5.335830000	-1.850350000	-3.278269000
H	-2.444875000	4.924996000	1.238867000
C	-2.299529000	5.020820000	-0.924082000
H	-2.116098000	4.741701000	-3.066366000
H	-7.113653000	-1.369833000	-1.566236000
H	-2.460201000	6.093483000	-0.979174000

61_{ls-hs}

Fe	-1.483617000	0.141956000	-0.460671000
O	-1.134936000	-0.487728000	-1.942152000
Fe	1.729125000	-0.294484000	-0.342114000
O	1.431630000	0.434675000	-1.943495000
H	0.526803000	0.144468000	-2.204900000
O	0.026399000	-0.030398000	0.387115000
N	-1.102218000	2.327396000	-0.751490000
N	-2.469597000	-1.518403000	0.687436000
N	-3.517296000	0.475941000	-1.011944000
C	-1.061437000	3.040254000	0.386310000
C	-0.694968000	4.384622000	0.397558000
H	-0.692448000	4.942744000	1.329055000
C	-0.336484000	4.989850000	-0.810426000
H	-0.053097000	6.038118000	-0.834136000
C	-0.358776000	4.234906000	-1.985070000
H	-0.090189000	4.670919000	-2.941600000
C	-0.753782000	2.898710000	-1.910271000
H	-0.793828000	2.256820000	-2.784068000
C	-2.874155000	-1.175869000	1.922869000
C	-3.669349000	-2.020842000	2.694386000
H	-3.991378000	-1.715318000	3.685304000
C	-4.040915000	-3.260151000	2.163930000
H	-4.664063000	-3.937171000	2.740695000
C	-3.608261000	-3.611515000	0.883591000
H	-3.881154000	-4.562729000	0.438518000
C	-2.825046000	-2.701294000	0.172675000
H	-2.468647000	-2.902612000	-0.833427000
C	-4.336975000	1.051485000	-0.114862000
C	-5.714565000	1.114781000	-0.317668000
H	-6.352127000	1.579199000	0.428582000
C	-6.248716000	0.582756000	-1.492129000
H	-7.318526000	0.622213000	-1.674163000
C	-5.388607000	0.001480000	-2.426834000
H	-5.762851000	-0.419035000	-3.354118000
C	-4.026358000	-0.039126000	-2.144093000
H	-3.295734000	-0.488836000	-2.808517000
C	-1.367086000	2.265202000	1.651392000
H	-1.730030000	2.931638000	2.446578000
C	-2.342015000	0.147786000	2.432582000
H	-1.299897000	-0.005106000	2.734086000
H	-2.908693000	0.486276000	3.311341000
C	-3.684829000	1.708189000	1.078883000
H	-3.588897000	2.777142000	0.854517000
H	-4.330174000	1.627564000	1.963534000
N	-2.327995000	1.174606000	1.368883000
H	-0.438503000	1.788440000	1.979875000
H	3.772986000	4.347055000	2.512068000
C	3.358605000	3.512405000	1.954572000
C	3.134962000	2.286455000	2.589575000
C	3.049167000	3.647820000	0.599910000
C	2.608744000	1.233558000	1.846415000
H	3.364319000	2.149758000	3.641886000
H	3.208869000	4.584276000	0.076450000
C	2.540826000	2.545909000	-0.085625000
N	2.333931000	1.376022000	0.532880000
C	2.212891000	-0.097154000	2.456918000
H	2.280801000	2.556229000	-1.138678000
H	1.163680000	-0.020776000	2.757975000
H	2.812680000	-0.320821000	3.348064000
N	2.293591000	-1.197563000	1.456924000
N	3.687210000	-0.579989000	-0.781717000

N	1.184917000	-2.156229000	-0.768789000
C	1.281123000	-2.274223000	1.648131000
C	3.669992000	-1.763651000	1.328847000
C	4.435222000	-1.150382000	0.180325000
C	4.277016000	-0.093726000	-1.887851000
C	1.030697000	-2.947791000	0.315596000
C	0.934282000	-2.636504000	-1.994269000
H	1.593558000	-2.995594000	2.413921000
H	0.351234000	-1.791287000	1.957452000
H	3.572440000	-2.837845000	1.132802000
H	4.217903000	-1.658602000	2.273034000
C	5.820792000	-1.241799000	0.074219000
C	5.655086000	-0.164202000	-2.072755000
H	3.597615000	0.353149000	-2.605314000
C	0.624002000	-4.271858000	0.193972000
C	0.512853000	-3.950731000	-2.192203000
H	1.079483000	-1.936347000	-2.807157000
H	6.398470000	-1.702197000	0.869937000
C	6.440665000	-0.741479000	-1.072451000
H	6.099160000	0.232974000	-2.979260000
H	0.524682000	-4.892344000	1.079150000
C	0.356253000	-4.780040000	-1.081309000
H	0.322327000	-4.309919000	-3.197719000
H	7.519222000	-0.801877000	-1.181980000
H	0.043103000	-5.812687000	-1.203431000

41_{ls-hs}

Fe	-1.485210000	0.140800000	-0.456208000
O	-1.129271000	-0.492011000	-1.932107000
Fe	1.727413000	-0.265153000	-0.332604000
O	1.438951000	0.483496000	-1.931310000
H	0.547357000	0.174312000	-2.209350000
O	0.030071000	0.010136000	0.394378000
N	-1.131221000	2.320806000	-0.782663000
N	-2.449250000	-1.516348000	0.714087000
N	-3.526032000	0.443671000	-1.009593000
C	-1.088732000	3.050175000	0.344798000
C	-0.725107000	4.395189000	0.335308000
H	-0.721533000	4.966857000	1.258550000
C	-0.371342000	4.983555000	-0.882430000
H	-0.089560000	6.031762000	-0.922008000
C	-0.396355000	4.211889000	-2.046002000
H	-0.131280000	4.634356000	-3.009518000
C	-0.788079000	2.876083000	-1.950769000
H	-0.830586000	2.221939000	-2.815138000
C	-2.856790000	-1.160032000	1.945002000
C	-3.641680000	-2.002623000	2.729559000
H	-3.966246000	-1.686173000	3.716201000
C	-3.999763000	-3.253745000	2.217952000
H	-4.614666000	-3.929129000	2.805382000
C	-3.564490000	-3.619061000	0.942429000
H	-3.827162000	-4.579669000	0.511623000
C	-2.792178000	-2.710745000	0.217400000
H	-2.434525000	-2.923512000	-0.785862000
C	-4.349785000	1.022108000	-0.118235000
C	-5.728797000	1.064878000	-0.316705000
H	-6.369551000	1.532468000	0.424808000
C	-6.260245000	0.508223000	-1.480934000
H	-7.331122000	0.531155000	-1.659478000
C	-5.396091000	-0.075833000	-2.410195000
H	-5.768269000	-0.514833000	-3.329712000
C	-4.032388000	-0.094489000	-2.132117000
H	-3.298883000	-0.544004000	-2.793484000
C	-1.387647000	2.293345000	1.622413000
H	-1.757850000	2.968758000	2.406525000
C	-2.339927000	0.176986000	2.435380000
H	-1.296071000	0.040779000	2.738595000
H	-2.910379000	0.521339000	3.309363000
C	-3.700684000	1.704967000	1.062318000
H	-3.614808000	2.770641000	0.819193000
H	-4.342587000	1.633756000	1.950259000
N	-2.338068000	1.188856000	1.357164000
H	-0.454545000	1.831212000	1.958432000
H	3.812696000	4.324432000	2.570547000
C	3.392186000	3.498998000	2.003990000

C	3.148432000	2.271427000	2.628481000
C	3.094439000	3.648188000	0.648120000
C	2.614424000	1.230934000	1.873681000
H	3.368001000	2.124322000	3.681473000
H	3.269768000	4.586530000	0.133003000
C	2.577340000	2.557731000	-0.049340000
N	2.352029000	1.385797000	0.559025000
C	2.196417000	-0.099694000	2.468606000
H	2.324499000	2.578990000	-1.104071000
H	1.143534000	-0.015558000	2.754178000
H	2.781239000	-0.337613000	3.366030000
N	2.280559000	-1.189953000	1.458603000
N	3.678134000	-0.579372000	-0.779926000
N	1.184344000	-2.125928000	-0.785450000
C	1.263150000	-2.265319000	1.630779000
C	3.656810000	-1.758787000	1.334798000
C	4.422596000	-1.159639000	0.178955000
C	4.269177000	-0.103475000	-1.890136000
C	1.026654000	-2.928235000	0.290236000
C	0.953457000	-2.599395000	-2.017286000
H	1.566079000	-2.993634000	2.393814000
H	0.331282000	-1.782186000	1.934073000
H	3.559461000	-2.835494000	1.153017000
H	4.205945000	-1.642130000	2.276810000
C	5.806107000	-1.272172000	0.065012000
C	5.644870000	-0.195119000	-2.082415000
H	3.592013000	0.353563000	-2.603312000
C	0.633055000	-4.255097000	0.153619000
C	0.546995000	-3.915699000	-2.231068000
H	1.102446000	-1.891875000	-2.823226000
H	6.381179000	-1.740189000	0.858191000
C	6.427169000	-0.782901000	-1.085617000
H	6.089885000	0.194506000	-2.991734000
H	0.530375000	-4.883879000	1.032556000
C	0.384561000	-4.755302000	-1.128571000
H	0.372014000	-4.268792000	-3.241564000
H	7.504096000	-0.859586000	-1.200845000
H	0.082461000	-5.789759000	-1.262745000

41_{Is-is}

Fe	1.611432000	0.073306000	-0.312827000
O	1.293920000	0.597347000	-1.827765000
Fe	-1.620503000	0.049119000	-0.316187000
O	-1.138072000	-0.715839000	-1.872563000
H	-0.321879000	-0.246586000	-2.143992000
O	0.010929000	0.092457000	0.533440000
N	1.409596000	-1.894042000	-0.595383000
N	2.027566000	1.846298000	0.501341000
N	3.644447000	-0.255683000	-0.800857000
C	1.546289000	-2.637599000	0.523144000
C	1.491456000	-4.027672000	0.475898000
H	1.616752000	-4.603263000	1.387616000
C	1.281201000	-4.656168000	-0.754218000
H	1.241227000	-5.739647000	-0.815927000
C	1.141114000	-3.874166000	-1.901244000
H	0.987654000	-4.322128000	-2.877102000
C	1.218264000	-2.488168000	-1.780970000
H	1.135191000	-1.823032000	-2.630089000
C	2.238145000	1.831777000	1.836998000
C	2.580048000	2.993198000	2.523140000
H	2.763508000	2.955213000	3.592521000
C	2.687879000	4.193620000	1.813795000
H	2.959530000	5.110225000	2.328740000
C	2.452957000	4.193979000	0.438571000
H	2.529341000	5.103626000	-0.147284000
C	2.127858000	2.991594000	-0.187090000
H	1.934946000	2.907826000	-1.250676000
C	4.443716000	-0.759093000	0.152503000
C	5.742236000	-1.185751000	-0.123890000
H	6.360381000	-1.595607000	0.669363000
C	6.224855000	-1.069327000	-1.427394000
H	7.232612000	-1.392950000	-1.669740000
C	5.392285000	-0.532552000	-2.413005000
H	5.729150000	-0.423392000	-3.438379000
C	4.103651000	-0.144080000	-2.059569000

H	3.391779000	0.260342000	-2.771195000
C	1.682609000	-1.871632000	1.820119000
H	2.164470000	-2.485273000	2.592324000
C	2.021708000	0.497954000	2.520562000
H	0.951870000	0.388577000	2.710048000
H	2.563676000	0.448120000	3.473796000
C	3.890257000	-0.771129000	1.558470000
H	4.181540000	-1.691753000	2.079250000
H	4.350280000	0.058128000	2.109618000
N	2.412847000	-0.597260000	1.599667000
H	0.672394000	-1.608668000	2.141893000
H	-3.264697000	-4.648513000	2.690467000
C	-2.920593000	-3.799049000	2.108115000
C	-2.903063000	-2.520250000	2.674271000
C	-2.498173000	-3.968050000	0.787975000
C	-2.461938000	-1.450687000	1.899916000
H	-3.226009000	-2.355686000	3.697678000
H	-2.500068000	-4.945454000	0.317313000
C	-2.085991000	-2.848188000	0.067300000
N	-2.075046000	-1.628289000	0.619697000
C	-2.290824000	-0.044956000	2.445013000
H	-1.751612000	-2.881614000	-0.964206000
H	-1.261125000	0.044596000	2.802457000
H	-2.968261000	0.139287000	3.288470000
N	-2.461925000	0.971654000	1.373680000
N	-3.587992000	0.056534000	-0.914520000
N	-1.339400000	1.958121000	-0.848270000
C	-1.637150000	2.198926000	1.545893000
C	-3.893872000	1.316219000	1.127833000
C	-4.477672000	0.552897000	-0.036962000
C	-4.022262000	-0.553950000	-2.030644000
C	-1.409737000	2.825306000	0.185839000
C	-1.100570000	2.411433000	-2.085644000
H	-2.102252000	2.908990000	2.242020000
H	-0.667645000	1.880250000	1.932747000
H	-3.944637000	2.384925000	0.888482000
H	-4.487073000	1.165493000	2.038058000
C	-5.851427000	0.441773000	-0.239220000
C	-5.379341000	-0.688950000	-2.311530000
H	-3.234873000	-0.929537000	-2.675256000
C	-1.247887000	4.194178000	-0.001700000
C	-0.911310000	3.767886000	-2.348502000
H	-1.068420000	1.655402000	-2.860140000
H	-6.544487000	0.847726000	0.491468000
C	-6.309556000	-0.188924000	-1.397273000
H	-5.695991000	-1.182724000	-3.224081000
H	-1.329314000	4.870458000	0.843609000
C	-0.988948000	4.672974000	-1.289645000
H	-0.723455000	4.100170000	-3.363896000
H	-7.375017000	-0.287794000	-1.581745000
H	-0.865778000	5.737933000	-1.463376000

21_{Is-is}

Fe	1.613218000	0.067759000	-0.306231000
O	1.276492000	0.611812000	-1.807736000
Fe	-1.608077000	0.008549000	-0.298443000
O	-1.133299000	-0.775872000	-1.863127000
H	-0.336382000	-0.289096000	-2.153189000
O	0.006720000	0.011383000	0.542562000
N	1.463059000	-1.898777000	-0.629325000
N	1.978749000	1.830556000	0.545866000
N	3.650818000	-0.183652000	-0.796543000
C	1.606395000	-2.662676000	0.474602000
C	1.571113000	-4.052040000	0.399844000
H	1.702046000	-4.644012000	1.300230000
C	1.371839000	-4.658634000	-0.843148000
H	1.346340000	-5.741096000	-0.926373000
C	1.222906000	-3.856057000	-1.974528000
H	1.076131000	-4.286579000	-2.959176000
C	1.280130000	-2.471774000	-1.826509000
H	1.188714000	-1.791424000	-2.662551000
C	2.202193000	1.791848000	1.879418000
C	2.528440000	2.945037000	2.586582000
H	2.721374000	2.888240000	3.653426000
C	2.608679000	4.161738000	1.901682000

H	2.868427000	5.072157000	2.433456000
C	2.361598000	4.186463000	0.528842000
H	2.416301000	5.109271000	-0.038526000
C	2.051944000	2.991921000	-0.119038000
H	1.851074000	2.927020000	-1.182496000
C	4.465521000	-0.687569000	0.143293000
C	5.780410000	-1.055127000	-0.141517000
H	6.411125000	-1.466931000	0.640771000
C	6.262249000	-0.878733000	-1.438271000
H	7.282227000	-1.156199000	-1.686634000
C	5.412682000	-0.342519000	-2.409662000
H	5.747940000	-0.188179000	-3.429738000
C	4.109572000	-0.014113000	-2.049470000
H	3.385759000	0.386248000	-2.751027000
C	1.724740000	-1.921054000	1.787252000
H	2.218478000	-2.539522000	2.547932000
C	2.017265000	0.440061000	2.536153000
H	0.950879000	0.302999000	2.727128000
H	2.563059000	0.383335000	3.486776000
C	3.909750000	-0.773112000	1.545831000
H	4.215160000	-1.712985000	2.021859000
H	4.356529000	0.035015000	2.137810000
N	2.429104000	-0.627708000	1.592508000
H	0.709035000	-1.685547000	2.112918000
H	-3.349023000	-4.653226000	2.704246000
C	-2.988477000	-3.809507000	2.123486000
C	-2.941945000	-2.533050000	2.693817000
C	-2.573415000	-3.983726000	0.801742000
C	-2.480189000	-1.471099000	1.921511000
H	-3.258292000	-2.364915000	3.718691000
H	-2.597842000	-4.959599000	0.328487000
C	-2.138395000	-2.870927000	0.083088000
N	-2.101100000	-1.653233000	0.639510000
C	-2.279116000	-0.068688000	2.464111000
H	-1.806076000	-2.906869000	-0.949274000
H	-1.242914000	0.006468000	2.805287000
H	-2.941805000	0.127806000	3.316583000
N	-2.450740000	0.942766000	1.389767000
N	-3.570548000	0.070609000	-0.919320000
N	-1.334600000	1.915946000	-0.851035000
C	-1.617545000	2.166160000	1.544044000
C	-3.883231000	1.290609000	1.149621000
C	-4.461553000	0.571671000	-0.046436000
C	-4.000893000	-0.506325000	-2.055124000
C	-1.413410000	2.788624000	0.177913000
C	-1.122370000	2.364998000	-2.094512000
H	-2.065825000	2.881252000	2.246160000
H	-0.643169000	1.842459000	1.915012000
H	-3.942035000	2.368360000	0.957090000
H	-4.479880000	1.097737000	2.049457000
C	-5.834204000	0.500847000	-0.274412000
C	-5.355775000	-0.600370000	-2.361167000
H	-3.210280000	-0.890029000	-2.691201000
C	-1.283919000	4.159519000	-0.021375000
C	-0.967064000	3.723250000	-2.369568000
H	-1.084612000	1.603310000	-2.863316000
H	-6.529307000	0.909748000	0.452748000
C	-6.288315000	-0.094243000	-1.452472000
H	-5.669462000	-1.068231000	-3.288287000
H	-1.370416000	4.840129000	0.819925000
C	-1.051398000	4.634181000	-1.315857000
H	-0.799956000	4.052604000	-3.389539000
H	-7.352689000	-0.161639000	-1.656483000
H	-0.954065000	5.700279000	-1.498832000

²¹Is-Is

Fe	1.606948000	0.084730000	-0.301987000
O	1.285709000	0.612240000	-1.829701000
Fe	-1.612879000	0.051082000	-0.312258000
O	-1.132116000	-0.712265000	-1.869712000
H	-0.322745000	-0.230487000	-2.144624000
O	0.018168000	0.130994000	0.536526000
N	1.381339000	-1.888879000	-0.603771000
N	2.049829000	1.845825000	0.506217000
N	3.617249000	-0.272816000	-0.804955000

C	1.509928000	-2.634468000	0.514094000
C	1.448553000	-4.024444000	0.467251000
H	1.566667000	-4.600811000	1.379472000
C	1.242179000	-4.651846000	-0.764098000
H	1.197827000	-5.735145000	-0.826423000
C	1.112091000	-3.868767000	-1.911585000
H	0.962546000	-4.315931000	-2.888451000
C	1.194144000	-2.482984000	-1.789595000
H	1.116451000	-1.818380000	-2.639819000
C	2.261221000	1.825045000	1.841769000
C	2.617546000	2.980219000	2.531205000
H	2.801182000	2.936982000	3.600355000
C	2.739081000	4.181431000	1.825549000
H	3.021579000	5.093218000	2.343201000
C	2.504034000	4.188759000	0.450300000
H	2.591657000	5.099223000	-0.132746000
C	2.164689000	2.992148000	-0.178790000
H	1.972812000	2.914111000	-1.243092000
C	4.418186000	-0.788794000	0.140663000
C	5.711426000	-1.224503000	-0.145619000
H	6.330073000	-1.643874000	0.642225000
C	6.188124000	-1.104940000	-1.450832000
H	7.191655000	-1.435896000	-1.700644000
C	5.354950000	-0.554220000	-2.428142000
H	5.687091000	-0.440738000	-3.454581000
C	4.072139000	-0.155873000	-2.065612000
H	3.362325000	0.263333000	-2.770380000
C	1.649507000	-1.870283000	1.812618000
H	2.119778000	-2.490909000	2.586509000
C	2.029382000	0.491877000	2.522438000
H	0.959597000	0.397475000	2.719534000
H	2.576610000	0.431058000	3.472030000
C	3.872259000	-0.805314000	1.548936000
H	4.149442000	-1.736200000	2.059027000
H	4.349426000	0.010063000	2.106153000
N	2.398616000	-0.606241000	1.595633000
H	0.642264000	-1.592528000	2.131382000
H	-3.229272000	-4.639973000	2.711818000
C	-2.889577000	-3.790775000	2.126499000
C	-2.877607000	-2.510066000	2.688697000
C	-2.467026000	-3.962010000	0.806773000
C	-2.442364000	-1.440684000	1.910954000
H	-3.200518000	-2.343885000	3.711838000
H	-2.463927000	-4.940920000	0.339319000
C	-2.060473000	-2.842669000	0.082207000
N	-2.055455000	-1.620821000	0.630657000
C	-2.278262000	-0.032136000	2.451193000
H	-1.725334000	-2.877894000	-0.948974000
H	-1.248496000	0.064826000	2.806389000
H	-2.954928000	0.150420000	3.295657000
N	-2.457867000	0.979074000	1.376644000
N	-3.581618000	0.057046000	-0.908847000
N	-1.342569000	1.961155000	-0.855796000
C	-1.639459000	2.211956000	1.540005000
C	-3.892136000	1.315157000	1.133779000
C	-4.472950000	0.552545000	-0.032770000
C	-4.013729000	-0.552537000	-2.026609000
C	-1.412218000	2.831230000	0.176132000
C	-1.103176000	2.411053000	-2.094420000
H	-2.109862000	2.924803000	2.229703000
H	-0.668972000	1.902662000	1.931906000
H	-3.950918000	2.384428000	0.898797000
H	-4.483319000	1.157067000	2.044079000
C	-5.846373000	0.441455000	-0.237780000
C	-5.370199000	-0.687428000	-2.310054000
H	-3.224959000	-0.927246000	-2.669950000
C	-1.247279000	4.199283000	-0.015376000
C	-0.910025000	3.766280000	-2.360819000
H	-1.073977000	1.653243000	-2.867379000
H	-6.540798000	0.846965000	0.491863000
C	-6.302250000	-0.188285000	-1.397131000
H	-5.684990000	-1.180437000	-3.223657000
H	-1.328162000	4.878173000	0.827913000
C	-0.985584000	4.674146000	-1.304226000
H	-0.720531000	4.095341000	-3.376951000

H	-7.367349000	-0.287044000	-1.583753000
H	-0.859000000	5.738300000	-1.480380000

Cyclopentane (CP)

H	2.176188000	-0.589958000	0.268899000
H	1.086754000	1.406023000	1.058924000
C	1.218177000	-0.362296000	-0.212674000
H	1.348437000	-0.505021000	-1.294092000
C	0.729218000	1.078312000	0.075485000
H	1.114218000	1.793801000	-0.659539000
C	-0.830366000	1.003510000	0.069495000
H	-1.274840000	1.670425000	-0.677632000
H	-1.226310000	1.307701000	1.045601000
C	0.061929000	-1.250833000	0.275040000
H	0.111244000	-2.276811000	-0.108037000
H	0.067152000	-1.299923000	1.373345000
C	-1.178084000	-0.480126000	-0.207700000
H	-1.301993000	-0.640595000	-1.287388000
H	-2.106094000	-0.797045000	0.282048000

²RC_{hs-hs}

Fe	1.516473000	-0.195661000	0.018127000
O	1.388827000	0.670210000	-1.367917000
Fe	-1.656579000	0.217844000	-0.290570000
O	-1.201173000	0.247714000	-2.058234000
H	-0.234619000	0.435141000	-2.117392000
O	-0.092876000	-0.014540000	0.700955000
N	1.066523000	-2.251995000	-0.736273000
N	2.482569000	1.137056000	1.488616000
N	3.488394000	-0.818984000	-0.510738000
C	1.051134000	-3.196964000	0.218470000
C	0.917469000	-4.548017000	-0.092646000
H	0.920767000	-5.293963000	0.696232000
C	0.786156000	-4.915472000	-1.435657000
H	0.690249000	-5.962266000	-1.708788000
C	0.789633000	-3.924018000	-2.419087000
H	0.693417000	-4.171732000	-3.471109000
C	0.938348000	-2.594037000	-2.022532000
H	0.954245000	-1.773137000	-2.732533000
C	2.505299000	0.651689000	2.744685000
C	3.084973000	1.361214000	3.793129000
H	3.104440000	0.939423000	4.793492000
C	3.640476000	2.617078000	3.526927000
H	4.101208000	3.191188000	4.325266000
C	3.603791000	3.116063000	2.224024000
H	4.027239000	4.083997000	1.977348000
C	3.015977000	2.337533000	1.226669000
H	2.961357000	2.667806000	0.195845000
C	4.118789000	-1.688622000	0.296908000
C	5.334035000	-2.270340000	-0.062391000
H	5.817396000	-2.974908000	0.607884000
C	5.912025000	-1.926634000	-1.284867000
H	6.859428000	-2.364393000	-1.584766000
C	5.253121000	-1.016713000	-2.115436000
H	5.667126000	-0.723259000	-3.074123000
C	4.035413000	-0.491300000	-1.695133000
H	3.455842000	0.203010000	-2.293516000
C	1.124806000	-2.672493000	1.636249000
H	1.394251000	-3.470740000	2.341636000
C	1.828581000	-0.691265000	2.925744000
H	0.747581000	-0.530653000	2.985831000
H	2.169912000	-1.187699000	3.844424000
C	3.488444000	-1.964949000	1.642507000
H	3.576045000	-3.030797000	1.888283000
H	4.062733000	-1.421027000	2.402021000
N	2.065261000	-1.532136000	1.727626000
H	0.135682000	-2.286104000	1.898159000
H	-3.529359000	-5.413856000	0.879581000
C	-3.157528000	-4.418374000	0.655512000
C	-3.128251000	-3.437699000	1.651584000
C	-2.718882000	-4.097124000	-0.630362000
C	-2.654404000	-2.167243000	1.330304000
H	-3.475642000	-3.649795000	2.658217000
H	-2.735655000	-4.827887000	-1.431772000

C	-2.269189000	-2.800484000	-0.875010000
N	-2.233129000	-1.869797000	0.087157000
C	-2.531255000	-1.053796000	2.351948000
H	-1.926349000	-2.475691000	-1.851778000
H	-1.487926000	-1.009283000	2.683019000
H	-3.161365000	-1.266919000	3.228056000
N	-2.846021000	0.251331000	1.749916000
N	-3.821839000	0.289530000	-0.858817000
N	-1.904632000	2.312812000	0.220426000
C	-2.216616000	1.397874000	2.439447000
C	-4.297695000	0.451317000	1.535575000
C	-4.751941000	0.230637000	0.104942000
C	-4.192476000	0.189874000	-2.148049000
C	-2.190146000	2.592309000	1.508424000
C	-1.833351000	3.302297000	-0.680368000
H	-2.726561000	1.648958000	3.380420000
H	-1.182670000	1.110786000	2.658078000
H	-4.545786000	1.486234000	1.802176000
H	-4.877796000	-0.189512000	2.213308000
C	-6.104282000	0.052401000	-0.189169000
C	-5.522945000	0.027409000	-2.524876000
H	-3.380084000	0.239914000	-2.865799000
C	-2.427761000	3.895439000	1.933969000
C	-2.053079000	4.634126000	-0.329206000
H	-1.587330000	3.002263000	-1.692894000
H	-6.833967000	0.002194000	0.613855000
C	-6.495606000	-0.048784000	-1.524530000
H	-5.786156000	-0.042863000	-3.575004000
H	-2.670045000	4.092057000	2.973863000
C	-2.356010000	4.933674000	0.998734000
H	-1.988314000	5.410284000	-1.083984000
H	-7.542419000	-0.184501000	-1.779668000
H	-2.542075000	5.958801000	1.304891000
H	0.131913000	2.446940000	-2.962487000
H	2.206448000	1.578585000	-3.686749000
C	0.882427000	3.236565000	-3.073864000
H	0.487374000	3.972542000	-3.783810000
C	2.239406000	2.669761000	-3.594417000
H	2.466567000	3.074819000	-4.586209000
C	3.311637000	3.118649000	-2.570033000
H	4.276118000	3.349958000	-3.035418000
H	3.477290000	2.317795000	-1.837528000
C	1.204817000	3.920509000	-1.724854000
H	0.547441000	4.769216000	-1.505336000
H	1.095041000	3.188773000	-0.914038000
C	2.680011000	4.330685000	-1.863149000
H	2.760992000	5.218959000	-2.502664000
H	3.158582000	4.576136000	-0.905519000

¹⁰RC_{hs-hs}

Fe	1.524946000	-0.200134000	0.019195000
O	1.376749000	0.684316000	-1.352477000
Fe	-1.672184000	0.219625000	-0.285664000
O	-1.217804000	0.210597000	-2.058964000
H	-0.255372000	0.407531000	-2.119314000
O	-0.092070000	-0.007418000	0.737985000
N	1.039880000	-2.249247000	-0.753281000
N	2.528692000	1.103338000	1.504102000
N	3.475801000	-0.834798000	-0.537963000
C	1.023633000	-3.201091000	0.194474000
C	0.875517000	-4.548720000	-0.125100000
H	0.878360000	-5.300207000	0.658511000
C	0.729979000	-4.905365000	-1.469529000
H	0.622784000	-5.949268000	-1.749477000
C	0.733490000	-3.906713000	-2.445675000
H	0.625889000	-4.145779000	-3.498599000
C	0.897193000	-2.581002000	-2.040584000
H	0.912721000	-1.755594000	-2.745309000
C	2.550830000	0.601655000	2.753335000
C	3.142047000	1.290765000	3.809090000
H	3.160299000	0.855637000	4.803757000
C	3.709893000	2.543998000	3.557495000
H	4.179837000	3.102467000	4.361550000
C	3.672903000	3.061055000	2.261576000
H	4.105197000	4.027935000	2.026338000

C	3.072951000	2.302045000	1.256540000
H	3.017253000	2.647826000	0.230796000
C	4.108098000	-1.716977000	0.255040000
C	5.318946000	-2.297784000	-0.120539000
H	5.804594000	-3.012306000	0.537411000
C	5.889550000	-1.940884000	-1.342591000
H	6.833370000	-2.378050000	-1.654412000
C	5.228115000	-1.018656000	-2.157558000
H	5.636446000	-0.714946000	-3.115469000
C	4.015521000	-0.494215000	-1.722337000
H	3.434698000	0.209956000	-2.307745000
C	1.111892000	-2.686598000	1.614669000
H	1.372151000	-3.492688000	2.314542000
C	1.856375000	-0.733805000	2.920188000
H	0.778597000	-0.556967000	2.989647000
H	2.197452000	-1.249091000	3.828548000
C	3.485897000	-2.011562000	1.600862000
H	3.560880000	-3.083494000	1.823280000
H	4.075108000	-1.491872000	2.365895000
N	2.069838000	-1.561165000	1.708551000
H	0.130404000	-2.284177000	1.881424000
H	-3.561451000	-5.393746000	0.923643000
C	-3.187483000	-4.400749000	0.692192000
C	-3.152845000	-3.413996000	1.682244000
C	-2.751352000	-4.089311000	-0.597016000
C	-2.676364000	-2.147041000	1.351649000
H	-3.497886000	-3.619031000	2.691128000
H	-2.772062000	-4.825468000	-1.393358000
C	-2.298641000	-2.795665000	-0.851339000
N	-2.257792000	-1.859331000	0.105163000
C	-2.544142000	-1.026551000	2.363908000
H	-1.956716000	-2.476767000	-1.830344000
H	-1.498116000	-0.983350000	2.686172000
H	-3.170771000	-1.229195000	3.244858000
N	-2.856176000	0.275457000	1.752074000
N	-3.832303000	0.307928000	-0.857845000
N	-1.901260000	2.319583000	0.206109000
C	-2.219800000	1.424433000	2.432419000
C	-4.307055000	0.479822000	1.538192000
C	-4.762592000	0.264056000	0.106966000
C	-4.204775000	0.209765000	-2.146995000
C	-2.185167000	2.610949000	1.491995000
C	-1.821129000	3.301748000	-0.702091000
H	-2.729098000	1.685678000	3.370882000
H	-1.187381000	1.133085000	2.651512000
H	-4.553196000	1.514360000	1.808199000
H	-4.888770000	-0.161985000	2.213505000
C	-6.117259000	0.103551000	-0.186799000
C	-5.537344000	0.063776000	-2.522529000
H	-3.392390000	0.246864000	-2.865289000
C	-2.411544000	3.919363000	1.907302000
C	-2.029173000	4.637922000	-0.361178000
H	-1.578197000	2.992428000	-1.712531000
H	-6.847194000	0.065527000	0.616659000
C	-6.510523000	0.003744000	-1.521570000
H	-5.801828000	-0.006167000	-3.572342000
H	-2.652424000	4.125921000	2.945574000
C	-2.330059000	4.949901000	0.964434000
H	-1.957205000	5.407787000	-1.121700000
H	-7.559203000	-0.118448000	-1.775855000
H	-2.507060000	5.978891000	1.262904000
H	0.177184000	2.460618000	-2.921475000
H	2.242983000	1.607074000	-3.679924000
C	0.922905000	3.254812000	-3.031065000
H	0.520952000	3.994924000	-3.732819000
C	2.278462000	2.695986000	-3.563656000
H	2.506506000	3.121605000	-4.546629000
C	3.351664000	3.122793000	-2.531506000
H	4.319322000	3.351267000	-2.991711000
H	3.508711000	2.312298000	-1.807707000
C	1.250092000	3.927063000	-1.676865000
H	0.596962000	4.777024000	-1.449938000
H	1.137968000	3.189374000	-0.871861000
C	2.727267000	4.331342000	-1.812719000
H	2.812686000	5.224911000	-2.444257000

H	3.207586000	4.565392000	-0.853169000
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⁸ RC _{hs-is}			
Fe	1.656347000	-0.275693000	0.101935000
O	1.594407000	0.667429000	-1.221242000
Fe	-1.545327000	0.180716000	-0.232709000
O	-1.054793000	0.307181000	-2.008013000
H	-0.102316000	0.531217000	-2.035254000
O	-0.036508000	-0.084110000	0.776233000
N	1.134887000	-1.996119000	-0.760445000
N	2.293588000	1.072478000	1.414220000
N	3.614969000	-0.846135000	-0.324554000
C	1.042249000	-3.045019000	0.085369000
C	0.829298000	-4.335283000	-0.388524000
H	0.770870000	-5.164346000	0.309431000
C	0.695830000	-4.536929000	-1.765115000
H	0.539201000	-5.536840000	-2.158670000
C	0.773755000	-3.440722000	-2.624654000
H	0.675494000	-3.554801000	-3.698920000
C	0.999446000	-2.176972000	-2.081816000
H	1.076686000	-1.282874000	-2.687308000
C	2.296978000	0.662150000	2.703127000
C	2.749913000	1.494526000	3.721402000
H	2.759780000	1.137821000	4.746684000
C	3.189064000	2.782598000	3.399804000
H	3.547340000	3.448468000	4.179055000
C	3.171088000	3.193943000	2.066890000
H	3.506936000	4.182822000	1.773769000
C	2.719735000	2.303613000	1.094600000
H	2.685590000	2.553977000	0.042632000
C	4.206313000	-1.720406000	0.506472000
C	5.452429000	-2.277098000	0.221135000
H	5.901108000	-2.985657000	0.910994000
C	6.104789000	-1.902630000	-0.953568000
H	7.077115000	-2.319789000	-1.197545000
C	5.486878000	-0.987088000	-1.809410000
H	5.958647000	-0.669015000	-2.732930000
C	4.235890000	-0.486880000	-1.463207000
H	3.688793000	0.211043000	-2.086653000
C	1.111214000	-2.700644000	1.555798000
H	1.368812000	-3.579855000	2.160292000
C	1.739204000	-0.723254000	2.946715000
H	0.651404000	-0.643883000	2.996406000
H	2.118451000	-1.149027000	3.884514000
C	3.483846000	-2.020905000	1.798920000
H	3.549963000	-3.089754000	2.036789000
H	3.997460000	-1.487548000	2.607740000
N	2.060446000	-1.582170000	1.778168000
H	0.121349000	-2.340841000	1.845110000
H	-3.715710000	-5.419160000	0.686143000
C	-3.283081000	-4.439263000	0.506959000
C	-3.217639000	-3.498519000	1.539472000
C	-2.804306000	-4.094015000	-0.757667000
C	-2.668474000	-2.245670000	1.274204000
H	-3.598942000	-3.725813000	2.530413000
H	-2.852106000	-4.790186000	-1.588460000
C	-2.272519000	-2.817891000	-0.942359000
N	-2.199228000	-1.926758000	0.053121000
C	-2.534962000	-1.166349000	2.330767000
H	-1.895153000	-2.480615000	-1.902360000
H	-1.493540000	-1.138640000	2.668920000
H	-3.174152000	-1.398216000	3.196030000
N	-2.832078000	0.155627000	1.761334000
N	-3.714525000	0.260327000	-0.882619000
N	-1.873651000	2.265116000	0.322641000
C	-2.226557000	1.281960000	2.501632000
C	-4.274372000	0.355810000	1.498448000
C	-4.675407000	0.164209000	0.046744000
C	-4.041854000	0.188752000	-2.184497000
C	-2.196408000	2.505338000	1.608615000
C	-1.817603000	3.275326000	-0.554511000
H	-2.755083000	1.498394000	3.441387000
H	-1.193653000	0.993785000	2.724684000
H	-4.536736000	1.383601000	1.778386000
H	-4.876938000	-0.301616000	2.140244000

C	-6.014809000	-0.026678000	-0.295931000
C	-5.356680000	0.015603000	-2.610278000
H	-3.206705000	0.271571000	-2.872658000
C	-2.479749000	3.790769000	2.060221000
C	-2.082846000	4.592341000	-0.178107000
H	-1.548720000	3.002244000	-1.569158000
H	-6.769617000	-0.107471000	0.481067000
C	-6.360603000	-0.100722000	-1.645532000
H	-5.584161000	-0.031569000	-3.670078000
H	-2.752161000	3.955468000	3.098273000
C	-2.418064000	4.852340000	1.150642000
H	-2.030001000	5.387529000	-0.913924000
H	-7.396199000	-0.245864000	-1.938610000
H	-2.640287000	5.864311000	1.476019000
H	0.001281000	2.435193000	-3.140557000
H	2.114645000	1.463912000	-3.618018000
C	0.796524000	3.185390000	-3.219174000
H	0.475219000	3.929931000	-3.956885000
C	2.153779000	2.557964000	-3.659842000
H	2.389267000	2.837589000	-4.691837000
C	3.224298000	3.106725000	-2.677182000
H	4.160169000	3.379381000	-3.176753000
H	3.459535000	2.340370000	-1.928189000
C	1.080730000	3.880056000	-1.870484000
H	0.409704000	4.723563000	-1.672097000
H	0.956883000	3.154436000	-1.056684000
C	2.552446000	4.307935000	-1.984396000
H	2.628243000	5.198107000	-2.621444000
H	3.011432000	4.561077000	-1.018832000

⁴RC_{hs-is}

Fe	1.636957000	-0.289596000	0.110365000
O	1.583349000	0.654669000	-1.217810000
Fe	-1.538252000	0.176236000	-0.238464000
O	-1.032132000	0.309626000	-2.000979000
H	-0.077453000	0.536637000	-2.016913000
O	-0.045329000	-0.114941000	0.789128000
N	1.117069000	-2.009094000	-0.751146000
N	2.267914000	1.064069000	1.421446000
N	3.591926000	-0.856926000	-0.315251000
C	1.027069000	-3.057783000	0.095252000
C	0.810415000	-4.347792000	-0.378003000
H	0.754186000	-5.176915000	0.320096000
C	0.671472000	-4.549435000	-1.754014000
H	0.511864000	-5.549196000	-2.146753000
C	0.748927000	-3.453592000	-2.614058000
H	0.647599000	-3.567754000	-3.688038000
C	0.978007000	-2.190138000	-2.072088000
H	1.053865000	-1.295919000	-2.677518000
C	2.270536000	0.654740000	2.710743000
C	2.716351000	1.490618000	3.729420000
H	2.726009000	1.134769000	4.755022000
C	3.149512000	2.780720000	3.407879000
H	3.502232000	3.449105000	4.187520000
C	3.133714000	3.190471000	2.074463000
H	3.466272000	4.180429000	1.781212000
C	2.689557000	2.296677000	1.101947000
H	2.658870000	2.544736000	0.049230000
C	4.190200000	-1.725463000	0.516861000
C	5.438111000	-2.277339000	0.230272000
H	5.891576000	-2.981100000	0.921900000
C	6.085570000	-1.904615000	-0.947574000
H	7.059215000	-2.318037000	-1.192648000
C	5.460287000	-0.995892000	-1.805197000
H	5.927291000	-0.679403000	-2.731672000
C	4.207937000	-0.500153000	-1.457760000
H	3.655204000	0.191667000	-2.082618000
C	1.103311000	-2.716542000	1.566493000
H	1.369913000	-3.596610000	2.165880000
C	1.722397000	-0.734561000	2.956358000
H	0.634340000	-0.663739000	3.010322000
H	2.107549000	-1.156060000	3.893779000
C	3.472063000	-2.024953000	1.811267000
H	3.544347000	-3.092475000	2.053399000
H	3.983663000	-1.485392000	2.617242000

N	2.047199000	-1.593308000	1.788604000
H	0.112880000	-2.365221000	1.863910000
H	-3.759861000	-5.406920000	0.651985000
C	-3.322313000	-4.428585000	0.476252000
C	-3.248660000	-3.493263000	1.513028000
C	-2.845225000	-4.079938000	-0.788078000
C	-2.693044000	-2.242187000	1.252678000
H	-3.628255000	-3.723384000	2.503976000
H	-2.899323000	-4.771707000	-1.622144000
C	-2.307149000	-2.805829000	-0.968109000
N	-2.226053000	-1.919824000	0.031537000
C	-2.548195000	-1.171220000	2.316436000
H	-1.930766000	-2.466468000	-1.927722000
H	-1.507134000	-1.159002000	2.656249000
H	-3.191402000	-1.401404000	3.179148000
N	-2.827725000	0.158495000	1.756432000
N	-3.705670000	0.306682000	-0.884928000
N	-1.828578000	2.260473000	0.330789000
C	-2.206838000	1.271594000	2.503617000
C	-4.267228000	0.380586000	1.495828000
C	-4.669683000	0.215419000	0.041334000
C	-4.031192000	0.256324000	-2.188169000
C	-2.154065000	2.498436000	1.616560000
C	-1.754050000	3.274388000	-0.540822000
H	-2.735208000	1.492337000	3.442444000
H	-1.179415000	0.966680000	2.728880000
H	-4.517239000	1.407153000	1.791261000
H	-4.878201000	-0.278889000	2.127408000
C	-6.011515000	0.051815000	-0.306095000
C	-5.347747000	0.110881000	-2.618684000
H	-3.193190000	0.332554000	-2.873845000
C	-2.420669000	3.785625000	2.073418000
C	-2.001448000	4.593127000	-0.158578000
H	-1.485554000	3.002839000	-1.555917000
H	-6.769284000	-0.025864000	0.468329000
C	-6.355503000	0.000162000	-1.657177000
H	-5.573858000	0.080191000	-3.679380000
H	-2.695809000	3.948686000	3.111012000
C	-2.339073000	4.851018000	1.169970000
H	-1.933485000	5.391200000	-0.889977000
H	-7.392774000	-0.123740000	-1.954053000
H	-2.548047000	5.864397000	1.499722000
H	0.056554000	2.406127000	-3.178446000
H	2.174080000	1.416338000	-3.599153000
C	0.857440000	3.150603000	-3.255583000
H	0.553954000	3.883237000	-4.012437000
C	2.219950000	2.509321000	-3.658587000
H	2.477099000	2.770381000	-4.690304000
C	3.273671000	3.070157000	-2.664627000
H	4.220367000	3.329693000	-3.150632000
H	3.491108000	2.316271000	-1.897860000
C	1.119164000	3.867776000	-1.914356000
H	0.448409000	4.717721000	-1.743884000
H	0.975912000	3.156989000	-1.090854000
C	2.594885000	4.286415000	-2.005910000
H	2.688338000	5.165497000	-2.655829000
H	3.035838000	4.552571000	-1.035494000

⁶RC_{is-is}

Fe	1.607718000	-0.301376000	0.072463000
O	1.657851000	0.679651000	-1.225787000
Fe	-1.607110000	0.186206000	-0.207432000
O	-0.950242000	0.322782000	-1.873241000
H	-0.010353000	0.602720000	-1.807629000
O	-0.087101000	-0.047407000	0.715647000
N	1.049476000	-1.978673000	-0.840457000
N	2.258648000	0.995491000	1.440886000
N	3.568524000	-0.953358000	-0.298466000
C	0.915190000	-3.045766000	-0.023466000
C	0.694124000	-4.320737000	-0.533783000
H	0.603850000	-5.164595000	0.142656000
C	0.591439000	-4.486756000	-1.917791000
H	0.429676000	-5.474060000	-2.340155000
C	0.703985000	-3.370347000	-2.747290000
H	0.628675000	-3.456614000	-3.825975000

C	0.940053000	-2.124048000	-2.168657000
H	1.050002000	-1.216857000	-2.748385000
C	2.202026000	0.558432000	2.719397000
C	2.652007000	1.349390000	3.771537000
H	2.613406000	0.969922000	4.787985000
C	3.153321000	2.625232000	3.494618000
H	3.510697000	3.259052000	4.300566000
C	3.199727000	3.064232000	2.171413000
H	3.586599000	4.043855000	1.912021000
C	2.747356000	2.213365000	1.164445000
H	2.762983000	2.485400000	0.117295000
C	4.091861000	-1.871072000	0.530120000
C	5.313553000	-2.489349000	0.267200000
H	5.705718000	-3.232622000	0.954960000
C	6.015758000	-2.129104000	-0.883054000
H	6.970743000	-2.593167000	-1.110325000
C	5.470654000	-1.165795000	-1.735766000
H	5.983931000	-0.855800000	-2.639718000
C	4.238367000	-0.606448000	-1.412527000
H	3.745665000	0.131477000	-2.035465000
C	0.940930000	-2.736413000	1.456164000
H	1.146422000	-3.636922000	2.049346000
C	1.587746000	-0.811629000	2.913691000
H	0.502898000	-0.695389000	2.931582000
H	1.921239000	-1.269532000	3.853825000
C	3.322253000	-2.144166000	1.800528000
H	3.344160000	-3.213484000	2.044939000
C	3.829887000	-1.623923000	2.621608000
N	1.916903000	-1.655649000	1.737672000
H	-0.047518000	-2.349295000	1.714282000
H	-4.045628000	-5.297601000	0.967269000
C	-3.539489000	-4.364048000	0.739855000
C	-3.439416000	-3.362321000	1.711046000
C	-2.994179000	-4.141813000	-0.525795000
C	-2.793069000	-2.173553000	1.378844000
H	-3.862505000	-3.497247000	2.702007000
H	-3.061330000	-4.891260000	-1.307606000
C	-2.367570000	-2.919694000	-0.774527000
N	-2.267392000	-1.968238000	0.158753000
C	-2.596988000	-1.035695000	2.359224000
H	-1.930403000	-2.679856000	-1.739227000
H	-1.568648000	-1.065753000	2.733781000
H	-3.276763000	-1.137975000	3.217058000
N	-2.767717000	0.267614000	1.686736000
N	-3.534309000	0.269700000	-0.980477000
N	-1.838297000	2.358044000	0.276108000
C	-2.157429000	1.380990000	2.451929000
C	-4.198836000	0.533866000	1.359472000
C	-4.546927000	0.292384000	-0.094133000
C	-3.795654000	0.160433000	-2.294572000
C	-2.088258000	2.611472000	1.572790000
C	-1.736927000	3.368814000	-0.593283000
H	-2.704613000	1.586270000	3.382740000
H	-1.135995000	1.065513000	2.689843000
H	-4.411452000	1.586809000	1.578482000
H	-4.855768000	-0.058915000	2.008872000
C	-5.874571000	0.179943000	-0.504059000
C	-5.096254000	0.058951000	-2.779815000
H	-2.917136000	0.162064000	-2.931778000
C	-2.260394000	3.907879000	2.049198000
C	-1.890534000	4.698955000	-0.198109000
H	-1.517319000	3.088800000	-1.618390000
H	-6.673142000	0.194724000	0.231662000
C	-6.153377000	0.061381000	-1.866474000
H	-5.272556000	-0.022884000	-3.847059000
H	-2.478351000	4.082355000	3.098637000
C	-2.156896000	4.970151000	1.144179000
H	-1.804068000	5.496338000	-0.928390000
H	-7.180386000	-0.024157000	-2.208856000
H	-2.291585000	5.992658000	1.484310000
H	0.162010000	2.437112000	-3.049584000
H	2.257600000	1.494762000	-3.629897000
C	0.943498000	3.199681000	-3.142298000
H	0.598943000	3.938121000	-3.875579000
C	2.301993000	2.588975000	-3.604332000

H	2.549972000	2.930331000	-4.614822000
C	3.365782000	3.075624000	-2.585571000
H	4.322312000	3.326203000	-3.057159000
H	3.555353000	2.284869000	-1.849024000
C	1.232706000	3.894502000	-1.792876000
H	0.582971000	4.757206000	-1.608100000
H	1.075584000	3.178304000	-0.977014000
C	2.717176000	4.284097000	-1.884844000
H	2.824901000	5.179518000	-2.509959000
H	3.170173000	4.513240000	-0.910422000

²RC_{is-is}

Fe	1.607591000	-0.285914000	0.072177000
O	1.668416000	0.688900000	-1.231691000
Fe	-1.609199000	0.175788000	-0.202032000
O	-0.950592000	0.309105000	-1.866183000
H	-0.007847000	0.577695000	-1.797355000
O	-0.088362000	-0.027520000	0.713226000
N	1.050242000	-1.969116000	-0.837564000
N	2.259389000	1.012596000	1.438439000
N	3.573591000	-0.954035000	-0.298255000
C	0.921731000	-3.034279000	-0.017113000
C	0.711108000	-4.312764000	-0.523130000
H	0.624860000	-5.154655000	0.156290000
C	0.614452000	-4.484952000	-1.906807000
H	0.461123000	-5.475018000	-2.325844000
C	0.722917000	-3.371086000	-2.740287000
H	0.653144000	-3.462211000	-3.818951000
C	0.947770000	-2.120922000	-2.165531000
H	1.055189000	-1.215620000	-2.748811000
C	2.199602000	0.579504000	2.718228000
C	2.649006000	1.372860000	3.768787000
H	2.607980000	0.996569000	4.786325000
C	3.153439000	2.646848000	3.488842000
H	3.510447000	3.282488000	4.293523000
C	3.203871000	3.081420000	2.164346000
H	3.593744000	4.059240000	1.902647000
C	2.751695000	2.228376000	1.159087000
H	2.770568000	2.496533000	0.110957000
C	4.091426000	-1.870223000	0.534873000
C	5.307096000	-2.500707000	0.273079000
H	5.695223000	-3.242741000	0.964471000
C	6.009151000	-2.153073000	-0.881343000
H	6.959667000	-2.626424000	-1.108243000
C	5.470381000	-1.189963000	-1.738307000
H	5.984611000	-0.889363000	-2.644908000
C	4.243315000	-0.618592000	-1.415260000
H	3.754809000	0.120664000	-2.040332000
C	0.944352000	-2.720196000	1.461707000
H	1.150679000	-3.618901000	2.057407000
C	1.584807000	-0.790108000	2.915069000
H	0.499756000	-0.674656000	2.929920000
H	1.916092000	-1.245027000	3.857457000
C	3.323457000	-2.123804000	1.810452000
H	3.346404000	-3.188814000	2.073150000
H	3.831567000	-1.588902000	2.621742000
N	1.917729000	-1.636955000	1.742209000
H	-0.045207000	-2.334827000	1.717884000
H	-4.030179000	-5.317107000	0.953353000
C	-3.526829000	-4.381252000	0.729251000
C	-3.431590000	-3.381870000	1.703372000
C	-2.980289000	-4.153764000	-0.534896000
C	-2.788724000	-2.190123000	1.375474000
H	-3.855696000	-3.520954000	2.693315000
H	-3.043719000	-4.901290000	-1.318835000
C	-2.357043000	-2.929096000	-0.779373000
N	-2.261493000	-1.979670000	0.156695000
C	-2.598731000	-1.053898000	2.358832000
H	-1.918650000	-2.685652000	-1.742589000
H	-1.571595000	-1.080976000	2.737194000
H	-3.280702000	-1.159827000	3.214422000
N	-2.772164000	0.249888000	1.687472000
N	-3.533199000	0.270019000	-0.982577000
N	-1.843177000	2.343871000	0.283091000
C	-2.169404000	1.364936000	2.456956000

C	-4.204363000	0.511893000	1.358302000
C	-4.548029000	0.284820000	-0.098600000
C	-3.791315000	0.172981000	-2.298333000
C	-2.099529000	2.595995000	1.578764000
C	-1.738998000	3.354890000	-0.585686000
H	-2.722849000	1.567551000	3.384581000
H	-1.148427000	1.053166000	2.701191000
H	-4.423845000	1.560895000	1.589277000
H	-4.859308000	-0.092226000	1.999074000
C	-5.874717000	0.177130000	-0.512844000
C	-5.090792000	0.077079000	-2.787694000
H	-2.911006000	0.178808000	-2.933055000
C	-2.276370000	3.891857000	2.054782000
C	-1.896788000	4.684492000	-0.190419000
H	-1.513637000	3.075718000	-1.609686000
H	-6.675160000	0.185472000	0.220949000
C	-6.150187000	0.071695000	-1.877025000
H	-5.264434000	0.005136000	-3.856084000
H	-2.499483000	4.065562000	3.103255000
C	-2.170390000	4.954624000	1.150619000
H	-1.807754000	5.482314000	-0.919879000
H	-7.176392000	-0.010000000	-2.222732000
H	-2.308543000	5.976752000	1.490473000
H	0.155948000	2.428183000	-3.035962000
H	2.248788000	1.560998000	-3.653684000
C	0.927691000	3.199165000	-3.139153000
H	0.566712000	3.932894000	-3.869243000
C	2.286793000	2.601077000	-3.616119000
H	2.526483000	2.955476000	-4.624160000
C	3.354126000	3.083175000	-2.599463000
H	4.309406000	3.334333000	-3.073325000
C	3.544176000	2.289672000	-1.866041000
H	1.224779000	3.897423000	-1.792844000
H	0.574448000	4.759118000	-1.605155000
H	1.074571000	3.181984000	-0.975079000
C	2.707957000	4.290033000	-1.894020000
H	2.810358000	5.185976000	-2.519342000
H	3.166342000	4.519621000	-0.922195000

⁴RC_{ls-is}

Fe	1.397921000	-0.358823000	0.332216000
O	1.387978000	0.947834000	-0.646710000
Fe	-1.765713000	0.118024000	-0.091592000
O	-1.042294000	0.232169000	-1.741388000
H	-0.166363000	0.643342000	-1.597142000
O	-0.336752000	-0.589618000	0.815897000
N	1.163398000	-1.798604000	-1.035021000
N	1.729953000	0.597672000	2.049256000
N	3.467095000	-0.618839000	0.020078000
C	1.046900000	-3.042845000	-0.523603000
C	0.916633000	-4.154411000	-1.350872000
H	0.837423000	-5.145014000	-0.914155000
C	0.895552000	-3.969504000	-2.735738000
H	0.800937000	-4.822752000	-3.400840000
C	1.013954000	-2.678072000	-3.249413000
H	1.012370000	-2.490393000	-4.317689000
C	1.151794000	-1.612593000	-2.362150000
H	1.259912000	-0.590342000	-2.696847000
C	1.709640000	-0.178922000	3.155834000
C	1.984829000	0.353209000	4.411873000
H	1.981378000	-0.291823000	5.285086000
C	2.268049000	1.718339000	4.523088000
H	2.491947000	2.152653000	5.492809000
C	2.268117000	2.508642000	3.373377000
H	2.483356000	3.570797000	3.417864000
C	1.996765000	1.907268000	2.145701000
H	1.980275000	2.451054000	1.208031000
C	4.062679000	-1.670832000	0.601916000
C	5.378125000	-2.028168000	0.306076000
H	5.829320000	-2.889941000	0.788935000
C	6.094456000	-1.258041000	-0.610356000
H	7.119748000	-1.515163000	-0.858805000
C	5.472884000	-0.154243000	-1.200514000
H	5.992179000	0.473719000	-1.916682000
C	4.153978000	0.128669000	-0.861799000

H	3.601845000	0.955864000	-1.291443000
C	0.985463000	-3.140621000	0.983772000
H	1.287650000	-4.138218000	1.328284000
C	1.313412000	-1.622923000	2.932753000
H	0.222509000	-1.667333000	2.895735000
H	1.672979000	-2.265150000	3.747121000
C	3.259204000	-2.407509000	1.649053000
H	3.402755000	-3.490509000	1.550560000
H	3.650957000	-2.129487000	2.635099000
N	1.808115000	-2.074206000	1.608791000
H	-0.051363000	-2.954266000	1.272707000
H	-4.327252000	-5.089601000	-0.447446000
C	-3.812074000	-4.134466000	-0.409034000
C	-3.802950000	-3.388651000	0.774221000
C	-3.158963000	-3.634745000	-1.537556000
C	-3.138875000	-2.165418000	0.789546000
H	-4.301918000	-3.749292000	1.668464000
H	-3.147705000	-4.186529000	-2.471510000
C	-2.528474000	-2.394107000	-1.452956000
N	-2.528389000	-1.688163000	-0.314857000
C	-2.965349000	-1.326330000	2.041000000
H	-2.005734000	-1.922682000	-2.278676000
H	-2.014179000	-1.612848000	2.498679000
H	-3.770706000	-1.513998000	2.762622000
N	-2.858425000	0.117121000	1.702214000
N	-3.560889000	0.800077000	-0.824188000
N	-1.254752000	1.941581000	0.566462000
C	-2.001543000	0.907657000	2.627126000
C	-4.191030000	0.765018000	1.512528000
C	-4.573218000	0.884149000	0.056238000
C	-3.797922000	0.990746000	-2.133703000
C	-1.479384000	2.121219000	1.887245000
C	-0.750433000	2.941930000	-0.167040000
H	-2.540968000	1.194367000	3.539230000
H	-1.146824000	0.278613000	2.883274000
H	-4.134619000	1.777289000	1.929894000
H	-4.961583000	0.229554000	2.080332000
C	-5.879600000	1.150032000	-0.348254000
C	-5.073261000	1.277263000	-2.613110000
H	-2.923072000	0.894736000	-2.767749000
C	-1.209532000	3.334283000	2.512155000
C	-0.435581000	4.179228000	0.393924000
H	-0.597183000	2.729205000	-1.216588000
H	-6.677156000	1.205520000	0.386572000
C	-6.133153000	1.350888000	-1.706133000
H	-5.229659000	1.430240000	-3.675647000
H	-1.418932000	3.457153000	3.570265000
C	-0.674051000	4.380025000	1.753278000
H	-0.021201000	4.959786000	-0.234237000
H	-7.141611000	1.561318000	-2.049286000
H	-0.459714000	5.338660000	2.216606000
H	0.341950000	1.949563000	-3.186810000
H	2.544855000	0.993143000	-3.167483000
C	1.134518000	2.614655000	-3.549412000
H	0.773188000	3.083322000	-4.473510000
C	2.463827000	1.866787000	-3.824170000
H	2.520862000	1.505682000	-4.856448000
C	3.599935000	2.885471000	-3.496405000
H	4.279485000	3.034876000	-4.341221000
H	4.210245000	2.523122000	-2.657936000
C	1.527405000	3.714594000	-2.548524000
H	0.783185000	4.518670000	-2.476821000
H	1.659802000	3.270031000	-1.553426000
C	2.882533000	4.195026000	-3.091309000
H	2.716326000	4.819473000	-3.977894000
H	3.457150000	4.788609000	-2.371566000

²RC_{ls-is}

Fe	1.392527000	-0.359948000	0.344794000
O	1.372555000	0.984606000	-0.579018000
Fe	-1.762552000	0.080533000	-0.106070000
O	-1.025889000	0.241576000	-1.757142000
H	-0.165694000	0.674689000	-1.592871000
O	-0.351533000	-0.655106000	0.777743000
N	1.226191000	-1.744002000	-1.091179000

N	1.657658000	0.525485000	2.107964000
N	3.469883000	-0.562142000	0.067015000
C	1.131405000	-3.012655000	-0.638607000
C	1.056351000	-4.089343000	-1.517146000
H	0.995078000	-5.100475000	-1.126975000
C	1.066270000	-3.842836000	-2.892780000
H	1.014633000	-4.667681000	-3.597257000
C	1.158309000	-2.526774000	-3.345360000
H	1.177543000	-2.291197000	-4.403912000
C	1.241092000	-1.498707000	-2.408401000
H	1.327636000	-0.460016000	-2.695310000
C	1.634481000	-0.300413000	3.178647000
C	1.870883000	0.181806000	4.462515000
H	1.865365000	-0.501477000	5.306105000
C	2.118417000	1.546782000	4.639872000
H	2.312070000	1.942570000	5.632328000
C	2.122560000	2.387409000	3.526462000
H	2.310904000	3.451257000	3.622412000
C	1.890708000	1.835579000	2.267999000
H	1.880147000	2.420234000	1.355076000
C	4.074579000	-1.631318000	0.607097000
C	5.398686000	-1.954729000	0.311680000
H	5.857072000	-2.831797000	0.758859000
C	6.114357000	-1.131264000	-0.557929000
H	7.146284000	-1.361504000	-0.805281000
C	5.483688000	-0.009423000	-1.102455000
H	6.001949000	0.659907000	-1.780903000
C	4.156204000	0.237076000	-0.768651000
H	3.596034000	1.074063000	-1.167259000
C	1.030512000	-3.177196000	0.860876000
H	1.344287000	-4.182257000	1.171593000
C	1.279681000	-1.742732000	2.884739000
H	0.191277000	-1.814774000	2.824869000
H	1.640462000	-2.410418000	3.677828000
C	3.269839000	-2.423020000	1.611599000
H	3.441718000	-3.498477000	1.480781000
H	3.635331000	-2.167846000	2.613749000
N	1.812598000	-2.121897000	1.553274000
H	-0.017484000	-3.023413000	1.128016000
H	-4.346855000	-5.098272000	-0.630508000
C	-3.827415000	-4.147310000	-0.559696000
C	-3.816742000	-3.441405000	0.648018000
C	-3.170264000	-3.613720000	-1.670193000
C	-3.147611000	-2.222446000	0.704810000
H	-4.318608000	-3.829468000	1.529047000
H	-3.160257000	-4.134542000	-2.621783000
C	-2.533447000	-2.379707000	-1.543587000
N	-2.533392000	-1.711920000	-0.382727000
C	-2.973184000	-1.420815000	1.980464000
H	-2.005376000	-1.882864000	-2.351019000
H	-2.018119000	-1.713881000	2.425520000
H	-3.774680000	-1.633339000	2.699578000
N	-2.876021000	0.030294000	1.677772000
N	-3.545260000	0.808822000	-0.829360000
N	-1.278423000	1.899344000	0.591326000
C	-2.027985000	0.807923000	2.621166000
C	-4.213252000	0.671250000	1.495463000
C	-4.567756000	0.870191000	0.040531000
C	-3.760657000	1.061855000	-2.132444000
C	-1.525449000	2.048436000	1.911873000
C	-0.791773000	2.925282000	-0.118033000
H	-2.568224000	1.063600000	3.542009000
H	-1.164160000	0.183407000	2.858035000
H	-4.184868000	1.656840000	1.974944000
H	-4.988002000	0.091171000	2.011213000
C	-5.863744000	1.177457000	-0.368816000
C	-5.024108000	1.391535000	-2.615019000
H	-2.877287000	0.978539000	-2.756681000
C	-1.295079000	3.256720000	2.561826000
C	-0.515861000	4.159718000	0.468835000
H	-0.621441000	2.734448000	-1.169271000
H	-6.670524000	1.213754000	0.357144000
C	-6.094975000	1.443431000	-1.719272000
H	-5.163410000	1.594201000	-3.671602000
H	-1.521183000	3.355227000	3.619032000

C	-0.776775000	4.329156000	1.828698000
H	-0.113854000	4.962505000	-0.139187000
H	-7.094901000	1.686855000	-2.065611000
H	-0.592839000	5.284320000	2.311860000
H	0.439043000	1.950734000	-3.152704000
H	2.680342000	1.081458000	-3.120585000
C	1.207739000	2.657290000	-3.486661000
H	0.845981000	3.121082000	-4.412910000
C	2.579102000	1.978800000	-3.741481000
H	2.685961000	1.664800000	-4.785069000
C	3.656776000	3.031900000	-3.336022000
H	4.377623000	3.219813000	-4.137860000
H	4.230565000	2.678045000	-2.468517000
C	1.518920000	3.760608000	-2.460609000
H	0.737720000	4.530253000	-2.406291000
H	1.636156000	3.310533000	-1.466174000
C	2.869580000	4.305737000	-2.950921000
H	2.707990000	4.928322000	-3.839745000
H	3.391173000	4.918614000	-2.207340000

²RC_{ls-ls}

Fe	1.399451000	-0.331699000	0.352731000
O	1.410150000	0.947008000	-0.694627000
Fe	-1.760567000	0.169002000	-0.073316000
O	-1.034025000	0.255198000	-1.709618000
H	-0.145016000	0.649344000	-1.567475000
O	-0.302800000	-0.422784000	0.904082000
N	1.067696000	-1.814160000	-0.966219000
N	1.838034000	0.680436000	2.003364000
N	3.433416000	-0.691806000	-0.033028000
C	0.933788000	-3.031363000	-0.397316000
C	0.775520000	-4.179169000	-1.168721000
H	0.681653000	-5.146136000	-0.684506000
C	0.747840000	-4.060891000	-2.560635000
H	0.633708000	-4.943077000	-3.183638000
C	0.885750000	-2.797548000	-3.135790000
H	0.881294000	-2.661177000	-4.211903000
C	1.050168000	-1.693917000	-2.300666000
H	1.171936000	-0.691406000	-2.686522000
C	1.807064000	-0.044825000	3.143574000
C	2.128693000	0.529809000	4.369647000
H	2.116163000	-0.075255000	5.270984000
C	2.468481000	1.885640000	4.414440000
H	2.726892000	2.353095000	5.359870000
C	2.482203000	2.623341000	3.230125000
H	2.744574000	3.675830000	3.223636000
C	2.165424000	1.979556000	2.035249000
H	2.161244000	2.478869000	1.072844000
C	4.008702000	-1.741283000	0.573703000
C	5.297259000	-2.164649000	0.248757000
H	5.731249000	-3.022335000	0.754104000
C	6.009654000	-1.464674000	-0.725184000
H	7.014330000	-1.773842000	-0.997382000
C	5.411263000	-0.361966000	-1.340585000
H	5.929345000	0.213993000	-2.100046000
C	4.118172000	-0.009967000	-0.968808000
H	3.586348000	0.824038000	-1.411147000
C	0.894615000	-3.056434000	1.114498000
H	1.156113000	-4.050838000	1.499797000
C	1.347734000	-1.480066000	2.992983000
H	0.255472000	-1.482415000	2.994084000
H	1.710082000	-2.103547000	3.820586000
C	3.215090000	-2.397523000	1.680166000
H	3.309846000	-3.489064000	1.625911000
H	3.653334000	-2.093248000	2.638464000
N	1.779145000	-2.002953000	1.672762000
H	-0.125848000	-2.806605000	1.414560000
H	-4.166802000	-5.122597000	-0.241103000
C	-3.676602000	-4.153655000	-0.237543000
C	-3.696697000	-3.360783000	0.914494000
C	-3.027895000	-3.682235000	-1.380549000
C	-3.065219000	-2.120482000	0.885826000
H	-4.194691000	-3.697790000	1.818444000
H	-2.994509000	-4.269834000	-2.291754000
C	-2.430737000	-2.423317000	-1.341312000

N	-2.455834000	-1.673019000	-0.232313000	H	2.972782000	2.474306000	-0.099658000
C	-2.930637000	-1.228767000	2.105686000	C	4.267015000	-1.666228000	0.422624000
H	-1.915428000	-1.973078000	-2.182999000	C	5.650212000	-1.853086000	0.407130000
H	-1.981388000	-1.475610000	2.589773000	H	6.130950000	-2.422773000	1.197083000
H	-3.742983000	-1.409568000	2.821100000	C	6.392792000	-1.304329000	-0.638492000
N	-2.852134000	0.205430000	1.718575000	H	7.470096000	-1.436229000	-0.674406000
N	-3.577315000	0.746316000	-0.834701000	C	5.729128000	-0.586273000	-1.636855000
N	-1.270903000	2.012716000	0.534068000	H	6.267486000	-0.149246000	-2.471291000
C	-2.022153000	1.043251000	2.627677000	C	4.349175000	-0.433397000	-1.536801000
C	-4.196274000	0.818434000	1.501320000	H	3.770609000	0.123063000	-2.265371000
C	-4.590595000	0.838071000	0.044145000	C	0.988224000	-2.740493000	1.573990000
C	-3.824432000	0.858450000	-2.151205000	H	1.155081000	-3.562539000	2.284930000
C	-1.486199000	2.227565000	1.851071000	C	1.974597000	-0.814551000	2.775248000
C	-0.744223000	2.983883000	-0.223503000	H	0.914189000	-0.573439000	2.904619000
H	-2.587085000	1.364838000	3.512255000	H	2.350351000	-1.279216000	3.698535000
H	-1.169235000	0.435757000	2.935413000	C	3.406362000	-2.335833000	1.474816000
H	-4.149255000	1.856725000	1.850190000	H	3.280580000	-3.383961000	1.175953000
H	-4.953416000	0.310815000	2.111410000	H	3.932398000	-2.348838000	2.438938000
C	-5.907325000	1.029372000	-0.368298000	N	2.064264000	-1.729836000	1.622439000
C	-5.111191000	1.068389000	-2.639952000	H	0.058750000	-2.226527000	1.830929000
H	-2.949060000	0.766593000	-2.784894000	H	-3.805739000	-5.310232000	0.520088000
C	-1.184876000	3.447651000	2.447024000	C	-3.391875000	-4.317569000	0.368879000
C	-0.395507000	4.224614000	0.309022000	C	-3.301150000	-3.422746000	1.438813000
H	-0.600925000	2.745059000	-1.268731000	C	-2.960512000	-3.912974000	-0.895589000
H	-6.704765000	1.092715000	0.365963000	C	-2.775234000	-2.152392000	1.210815000
C	-6.171488000	1.147281000	-1.733994000	H	-3.642093000	-3.699277000	2.431955000
H	-5.275305000	1.159624000	-3.708394000	H	-3.025312000	-4.574528000	-1.752775000
H	-1.388224000	3.599866000	3.502543000	C	-2.454802000	-2.622318000	-1.044055000
C	-0.624056000	4.461795000	1.663947000	N	-2.360278000	-1.774446000	-0.011957000
H	0.037241000	4.979234000	-0.338090000	C	-2.593534000	-1.133515000	2.320017000
H	-7.188164000	1.299025000	-2.083757000	H	-2.116010000	-2.235448000	-1.999849000
H	-0.383106000	5.424295000	2.105598000	H	-1.551502000	-1.170118000	2.655375000
H	0.222465000	1.968458000	-3.211667000	H	-3.233200000	-1.389249000	3.177972000
H	2.379097000	0.920641000	-3.176654000	N	-2.841500000	0.232956000	1.837073000
C	1.039377000	2.578531000	-3.614289000	N	-3.888133000	0.505999000	-0.729489000
H	0.682842000	3.036219000	-4.545866000	N	-1.855697000	2.369976000	0.463640000
C	2.318294000	1.750877000	-3.889008000	C	-2.128258000	1.276415000	2.603041000
H	2.320190000	1.321597000	-4.896637000	C	-4.281624000	0.535084000	1.680055000
C	3.513703000	2.727645000	-3.662306000	C	-4.788841000	0.395885000	0.257425000
H	4.144677000	2.822840000	-4.551483000	C	-4.299708000	0.480223000	-2.008734000
H	4.159710000	2.362692000	-2.852248000	C	-2.068714000	2.548144000	1.781902000
C	1.518194000	3.686888000	-2.660397000	C	-1.787143000	3.429312000	-0.353377000
H	0.818655000	4.530290000	-2.591282000	H	-2.591108000	1.468066000	3.581967000
H	1.660023000	3.264805000	-1.656699000	H	-1.105188000	0.915961000	2.754348000
C	2.877904000	4.080882000	-3.259625000	H	-4.449063000	1.574759000	1.987385000
H	2.714206000	4.696275000	-4.152852000	H	-4.883620000	-0.088247000	2.355539000
H	3.507473000	4.657419000	-2.572775000	C	-6.150829000	0.240086000	-0.002344000
I²TS_{Hhs-hs}				C	-5.642817000	0.345477000	-2.352698000
Fe	1.498581000	-0.330829000	-0.162171000	H	-3.508112000	0.563227000	-2.746654000
O	1.430009000	0.459769000	-1.724988000	C	-2.220419000	3.819111000	2.329066000
Fe	-1.688583000	0.311351000	-0.235587000	C	-1.922607000	4.734381000	0.119404000
O	-1.309326000	0.521025000	-2.019203000	H	-1.618155000	3.202358000	-1.400166000
H	-0.327591000	0.510643000	-2.123089000	H	-6.854895000	0.145875000	0.819376000
O	-0.110308000	-0.053101000	0.608178000	C	-6.584259000	0.216554000	-1.328640000
N	0.999193000	-2.353821000	-0.813081000	H	-5.939229000	0.334732000	-3.396332000
N	2.559126000	0.974830000	1.248519000	H	-2.405648000	3.934878000	3.392570000
N	3.637205000	-0.959682000	-0.526958000	C	-2.141063000	4.930421000	1.483434000
C	0.846951000	-3.269571000	0.161564000	H	-1.864984000	5.570451000	-0.569369000
C	0.553645000	-4.598998000	-0.131156000	H	-7.639187000	0.098756000	-1.558121000
H	0.450996000	-5.322459000	0.671763000	H	-2.261024000	5.932291000	1.884905000
C	0.407424000	-4.977245000	-1.469291000	H	-0.210956000	2.583488000	-3.053042000
H	0.189649000	-6.010293000	-1.724214000	H	1.751907000	1.329267000	-2.641484000
C	0.558231000	-4.016743000	-2.471144000	C	0.713449000	3.166528000	-3.136705000
H	0.459573000	-4.274366000	-3.520488000	H	0.593970000	3.878097000	-3.968260000
C	0.857620000	-2.706588000	-2.097198000	C	1.930267000	2.285711000	-3.395108000
H	0.995834000	-1.905359000	-2.816325000	H	2.016974000	1.835059000	-4.388659000
C	2.711291000	0.479171000	2.491717000	C	3.163356000	3.018436000	-2.849674000
C	3.462151000	1.149114000	3.454627000	H	3.832917000	3.326877000	-3.661788000
H	3.579811000	0.722087000	4.445868000	H	3.753909000	2.360621000	-2.196616000
C	4.056935000	2.369213000	3.119114000	C	1.105596000	3.914145000	-1.850146000
H	4.648977000	2.909114000	3.852070000	H	0.503639000	4.809745000	-1.664364000
C	3.886873000	2.877550000	1.830339000	H	0.979915000	3.237489000	-0.994454000
H	4.335436000	3.818627000	1.529800000	C	2.596251000	4.238666000	-2.071707000
C	3.131459000	2.140015000	0.919543000	H	2.683635000	5.138356000	-2.691145000
				H	3.136337000	4.438426000	-1.138625000

I-¹⁰TS_{Hhs-hs}

Fe	1.512775000	-0.317079000	-0.148944000
O	1.419936000	0.492954000	-1.698697000
Fe	-1.704193000	0.305168000	-0.224522000
O	-1.305118000	0.493559000	-2.004343000
H	-0.322996000	0.505859000	-2.101368000
O	-0.109836000	-0.050579000	0.683006000
N	0.994926000	-2.332752000	-0.814348000
N	2.598545000	0.971591000	1.261047000
N	3.640446000	-0.951362000	-0.551438000
C	0.857724000	-3.257070000	0.154802000
C	0.564605000	-4.584942000	-0.145376000
H	0.474646000	-5.315194000	0.652890000
C	0.402094000	-4.952780000	-1.484490000
H	0.184537000	-5.984460000	-1.745088000
C	0.535654000	-3.983299000	-2.480102000
H	0.423231000	-4.232247000	-3.530162000
C	0.836140000	-2.675502000	-2.099092000
H	0.961361000	-1.868540000	-2.814084000
C	2.759933000	0.464894000	2.498589000
C	3.519008000	1.126047000	3.461234000
H	3.644027000	0.690485000	4.447831000
C	4.111577000	2.348791000	3.131759000
H	4.709638000	2.881998000	3.864737000
C	3.931136000	2.869008000	1.849042000
H	4.377185000	3.812898000	1.553622000
C	3.168186000	2.139757000	0.938094000
H	3.000344000	2.483480000	-0.076441000
C	4.280410000	-1.670664000	0.381987000
C	5.661758000	-1.867740000	0.340807000
H	6.151310000	-2.447663000	1.117787000
C	6.390920000	-1.315920000	-0.712433000
H	7.466412000	-1.455712000	-0.767570000
C	5.716182000	-0.584453000	-1.693556000
H	6.243743000	-0.144466000	-2.533301000
C	4.339471000	-0.422172000	-1.569051000
H	3.753925000	0.144050000	-2.284247000
C	1.014649000	-2.738711000	1.569130000
H	1.184303000	-3.566031000	2.273198000
C	2.021400000	-0.828452000	2.776916000
H	0.963558000	-0.582261000	2.914829000
H	2.403434000	-1.303854000	3.692043000
C	3.434337000	-2.341467000	1.445364000
H	3.303184000	-3.388982000	1.146502000
H	3.975354000	-2.357047000	2.401105000
N	2.096281000	-1.733349000	1.614402000
H	0.090744000	-2.219043000	1.835409000
H	-3.791346000	-5.325370000	0.546958000
C	-3.382595000	-4.331279000	0.391248000
C	-3.295679000	-3.431445000	1.457415000
C	-2.954051000	-3.929989000	-0.875204000
C	-2.776412000	-2.159520000	1.223685000
H	-3.634399000	-3.705498000	2.451981000
H	-3.015935000	-4.595649000	-1.729417000
C	-2.455064000	-2.637409000	-1.029554000
N	-2.364183000	-1.784663000	-0.001316000
C	-2.597711000	-1.133718000	2.326198000
H	-2.118630000	-2.253210000	-1.987198000
H	-1.550914000	-1.154901000	2.646830000
H	-3.226820000	-1.391196000	3.191324000
N	-2.865641000	0.227278000	1.836444000
N	-3.894905000	0.486707000	-0.738817000
N	-1.889645000	2.367966000	0.456597000
C	-2.167439000	1.283408000	2.599504000
C	-4.308430000	0.508189000	1.670488000
C	-4.802566000	0.376044000	0.242006000
C	-4.297161000	0.464402000	-2.021370000
C	-2.117080000	2.550891000	1.772006000
C	-1.820289000	3.423914000	-0.364827000
H	-2.636271000	1.474436000	3.575584000
H	-1.140506000	0.935328000	2.752019000
H	-4.496083000	1.541370000	1.988144000
H	-4.906192000	-0.132444000	2.333361000
C	-6.162887000	0.223461000	-0.028876000
C	-5.637696000	0.332215000	-2.375197000

H	-3.500532000	0.548071000	-2.753611000
C	-2.284988000	3.823489000	2.310702000
C	-1.970902000	4.730121000	0.099635000
H	-1.638014000	3.193590000	-1.408670000
H	-6.873090000	0.128912000	0.787506000
C	-6.586750000	0.203102000	-1.358110000
H	-5.926468000	0.323786000	-3.420977000
H	-2.481414000	3.943132000	3.371743000
C	-2.206023000	4.931070000	1.460292000
H	-1.912177000	5.563235000	-0.592628000
H	-7.640201000	0.087640000	-1.595411000
H	-2.338388000	5.933934000	1.855335000
H	-0.201942000	2.596758000	-3.028737000
H	1.761904000	1.354686000	-2.608841000
C	0.719247000	3.185942000	-3.105499000
H	0.598172000	3.902328000	-3.932750000
C	1.941157000	2.313440000	-3.365379000
H	2.030836000	1.861446000	-4.358064000
C	3.169163000	3.050999000	-2.816754000
H	3.833080000	3.371605000	-3.628948000
H	3.768315000	2.392973000	-2.171773000
C	1.103932000	3.925984000	-1.812211000
H	0.496801000	4.816885000	-1.621195000
H	0.979947000	3.241674000	-0.962387000
C	2.593492000	4.260498000	-2.027976000
H	2.677483000	5.166476000	-2.638627000
H	3.130374000	4.454230000	-1.091909000

I-⁸TS_{Hhs-is}

Fe	1.648001000	-0.213256000	-0.052757000
O	1.586945000	0.632095000	-1.602663000
Fe	-1.585844000	0.196171000	-0.264977000
O	-1.134751000	0.354768000	-2.041866000
H	-0.154811000	0.463080000	-2.073531000
O	-0.010932000	-0.002440000	0.650548000
N	1.166006000	-2.097084000	-0.709760000
N	2.337924000	1.184956000	1.300909000
N	3.654945000	-0.798832000	-0.392231000
C	1.138829000	-3.075560000	0.215622000
C	0.978467000	-4.408957000	-0.151886000
H	0.971258000	-5.181212000	0.610999000
C	0.835871000	-4.727417000	-1.504859000
H	0.721373000	-5.762122000	-1.814181000
C	0.852432000	-3.701302000	-2.450637000
H	0.748107000	-3.906328000	-3.510887000
C	1.023343000	-2.389716000	-2.010904000
H	1.053495000	-1.538750000	-2.681131000
C	2.370450000	0.817293000	2.596852000
C	2.839594000	1.685642000	3.579829000
H	2.872703000	1.362185000	4.615830000
C	3.265195000	2.964306000	3.208859000
H	3.635419000	3.656698000	3.958976000
C	3.219397000	3.332881000	1.863250000
H	3.546337000	4.313107000	1.532689000
C	2.751969000	2.405513000	0.934373000
H	2.696328000	2.617175000	-0.125965000
C	4.282493000	-1.582918000	0.501039000
C	5.569729000	-2.072228000	0.270552000
H	6.044482000	-2.707950000	1.012317000
C	6.226883000	-1.730163000	-0.909241000
H	7.229239000	-2.097872000	-1.107056000
C	5.571208000	-0.910007000	-1.831147000
H	6.041587000	-0.619112000	-2.764391000
C	4.285100000	-0.471935000	-1.537374000
H	3.706111000	0.146972000	-2.212130000
C	1.227049000	-2.630947000	1.662210000
H	1.498525000	-3.479833000	2.306139000
C	1.828866000	-0.564379000	2.911602000
H	0.739106000	-0.490347000	2.957786000
H	2.205499000	-0.912208000	3.884136000
C	3.577137000	-1.890296000	1.806813000
H	3.683181000	-2.959061000	2.037233000
H	4.099787000	-1.351425000	2.607311000
N	2.154793000	-1.498808000	1.818811000
H	0.233136000	-2.279540000	1.948275000

H	-3.366836000	-5.530171000	0.719032000	C	2.353123000	0.733698000	2.630066000
C	-3.006689000	-4.523563000	0.527968000	C	2.826527000	1.584461000	3.626427000
C	-2.973436000	-3.579659000	1.558765000	H	2.862956000	1.242418000	4.656339000
C	-2.590003000	-4.148132000	-0.749926000	C	3.252273000	2.869137000	3.277261000
C	-2.517006000	-2.293213000	1.278082000	H	3.625706000	3.547468000	4.038556000
H	-3.308967000	-3.830809000	2.560489000	C	3.202544000	3.261846000	1.938688000
H	-2.614157000	-4.846868000	-1.579436000	H	3.529561000	4.247511000	1.624761000
C	-2.152783000	-2.838937000	-0.949494000	C	2.731345000	2.351827000	0.994697000
N	-2.108889000	-1.944162000	0.044310000	H	2.672416000	2.581735000	-0.061712000
C	-2.423850000	-1.209137000	2.333832000	C	4.236459000	-1.662438000	0.485701000
H	-1.828286000	-2.477289000	-1.919585000	C	5.512459000	-2.169710000	0.232953000
H	-1.381823000	-1.128430000	2.661016000	H	5.982872000	-2.826649000	0.958802000
H	-3.037554000	-1.474955000	3.207826000	C	6.163942000	-1.818097000	-0.946960000
N	-2.797071000	0.097545000	1.774192000	H	7.157555000	-2.199593000	-1.161955000
N	-3.767575000	0.148754000	-0.845629000	C	5.513282000	-0.969521000	-1.846337000
N	-2.013659000	2.261816000	0.324848000	H	5.978968000	-0.668938000	-2.778850000
C	-2.224739000	1.246507000	2.505538000	C	4.238001000	-0.515012000	-1.531843000
C	-4.254636000	0.230570000	1.551456000	H	3.666462000	0.126571000	-2.190434000
C	-4.689690000	-0.002145000	0.115507000	C	1.182835000	-2.689916000	1.637692000
C	-4.128619000	0.039637000	-2.135557000	H	1.454752000	-3.561030000	2.251037000
C	-2.290830000	2.476935000	1.625299000	C	1.810797000	-0.652248000	2.927186000
C	-2.057341000	3.279830000	-0.543850000	H	0.722127000	-0.576046000	2.986531000
H	-2.729316000	1.427311000	3.465904000	H	2.196221000	-1.015010000	3.890800000
H	-1.171178000	1.009884000	2.690454000	C	3.540522000	-1.976742000	1.794142000
H	-4.552911000	1.250699000	1.823073000	H	3.640449000	-3.048163000	2.015221000
H	-4.808995000	-0.441624000	2.220846000	H	4.073953000	-1.447789000	2.594185000
C	-6.023061000	-0.285966000	-0.183079000	N	2.123736000	-1.572193000	1.818421000
C	-5.441742000	-0.224615000	-2.518033000	H	0.195951000	-2.339763000	1.948795000
H	-3.321227000	0.165998000	-2.850055000	H	-3.549688000	-5.467856000	0.709169000
C	-2.620614000	3.742706000	2.101714000	C	-3.157863000	-4.473498000	0.516302000
C	-2.374851000	4.578158000	-0.145081000	C	-3.086261000	-3.532151000	1.547485000
H	-1.827914000	3.025684000	-1.572404000	C	-2.738355000	-4.110690000	-0.764227000
H	-6.746130000	-0.410180000	0.617956000	C	-2.589168000	-2.261217000	1.265347000
C	-6.404986000	-0.396489000	-1.520668000	H	-3.423059000	-3.773069000	2.551277000
H	-5.698344000	-0.299855000	-3.569541000	H	-2.792149000	-4.807137000	-1.594324000
H	-2.853634000	3.884892000	3.152561000	C	-2.258707000	-2.816651000	-0.965461000
C	-2.657733000	4.812175000	1.200912000	N	-2.177403000	-1.924800000	0.028672000
H	-2.404387000	5.379150000	-0.876079000	C	-2.452416000	-1.183176000	2.322594000
H	-7.437090000	-0.613862000	-1.779395000	H	-1.928886000	-2.466342000	-1.937856000
H	-2.917531000	5.808701000	1.545503000	H	-1.404599000	-1.135685000	2.636776000
H	-0.298603000	2.544377000	-3.058553000	H	-3.065519000	-1.432311000	3.201909000
H	1.755819000	1.488329000	-2.452155000	N	-2.789479000	0.135824000	1.769315000
C	0.568744000	3.211787000	-3.121661000	N	-3.750523000	0.246950000	-0.847529000
H	0.414645000	3.890410000	-3.975841000	N	-1.915044000	2.270941000	0.319495000
C	1.867599000	2.447308000	-3.309916000	C	-2.181226000	1.265924000	2.500225000
H	2.025038000	1.929610000	-4.260440000	C	-4.241924000	0.312957000	1.548988000
C	3.010045000	3.301976000	-2.761952000	C	-4.681522000	0.122306000	0.108119000
H	3.649573000	3.674376000	-3.572340000	C	-4.111045000	0.170725000	-2.139951000
C	3.664485000	2.710521000	-2.104669000	C	-2.199175000	2.495844000	1.616887000
H	0.841178000	4.019412000	-1.839546000	C	-1.913208000	3.289045000	-0.550217000
H	0.160413000	4.865811000	-1.703002000	H	-2.684271000	1.466928000	3.457335000
H	0.730800000	3.353375000	-0.974183000	H	-1.137236000	0.994447000	2.689867000
C	2.310578000	4.463612000	-1.999618000	H	-4.513832000	1.334409000	1.842876000
H	2.351974000	5.374966000	-2.606266000	H	-4.814918000	-0.358500000	2.203226000
H	2.792510000	4.694645000	-1.042225000	C	-6.024941000	-0.099888000	-0.198421000
I-⁴TS_{Hhs-is}				C	-5.432470000	-0.032752000	-2.530416000
Fe	1.623505000	-0.247555000	-0.025807000	H	-3.296285000	0.272355000	-2.850100000
O	1.565403000	0.659588000	-1.548190000	C	-2.491593000	3.772717000	2.088252000
Fe	-1.563537000	0.191974000	-0.267815000	C	-2.191109000	4.597718000	-0.155772000
O	-1.099249000	0.344493000	-2.035091000	H	-1.680422000	3.026369000	-1.576140000
H	-0.119962000	0.484347000	-2.053160000	H	-6.755691000	-0.203888000	0.598550000
O	-0.021865000	-0.052462000	0.702950000	C	-6.406023000	-0.176567000	-1.538452000
N	1.101025000	-2.092433000	-0.723366000	H	-5.688124000	-0.083288000	-3.583638000
N	2.317182000	1.125261000	1.340638000	H	-2.731500000	3.923753000	3.136320000
N	3.612322000	-0.852091000	-0.386459000	C	-2.482504000	4.842007000	1.186565000
C	1.068850000	-3.092264000	0.179748000	H	-2.184174000	5.398719000	-0.887271000
C	0.877180000	-4.412672000	-0.218875000	H	-7.445419000	-0.346413000	-1.803475000
H	0.866620000	-5.203559000	0.524653000	H	-2.712976000	5.846939000	1.527621000
C	0.707805000	-4.694830000	-1.576731000	H	-0.155414000	2.576458000	-3.122891000
H	0.568641000	-5.719260000	-1.909240000	H	1.827366000	1.460390000	-2.411200000
C	0.729355000	-3.646314000	-2.497368000	C	0.736195000	3.214062000	-3.159300000
H	0.603885000	-3.822835000	-3.560433000	H	0.636266000	3.886798000	-4.025906000
C	0.931950000	-2.349509000	-2.028735000	C	2.016132000	2.405412000	-3.285251000
H	0.963161000	-1.482593000	-2.677678000	H	2.195896000	1.868444000	-4.221008000
				C	3.162438000	3.224202000	-2.693407000

H	3.854784000	3.561808000	-3.475166000
H	3.760400000	2.617866000	-1.996723000
C	0.982728000	4.026799000	-1.875169000
H	0.324777000	4.896071000	-1.774452000
H	0.816277000	3.372878000	-1.009910000
C	2.471298000	4.420360000	-1.978663000
H	2.568425000	5.320057000	-2.596193000
H	2.920313000	4.649796000	-1.004996000

I-⁶TS_{His-is}

Fe	1.542521000	-0.330067000	-0.142708000
O	1.577052000	0.813113000	-1.450070000
Fe	-1.656362000	0.283185000	-0.124393000
O	-1.142541000	0.500567000	-1.834504000
H	-0.171121000	0.646409000	-1.865293000
O	-0.066672000	-0.081136000	0.630416000
N	0.852656000	-2.076939000	-1.185999000
N	2.493385000	0.653843000	1.603594000
N	3.552086000	-0.844820000	-0.558990000
C	0.662125000	-3.178951000	-0.439637000
C	0.300426000	-4.396274000	-1.011201000
H	0.170510000	-5.272804000	-0.383867000
C	0.110367000	-4.459604000	-2.394234000
H	-0.162481000	-5.398213000	-2.867648000
C	0.283990000	-3.303860000	-3.157747000
H	0.148037000	-3.311548000	-4.234100000
C	0.661448000	-2.126105000	-2.511766000
H	0.820165000	-1.196658000	-3.046011000
C	2.619445000	-0.116126000	2.697361000
C	3.359750000	0.295547000	3.803666000
H	3.454341000	-0.352944000	4.669574000
C	3.974076000	1.550992000	3.770461000
H	4.559355000	1.896734000	4.617312000
C	3.832852000	2.347541000	2.632681000
H	4.299325000	3.325009000	2.567117000
C	3.085770000	1.852573000	1.563122000
H	2.955819000	2.413465000	0.642076000
C	4.142360000	-1.799434000	0.182690000
C	5.514350000	-2.040418000	0.112006000
H	5.959118000	-2.813417000	0.731598000
C	6.291955000	-1.283113000	-0.763488000
H	7.361711000	-1.454491000	-0.836446000
C	5.671136000	-0.302434000	-1.540017000
H	6.235465000	0.309667000	-2.235504000
C	4.300411000	-0.108962000	-1.401629000
H	3.755172000	0.647930000	-1.954674000
C	0.818401000	-2.982390000	1.052376000
H	0.958934000	-3.945188000	1.563667000
C	1.854797000	-1.423592000	2.658350000
H	0.799916000	-1.197523000	2.843430000
C	2.210491000	-2.108269000	3.441346000
C	3.247810000	-2.660935000	1.044454000
H	3.081800000	-3.604686000	0.510608000
H	3.758020000	-2.917268000	1.982281000
N	1.926903000	-2.044059000	1.320857000
H	-0.096325000	-2.511061000	1.418708000
H	-4.249049000	-5.173568000	0.679787000
C	-3.715687000	-4.243034000	0.509359000
C	-3.476086000	-3.364000000	1.571203000
C	-3.272186000	-3.902813000	-0.769621000
C	-2.798928000	-2.175071000	1.311247000
H	-3.815638000	-3.592440000	2.577026000
H	-3.444977000	-4.556277000	-1.618342000
C	-2.604413000	-2.689262000	-0.942034000
N	-2.373558000	-1.855662000	0.076773000
C	-2.448923000	-1.164288000	2.382802000
H	-2.237185000	-2.361669000	-1.909940000
H	-1.389711000	-1.276301000	2.638316000
H	-3.043564000	-1.332213000	3.291826000
N	-2.614775000	0.212224000	1.873714000
N	-3.634513000	0.528746000	-0.692974000
N	-1.737695000	2.399481000	0.605186000
C	-1.871027000	1.202626000	2.689031000
C	-4.052928000	0.579803000	1.720389000
C	-4.552880000	0.513237000	0.291631000

C	-4.027498000	0.558092000	-1.978104000
C	-1.806496000	2.517455000	1.941970000
C	-1.674209000	3.496372000	-0.157833000
H	-2.319385000	1.331915000	3.684118000
H	-0.852933000	0.813031000	2.794448000
H	-4.183468000	1.610813000	2.069140000
H	-4.677601000	-0.049878000	2.366857000
C	-5.918268000	0.508934000	0.010057000
C	-5.372630000	0.570372000	-2.335126000
H	-3.215806000	0.569814000	-2.698570000
C	-1.810107000	3.760148000	2.571242000
C	-1.662733000	4.779139000	0.390942000
H	-1.625496000	3.322456000	-1.226754000
H	-6.639931000	0.489455000	0.821222000
C	-6.333934000	0.538963000	-1.321975000
H	-5.656497000	0.598406000	-3.381761000
H	-1.882300000	3.826323000	3.652695000
C	-1.729586000	4.910123000	1.779528000
H	-1.611228000	5.648754000	-0.255960000
H	-7.392544000	0.538653000	-1.564118000
H	-1.733174000	5.892965000	2.241424000
H	1.355235000	2.177620000	-1.361503000
H	3.555983000	3.120913000	-1.393731000
C	2.805637000	3.636939000	-2.006602000
H	3.006038000	4.717093000	-1.937668000
C	1.372271000	3.352499000	-1.564664000
H	1.043057000	3.802815000	-0.621514000
C	0.470028000	3.580489000	-2.788501000
H	-0.140678000	4.484474000	-2.661994000
H	-0.224798000	2.740065000	-2.913567000
C	2.798578000	3.192449000	-3.478954000
H	3.648789000	3.576265000	-4.051635000
H	2.815372000	2.095476000	-3.522074000
C	1.441957000	3.715077000	-3.994945000
H	1.540935000	4.771275000	-4.271058000
H	1.089521000	3.175275000	-4.879054000

I-²TS_{His-is}

Fe	-1.626098000	-0.233991000	-0.127820000
O	-1.675087000	0.721215000	1.357143000
Fe	1.603365000	0.183279000	0.189731000
O	0.950392000	0.259331000	1.860703000
H	-0.015057000	0.450335000	1.802366000
O	0.070755000	0.045393000	-0.715448000
N	-1.111593000	-1.908360000	0.846737000
N	-2.247737000	1.087634000	-1.514262000
N	-3.590438000	-0.867246000	0.235890000
C	-0.964780000	-2.973801000	0.030358000
C	-0.774481000	-4.256265000	0.535148000
H	-0.671883000	-5.095890000	-0.144938000
C	-0.718914000	-4.434292000	1.920259000
H	-0.580568000	-5.426269000	2.340075000
C	-0.852489000	-3.322960000	2.753438000
H	-0.818952000	-3.419078000	3.833465000
C	-1.055941000	-2.070089000	2.175509000
H	-1.191055000	-1.168099000	2.759151000
C	-2.138143000	0.634751000	-2.784723000
C	-2.555227000	1.398764000	-3.870299000
H	-2.470417000	0.999619000	-4.876440000
C	-3.089061000	2.670117000	-3.640446000
H	-3.422189000	3.283833000	-4.471928000
C	-3.205746000	3.125371000	-2.327556000
H	-3.629165000	4.098225000	-2.101593000
C	-2.780399000	2.296539000	-1.290081000
H	-2.865634000	2.585359000	-0.252356000
C	-4.099072000	-1.781188000	-0.606507000
C	-5.324455000	-2.402500000	-0.370973000
H	-5.702071000	-3.143693000	-1.069008000
C	-6.049474000	-2.046746000	0.766639000
H	-7.008010000	-2.512813000	0.974052000
C	-5.522612000	-1.084484000	1.631677000
H	-6.054986000	-0.778263000	2.525931000
C	-4.284139000	-0.522947000	1.335246000
H	-3.798607000	0.210958000	1.969142000
C	-0.942332000	-2.657948000	-1.448240000

H	-1.143236000	-3.552388000	-2.051987000	C	0.484372000	-3.255167000	0.087469000
C	-1.520938000	-0.739028000	-2.937256000	C	0.189785000	-4.538825000	-0.367360000
H	-0.435720000	-0.630710000	-2.916368000	H	0.111646000	-5.357068000	0.341927000
H	-1.825230000	-1.211230000	-3.880368000	C	0.010124000	-4.748272000	-1.736570000
C	-3.305298000	-2.037545000	-1.864721000	H	-0.209621000	-5.742320000	-2.114975000
H	-3.329607000	-3.100718000	-2.133891000	C	0.133402000	-3.666576000	-2.610020000
H	-3.787949000	-1.493106000	-2.685042000	H	0.012549000	-3.787580000	-3.681410000
N	-1.895949000	-4.876234000	-1.759261000	C	0.436936000	-2.412461000	-2.082678000
H	0.057107000	-2.281534000	-1.677731000	H	0.546946000	-1.531579000	-2.701259000
H	4.043166000	-5.304677000	-0.870913000	C	2.129616000	0.269077000	2.803846000
C	3.527231000	-4.369649000	-0.673531000	C	2.669403000	0.984994000	3.870873000
C	3.462151000	-3.379507000	-1.659472000	H	2.648727000	0.563400000	4.871408000
C	2.932618000	-4.134968000	0.567374000	C	3.238230000	2.238455000	3.627196000
C	2.800824000	-2.189117000	-1.365820000	H	3.668133000	2.812377000	4.442727000
H	3.921584000	-3.525171000	-2.632557000	C	3.255913000	2.733104000	2.322027000
H	2.969858000	-4.876234000	1.358895000	H	3.693420000	3.697846000	2.087134000
C	2.294836000	-2.911711000	0.779139000	C	2.707772000	1.951554000	1.306471000
N	2.229413000	-1.970906000	-0.168736000	H	2.692731000	2.264959000	0.271266000
C	2.630903000	-1.067309000	-2.369425000	C	3.689000000	-2.275570000	0.381056000
H	1.821056000	-2.661387000	1.723729000	C	4.804589000	-3.035768000	0.027175000
H	1.616449000	-1.114951000	-2.779697000	H	5.184212000	-3.787571000	0.712790000
H	3.337758000	-1.181119000	-3.203875000	C	5.415284000	-2.812695000	-1.206026000
N	2.770939000	0.249583000	-1.717496000	H	6.286118000	-3.390477000	-1.500845000
N	3.537893000	0.256023000	0.958487000	C	4.880535000	-1.842186000	-2.056172000
N	1.850762000	2.354405000	-0.339322000	H	5.316268000	-1.640193000	-3.028926000
C	2.149340000	1.337607000	-2.505406000	C	3.757288000	-1.136476000	-1.637630000
C	4.192110000	0.548189000	-1.379494000	H	3.274403000	-0.392573000	-2.256824000
C	4.546135000	0.272937000	0.066685000	C	0.628843000	-2.934103000	1.562216000
C	3.804151000	0.117305000	2.268317000	H	0.818486000	-3.854431000	2.134030000
C	2.033982000	2.582120000	-1.650511000	C	1.439165000	-1.069765000	2.981637000
C	1.716098000	3.386009000	0.501597000	H	0.363523000	-0.885175000	3.042101000
H	2.704678000	1.543808000	-3.431586000	H	1.769165000	-1.553226000	3.912523000
H	1.138302000	1.000270000	-2.755049000	C	3.043387000	-2.438633000	1.740927000
H	4.369946000	1.614130000	-1.562507000	H	3.077393000	-3.493310000	2.048781000
H	4.868908000	-0.001445000	-2.046691000	H	3.651472000	-1.882727000	2.465418000
C	5.873502000	0.127889000	0.466742000	N	1.665658000	-1.916219000	1.797978000
C	5.105571000	-0.015029000	2.744900000	H	-0.322882000	-2.506209000	1.890442000
H	2.927912000	0.115299000	2.908848000	H	-4.413506000	-4.781445000	0.888445000
C	2.094048000	3.872526000	-2.172415000	C	-3.892454000	-3.856802000	0.658867000
C	1.748941000	4.709620000	0.061347000	C	-3.745859000	-2.870776000	1.639762000
H	1.573618000	3.126944000	1.544230000	C	-3.374645000	-3.631481000	-0.617775000
H	6.668019000	0.137102000	-0.273404000	C	-3.078684000	-1.693426000	1.313206000
C	6.157467000	-0.017024000	1.825855000	H	-4.147305000	-3.009548000	2.638904000
H	5.286112000	-0.119707000	3.809471000	H	-3.476312000	-4.369911000	-1.405684000
H	2.263282000	4.026384000	-3.234034000	C	-2.730145000	-2.422975000	-0.875791000
C	1.940863000	4.954219000	-1.299937000	N	-2.584343000	-1.490495000	0.073442000
H	1.637578000	5.523311000	0.770505000	C	-2.795908000	-0.592635000	2.317182000
H	7.184455000	-0.128420000	2.160829000	H	-2.308665000	-2.161000000	-1.839431000
H	1.984833000	5.971640000	-1.677225000	H	-1.801745000	-0.768824000	2.736595000
H	-1.542347000	1.950941000	1.398205000	H	-3.528178000	-0.605040000	3.134572000
H	-3.705761000	3.061136000	1.616634000	N	-2.745759000	0.733357000	1.646810000
C	-2.920943000	3.451376000	2.277854000	N	-3.669136000	0.812641000	-0.900263000
H	-3.088319000	4.535507000	2.378815000	N	-1.265175000	2.229623000	-0.007541000
C	-1.503636000	3.195584000	1.777649000	C	-1.827406000	1.714488000	2.289906000
H	-1.158224000	3.742574000	0.894479000	C	-4.100501000	1.321947000	1.428514000
C	-0.583091000	3.184437000	3.002306000	C	-4.602686000	1.113321000	0.018920000
H	0.073572000	4.065499000	3.006486000	C	-4.018783000	0.697253000	-2.193305000
H	0.070199000	2.302451000	2.987982000	C	-1.391498000	2.719246000	1.245565000
C	-2.912913000	2.788185000	3.666497000	C	-0.847085000	3.026578000	-0.997912000
H	-3.743975000	3.108125000	4.302811000	H	-2.295545000	2.205400000	3.152769000
H	-2.967459000	1.698821000	3.541445000	H	-0.941566000	1.160954000	2.608028000
C	-1.533556000	3.179822000	4.231752000	H	-4.031093000	2.401736000	1.605677000
H	-1.589208000	4.188116000	4.658375000	H	-4.812923000	0.925461000	2.162177000
H	-1.192000000	2.505648000	5.023298000	C	-5.940496000	1.297440000	-0.325107000
I-⁴TS_{HLS-is}				C	-5.331708000	0.882612000	-2.616982000
Fe	1.302135000	-0.437468000	0.040104000	H	-3.201279000	0.446620000	-2.860783000
O	1.368436000	0.708301000	-1.330607000	C	-1.109167000	4.049832000	1.537411000
Fe	-1.810284000	0.314339000	-0.187917000	C	-0.537470000	4.368054000	-0.779745000
O	-1.212880000	0.059291000	-1.858271000	H	-0.769933000	2.557667000	-1.970875000
H	-0.293027000	0.421065000	-1.881915000	H	-6.672620000	1.533313000	0.441358000
O	-0.294398000	-0.124155000	0.786244000	C	-6.310340000	1.181525000	-1.665772000
N	0.599760000	-2.220723000	-0.766103000	H	-5.579338000	0.787198000	-3.668855000
N	2.161374000	0.753066000	1.547910000	H	-1.237103000	4.421951000	2.549197000
N	3.180980000	-1.339161000	-0.439251000	C	-0.672075000	4.888162000	0.507398000
				H	-0.198534000	4.983478000	-1.605202000

H	-7.345380000	1.322238000	-1.962274000
H	-0.450815000	5.932253000	0.707433000
H	1.118434000	3.454898000	-3.042731000
H	2.083595000	1.427444000	-2.040656000
C	2.209001000	3.497284000	-2.937490000
H	2.601716000	3.993880000	-3.838242000
C	2.848149000	2.122049000	-2.804028000
H	2.891453000	1.517388000	-3.715628000
C	4.156463000	2.289863000	-2.022513000
H	5.028498000	2.094067000	-2.659154000
H	4.213564000	1.570801000	-1.194493000
C	2.688000000	4.239909000	-1.678274000
H	2.614453000	5.329226000	-1.766288000
H	2.072492000	3.933853000	-0.823623000
C	4.143604000	3.756315000	-1.505645000
H	4.806297000	4.370184000	-2.125266000
H	4.499047000	3.838959000	-0.472005000

I⁻²TS_{Hls-is}

Fe	-1.290734000	0.471625000	0.031276000
O	-1.351459000	-0.673556000	-1.333523000
Fe	1.808714000	-0.240618000	-0.214799000
O	1.217202000	0.076291000	-1.898081000
H	0.312401000	-0.308076000	-1.947970000
O	0.359953000	0.320737000	0.741303000
N	-0.689745000	2.302383000	-0.766935000
N	-1.959526000	-0.806678000	1.555893000
N	-3.219983000	1.298122000	-0.391850000
C	-0.594390000	3.324273000	0.102887000
C	-0.291717000	4.614703000	-0.328792000
H	-0.231737000	5.424381000	0.392165000
C	-0.074826000	4.841058000	-1.689739000
H	0.155021000	5.839791000	-2.049310000
C	-0.171760000	3.770039000	-2.579513000
H	-0.019368000	3.903747000	-3.645335000
C	-0.490263000	2.510004000	-2.075777000
H	-0.580431000	1.637402000	-2.708887000
C	-1.937676000	-0.333035000	2.816078000
C	-2.361192000	-1.115216000	3.889400000
H	-2.353884000	-0.703982000	4.894446000
C	-2.796192000	-2.421498000	3.647250000
H	-3.135338000	-3.046022000	4.468410000
C	-2.796472000	-2.905246000	2.337587000
H	-3.128119000	-3.911603000	2.104226000
C	-2.370824000	-2.058291000	1.316253000
H	-2.343380000	-2.357003000	0.276837000
C	-3.750768000	2.196520000	0.456624000
C	-4.882788000	2.941985000	0.126406000
H	-5.279742000	3.662140000	0.835630000
C	-5.486150000	2.746201000	-1.115375000
H	-6.369177000	3.313688000	-1.393405000
C	-4.926448000	1.818483000	-1.996199000
H	-5.353498000	1.641051000	-2.977572000
C	-3.787781000	1.125178000	-1.598523000
H	-3.285338000	0.418525000	-2.244279000
C	-0.735991000	2.993211000	1.577184000
H	-0.996573000	3.899401000	2.143428000
C	-1.375425000	1.064941000	2.995647000
H	-0.286927000	0.980131000	3.047063000
H	-1.736689000	1.506140000	3.935934000
C	-3.104798000	2.322786000	1.818170000
H	-3.213629000	3.349389000	2.196258000
H	-3.657423000	1.673290000	2.508495000
N	-1.692563000	1.900795000	1.825504000
H	0.245260000	2.644333000	1.912027000
H	4.593584000	4.748896000	0.856404000
C	4.047887000	3.838086000	0.628760000
C	3.891524000	2.850324000	1.606668000
C	3.502958000	3.635856000	-0.640598000
C	3.190271000	1.692439000	1.283093000
H	4.306638000	2.975753000	2.601980000
H	3.607008000	4.379670000	-1.423210000
C	2.828548000	2.443480000	-0.898543000
N	2.682047000	1.506566000	0.047071000
C	2.866509000	0.603668000	2.287348000

H	2.380277000	2.196552000	-1.854575000
H	1.886526000	0.830527000	2.716237000
H	3.605242000	0.576052000	3.098501000
N	2.742721000	-0.713110000	1.610913000
N	3.617795000	-0.882934000	-0.952425000
N	1.184673000	-2.138990000	-0.051259000
C	1.775013000	-1.648876000	2.247372000
C	4.064506000	-1.370565000	1.381123000
C	4.545954000	-1.230042000	-0.044566000
C	3.948206000	-0.815072000	-2.253947000
C	1.300248000	-2.634642000	1.200954000
C	0.746058000	-2.923319000	-1.043264000
H	2.212365000	-2.162616000	3.113264000
H	0.915873000	-1.052114000	2.560463000
H	3.954188000	-2.439572000	1.598326000
H	4.810960000	-0.981474000	2.084026000
C	5.860050000	-1.515422000	-0.410182000
C	5.236003000	-1.101144000	-2.698406000
H	3.135958000	-0.514031000	-2.907178000
C	0.978216000	-3.956738000	1.491864000
C	0.404172000	-4.257118000	-0.827282000
H	0.677648000	-2.450810000	-2.014928000
H	6.589554000	-1.787439000	0.346817000
C	6.209828000	-1.451474000	-1.759729000
H	5.469159000	-1.041284000	-3.756189000
H	1.094841000	-4.332870000	2.503466000
C	0.521229000	-4.781657000	0.460194000
H	0.054384000	-4.864456000	-1.654056000
H	7.226417000	-1.670246000	-2.072383000
H	0.272549000	-5.820074000	0.657918000
H	-1.287761000	-3.473358000	-3.023573000
H	-2.115562000	-1.406359000	-1.987330000
C	-2.377804000	-3.476006000	-2.903893000
H	-2.799263000	-3.895744000	-3.829792000
C	-2.955333000	-2.082677000	-2.680275000
H	-3.059583000	-1.464584000	-3.577857000
C	-4.200363000	-2.221205000	-1.792770000
H	-5.104066000	-1.865797000	-2.302472000
H	-4.096263000	-1.608893000	-0.886928000
C	-2.872720000	-4.287659000	-1.693369000
H	-2.871172000	-5.367829000	-1.874767000
H	-2.221757000	-4.099374000	-0.830769000
C	-4.288009000	-3.730597000	-1.440329000
H	-4.995980000	-4.223585000	-2.115959000
H	-4.639128000	-3.903151000	-0.416727000

I⁻²TS_{Hls-ls}

Fe	-1.310526000	0.547076000	0.118546000
O	-1.311964000	-0.353167000	-1.462183000
Fe	1.799678000	-0.323691000	-0.252482000
O	1.252337000	0.091294000	-1.907212000
H	0.314057000	-0.216260000	-1.962708000
O	0.311658000	0.126769000	0.736932000
N	-0.604010000	2.238329000	-0.717648000
N	-2.021313000	-0.815027000	1.392395000
N	-3.153878000	1.468623000	-0.331391000
C	-0.389720000	3.223280000	0.178659000
C	-0.018669000	4.503392000	-0.223381000
H	0.136461000	5.280875000	0.518234000
C	0.140946000	4.761374000	-1.587695000
H	0.421664000	5.753884000	-1.927863000
C	-0.080890000	3.732617000	-2.504228000
H	0.022751000	3.895482000	-3.571814000
C	-0.462354000	2.479209000	-2.026804000
H	-0.670481000	1.637133000	-2.673920000
C	-1.942282000	-0.462245000	2.695602000
C	-2.346649000	-1.328418000	3.707584000
H	-2.294875000	-1.010537000	4.744486000
C	-2.810669000	-2.602973000	3.366510000
H	-3.135435000	-3.292268000	4.140172000
C	-2.843714000	-2.972332000	2.021964000
H	-3.180669000	-3.954210000	1.707389000
C	-2.439974000	-2.043274000	1.066031000
H	-2.422868000	-2.266629000	0.012464000
C	-3.615301000	2.354077000	0.568662000

C	-4.690773000	3.197821000	0.297417000
H	-5.030147000	3.903754000	1.049395000
C	-5.310957000	3.116266000	-0.949780000
H	-6.153314000	3.758894000	-1.187394000
C	-4.817529000	2.208886000	-1.889611000
H	-5.256692000	2.125771000	-2.878140000
C	-3.728477000	1.414057000	-1.544901000
H	-3.263225000	0.726765000	-2.236409000
C	-0.502608000	2.828173000	1.636383000
H	-0.683140000	3.705571000	2.271418000
C	-1.297495000	0.879400000	2.972802000
H	-0.219095000	0.721098000	3.030845000
H	-1.647375000	1.306209000	3.922136000
C	-2.927041000	2.342358000	1.909161000
H	-2.915736000	3.344712000	2.356039000
C	-3.506950000	1.699399000	2.582027000
N	-1.546720000	1.789150000	1.829780000
H	0.449322000	2.369662000	1.917190000
H	4.714391000	4.507429000	1.158315000
C	4.132695000	3.636264000	0.872163000
C	3.955560000	2.582505000	1.774746000
C	3.562403000	3.549361000	-0.399000000
C	3.211028000	1.475899000	1.376267000
H	4.390459000	2.616498000	2.768938000
H	3.681398000	4.346142000	-1.125343000
C	2.840702000	2.404802000	-0.733707000
N	2.674659000	1.403136000	0.139361000
C	2.875755000	0.323375000	2.304007000
H	2.371645000	2.246828000	-1.698602000
H	1.908361000	0.539866000	2.765025000
H	3.624536000	0.226668000	3.100751000
N	2.714582000	-0.944868000	1.547005000
C	3.646729000	-0.884814000	-0.996145000
N	1.118035000	-2.210627000	-0.197896000
C	1.726323000	-1.892608000	2.129031000
C	4.015408000	-1.622654000	1.275812000
C	4.554554000	-1.303781000	-0.098192000
C	4.019978000	-0.671010000	-2.269546000
C	1.199569000	-2.783438000	1.023377000
C	0.623811000	-2.905709000	-1.229701000
H	2.158503000	-2.482504000	2.947851000
H	0.890765000	-1.295888000	2.499456000
H	3.845707000	-2.704631000	1.326700000
H	4.747081000	-1.378063000	2.055777000
C	5.889013000	-1.511245000	-0.440603000
C	5.330877000	-0.873002000	-2.693594000
H	3.224035000	-0.326193000	-2.920887000
C	0.790129000	-4.095334000	1.240416000
C	0.187751000	-4.222629000	-1.086576000
H	0.589814000	-2.374999000	-2.173165000
H	6.599445000	-1.843160000	0.310530000
C	6.283023000	-1.292853000	-1.761795000
H	5.597513000	-0.695771000	-3.730133000
H	0.883815000	-4.535208000	2.228457000
C	0.273363000	-4.827041000	0.167533000
H	-0.204180000	-4.757862000	-1.943653000
H	7.316145000	-1.448027000	-2.057841000
H	-0.044845000	-5.855811000	0.307670000
H	-1.610229000	-3.273204000	-2.973184000
H	-2.212008000	-1.171989000	-1.806464000
C	-2.692368000	-3.197927000	-2.818276000
H	-3.169310000	-3.485967000	-3.767061000
C	-3.144901000	-1.786822000	-2.457965000
H	-3.217856000	-1.110208000	-3.315171000
C	-4.410027000	-1.904906000	-1.598555000
H	-5.284747000	-1.526802000	-2.142185000
H	-4.334722000	-1.297863000	-0.687620000
C	-3.226771000	-4.088440000	-1.681539000
H	-3.364946000	-5.128556000	-1.994702000
H	-2.515708000	-4.100111000	-0.846208000
C	-4.561915000	-3.420570000	-1.274827000
H	-5.374500000	-3.841255000	-1.876277000
H	-4.816422000	-3.596561000	-0.223816000

Fe	1.456664097	0.273339629	-0.015342965
O	1.245995459	0.243488211	1.826850041
Fe	-1.741397970	-0.016182769	0.157916545
O	-1.230860989	-0.883615937	1.693342325
H	-0.323330474	-0.569108435	1.933493545
O	-0.208890073	0.540297909	-0.662545791
N	2.149688381	2.279094973	-0.530975922
N	1.365067748	-1.874848534	-0.505389673
N	3.764300773	0.080252905	0.147121330
C	2.420786414	2.491469149	-1.832296863
C	3.001930457	3.679086832	-2.269450188
H	3.220669577	3.821783710	-3.323267520
C	3.294998342	4.672015971	-1.329917679
H	3.749597054	5.606349843	-1.645541215
C	3.003479359	4.444463933	0.016315064
H	3.219505387	5.189624347	0.774604894
C	2.434701659	3.223192694	0.375877775
H	2.198513449	2.970734929	1.405385763
C	1.349053257	-2.184757486	-1.815552107
C	1.273225332	-3.504770554	-2.251983635
H	1.283006645	-3.726304259	-3.314662569
C	1.192729535	-4.525733917	-1.300352546
H	1.145208889	-5.564249560	-1.614814538
C	1.180610847	-4.192876665	0.054629084
H	1.116878856	-4.953346706	0.825803852
C	1.268119830	-2.847193208	0.409852013
H	1.261018272	-2.524502509	1.441332244
C	4.447316728	0.056442045	-1.009160064
C	5.819232030	0.302024740	-1.067748982
H	6.334089742	0.280202528	-2.023685986
C	6.508917205	0.569039113	0.115514102
H	7.577561026	0.761092353	0.097913666
C	5.799181504	0.591709595	1.317405812
H	6.291665602	0.798977740	2.261663345
C	4.427490573	0.352598739	1.282294372
H	3.829899702	0.385507743	2.185361806
C	1.991888783	1.388911417	-2.778558919
H	2.477672439	1.507497922	-3.758000918
C	1.383100521	-1.003764573	-2.762095686
H	0.371182385	-0.593921556	-2.824261312
H	1.706410358	-1.316005080	-3.765626362
C	3.674461822	-0.330655346	-2.250515697
H	4.158397063	0.083952383	-3.145861377
H	3.726013741	-1.422371294	-2.340066246
N	2.246884483	0.054715340	-2.201408048
H	0.908024767	1.473813144	-2.912714348
H	-3.561681980	5.424397538	2.006323151
C	-3.186987974	4.455977772	1.688340013
C	-3.248846149	4.085661650	0.341270112
C	-2.646941954	3.564996746	2.617760474
C	-2.763401695	2.835421131	-0.032945517
H	-3.666579198	4.753334639	-0.406073158
H	-2.586392434	3.816371815	3.671378836
C	-2.194707077	2.325503817	2.165787011
N	-2.254261213	1.981136431	0.872872580
C	-2.708822354	2.365532901	-1.472569577
H	-1.779163233	1.572816915	2.828549235
H	-1.674574525	2.479130852	-1.815765365
H	-3.361602708	2.983161598	-2.106635578
N	-3.040647710	0.931927174	-1.573821823
N	-3.905222262	-0.321981072	0.753487547
N	-2.092408648	-1.609237010	-1.290516199
C	-2.484604132	0.271236149	-2.768583399
C	-4.484783535	0.657751974	-1.404753925
C	-4.866574337	0.228855931	-0.001415549
C	-4.209612953	-0.788358211	1.976819932
C	-2.422010401	-1.227402287	-2.539794144
C	-2.000093147	-2.909634536	-0.985263478
H	-3.056201817	0.497772696	-3.680524606
H	-1.463923879	0.649057592	-2.891727707
H	-4.761351674	-0.157590572	-2.084845646
H	-5.081178466	1.529606947	-1.706992453
C	-6.182836597	0.340988590	0.447070636
C	-5.502873466	-0.732057985	2.491137355
H	-3.370643701	-1.192778749	2.533891172

I-²Int_{hs-hs}

C	-2.674396198	-2.163368142	-3.540099486
C	-2.234966353	-3.905846162	-1.932339409
H	-1.729457085	-3.128289517	0.042807794
H	-6.936468080	0.801102916	-0.185400424
C	-6.506427426	-0.151123497	1.712197440
H	-5.712644619	-1.123881988	3.480889314
H	-2.954672812	-1.833096449	-4.535754946
C	-2.577700169	-3.523907191	-3.230279965
H	-2.159861813	-4.951271272	-1.653000498
H	-7.523957487	-0.078030890	2.084626038
H	-2.780894707	-4.272529482	-3.990428266
H	1.850239676	-0.107705562	2.516530454
H	0.697027510	-0.349462834	4.740801605
C	1.394603776	-1.194282141	4.819680766
H	1.561942852	-1.361059231	5.898232372
C	2.707299381	-0.948698388	4.131252916
H	3.364603143	-0.125606041	4.403997220
C	3.193438116	-2.183251448	3.418037345
H	4.215688437	-2.462376571	3.709931515
H	3.228958080	-2.031328364	2.324642317
C	0.866025556	-2.483237797	4.151638411
H	0.197774705	-3.052734648	4.805282911
H	0.295287784	-2.218897885	3.252932455

I-¹⁰Int_{hs-hs}

Fe	1.508371000	-0.313556000	-0.197489000
O	1.412045000	0.377948000	-1.909949000
Fe	-1.701113000	0.305454000	-0.229332000
O	-1.310121000	0.485697000	-2.008623000
H	-0.330522000	0.450456000	-2.153718000
O	-0.091906000	-0.009525000	0.680089000
N	0.988880000	-2.338263000	-0.836741000
N	2.633040000	0.958248000	1.217490000
N	3.660425000	-0.963237000	-0.582409000
C	0.862939000	-3.265255000	0.130652000
C	0.592704000	-4.597253000	-0.170766000
H	0.511107000	-5.328976000	0.627018000
C	0.443270000	-4.966930000	-1.511055000
H	0.243779000	-6.001870000	-1.773299000
C	0.568360000	-3.995175000	-2.505384000
H	0.468386000	-4.246080000	-3.556241000
C	0.846419000	-2.682357000	-2.123632000
H	0.971210000	-1.871867000	-2.834700000
C	2.775963000	0.453342000	2.459009000
C	3.542327000	1.101715000	3.424707000
H	3.649577000	0.665205000	4.412914000
C	4.166036000	2.309046000	3.097857000
H	4.769602000	2.831152000	3.834256000
C	4.010761000	2.825306000	1.810708000
H	4.482929000	3.755278000	1.511938000
C	3.238407000	2.109434000	0.897838000
H	3.095018000	2.455221000	-0.117954000
C	4.294860000	-1.661590000	0.369889000
C	5.680243000	-1.831549000	0.360368000
H	6.164484000	-2.396663000	1.151473000
C	6.420815000	-1.272609000	-0.681524000
H	7.499855000	-1.390967000	-0.712540000
C	5.752870000	-0.563643000	-1.683457000
H	6.289466000	-0.121093000	-2.516139000
C	4.370275000	-0.429598000	-1.590185000
H	3.786986000	0.110932000	-2.327616000
C	1.017611000	-2.743476000	1.542999000
H	1.187977000	-3.568680000	2.249436000
C	2.021525000	-0.828637000	2.739464000
H	0.965103000	-0.571676000	2.867105000
H	2.394000000	-1.301746000	3.659919000
C	3.437246000	-2.345404000	1.416877000
H	3.305967000	-3.387439000	1.099655000
H	3.969757000	-2.377368000	2.377153000
N	2.099016000	-1.738687000	1.583041000
H	0.094229000	-2.223753000	1.809646000
H	-3.674044000	-5.362390000	0.584044000
C	-3.282728000	-4.362375000	0.421604000
C	-3.201822000	-3.457347000	1.483909000
C	-2.871197000	-3.958506000	-0.849566000

C	-2.706015000	-2.177716000	1.241434000
H	-3.528632000	-3.733037000	2.482008000
H	-2.928863000	-4.627902000	-1.701081000
C	-2.394000000	-2.658753000	-1.012269000
N	-2.308716000	-1.800759000	0.011963000
C	-2.543691000	-1.141483000	2.336681000
H	-2.071050000	-2.273321000	-1.973921000
H	-1.493894000	-1.128933000	2.647362000
H	-3.157084000	-1.411053000	3.209451000
N	-2.856504000	0.206602000	1.838992000
N	-3.898144000	0.423210000	-0.735341000
N	-1.965918000	2.367668000	0.436999000
C	-2.187492000	1.290377000	2.588859000
C	-4.308207000	0.438444000	1.676425000
C	-4.800787000	0.296899000	0.247960000
C	-4.302926000	0.389802000	-2.016972000
C	-2.196555000	2.552223000	1.751933000
C	-1.963494000	3.416886000	-0.395637000
H	-2.651240000	1.470679000	3.569448000
H	-1.147065000	0.979566000	2.730014000
H	-4.532958000	1.461827000	2.001650000
H	-4.882085000	-0.227438000	2.335484000
C	-6.158639000	0.117328000	-0.019497000
C	-5.641404000	0.230947000	-2.367265000
H	-3.509251000	0.486628000	-2.750855000
C	-2.429978000	3.819393000	2.278808000
C	-2.185965000	4.717561000	0.055790000
H	-1.775941000	3.185938000	-1.438465000
H	-6.864840000	0.010496000	0.798878000
C	-6.585397000	0.085980000	-1.347472000
H	-5.932405000	0.214328000	-3.412326000
H	-2.625846000	3.939060000	3.339921000
C	-2.419637000	4.920427000	1.416412000
H	-2.182096000	5.544697000	-0.646217000
H	-7.637022000	-0.050318000	-1.581815000
H	-2.604945000	5.918593000	1.801916000
H	-0.140204000	2.606616000	-2.854973000
H	1.730669000	1.197177000	-2.356644000
C	0.671335000	3.344609000	-2.909393000
H	0.326100000	4.157963000	-3.572407000
C	1.955730000	2.763381000	-3.430871000
H	2.026455000	2.238277000	-4.379922000
C	3.149277000	3.349713000	-2.724130000
H	3.874492000	3.792585000	-3.421119000
H	3.711571000	2.575426000	-2.169972000
C	1.085119000	3.911567000	-1.533108000
H	0.426224000	4.707795000	-1.174399000
H	1.060121000	3.098658000	-0.793779000
C	2.529977000	4.399008000	-1.763618000
H	2.507891000	5.373704000	-2.264420000
H	3.098807000	4.526148000	-0.835210000

I-¹²Int_{hs-hs}

Fe	1.512361000	-0.304513000	-0.200647000
O	1.409438000	0.398960000	-1.923118000
Fe	-1.700546000	0.294341000	-0.232664000
O	-1.310012000	0.464733000	-2.010811000
H	-0.329900000	0.454758000	-2.161244000
O	-0.080949000	0.004469000	0.678915000
N	0.983939000	-2.321828000	-0.853853000
N	2.662353000	0.942676000	1.214990000
N	3.653661000	-0.966914000	-0.611298000
C	0.868543000	-3.259213000	0.104747000
C	0.607093000	-4.589918000	-0.209155000
H	0.534062000	-5.330398000	0.581324000
C	0.454589000	-4.946689000	-1.552721000
H	0.261720000	-5.980320000	-1.824897000
C	0.567676000	-3.963777000	-2.537476000
H	0.464709000	-4.204521000	-3.590409000
C	0.838590000	-2.652915000	-2.143672000
H	0.955786000	-1.834631000	-2.847141000
C	2.796906000	0.434372000	2.456161000
C	3.571509000	1.070478000	3.423191000
H	3.671158000	0.631612000	4.411133000
C	4.214232000	2.268199000	3.097485000

H	4.824367000	2.780969000	3.835018000
C	4.070968000	2.785671000	1.809493000
H	4.559668000	3.706942000	1.510460000
C	3.288741000	2.082568000	0.895190000
H	3.156456000	2.429991000	-0.121383000
C	4.293695000	-1.671623000	0.332501000
C	5.677151000	-1.854189000	0.305024000
H	6.166461000	-2.424752000	1.089101000
C	6.409349000	-1.300679000	-0.745703000
H	7.486798000	-1.428728000	-0.790484000
C	5.735213000	-0.584713000	-1.738453000
H	6.265150000	-0.146045000	-2.577405000
C	4.355090000	-0.438519000	-1.628041000
H	3.766774000	0.106680000	-2.358204000
C	1.025805000	-2.748945000	1.520786000
H	1.200045000	-3.579173000	2.220222000
C	2.030402000	-0.841592000	2.729172000
H	0.975258000	-0.578623000	2.855170000
H	2.397449000	-1.323915000	3.646904000
C	3.445267000	-2.347788000	1.392266000
H	3.314657000	-3.393465000	1.086985000
H	3.985450000	-2.368630000	2.348368000
N	2.106174000	-1.743103000	1.565358000
H	0.102486000	-2.233272000	1.795207000
H	-3.639411000	-5.376582000	0.637612000
C	-3.251294000	-4.377006000	0.465135000
C	-3.164611000	-3.464076000	1.520327000
C	-2.850148000	-3.981337000	-0.811853000
C	-2.674034000	-2.185045000	1.264928000
H	-3.484055000	-3.733073000	2.522620000
H	-2.912950000	-4.656762000	-1.658222000
C	-2.376268000	-2.682013000	-0.987321000
N	-2.285316000	-1.816347000	0.029909000
C	-2.512256000	-1.137039000	2.348849000
H	-2.060538000	-2.303695000	-1.954079000
H	-1.459336000	-1.106429000	2.647567000
H	-3.113103000	-1.405178000	3.230694000
N	-2.848726000	0.200606000	1.838458000
N	-3.896475000	0.382800000	-0.736326000
N	-2.000762000	2.358126000	0.408799000
C	-2.195171000	1.303953000	2.573739000
C	-4.304878000	0.405718000	1.677360000
C	-4.797365000	0.260241000	0.248872000
C	-4.302784000	0.344693000	-2.017513000
C	-2.233119000	2.555075000	1.721793000
C	-2.030040000	3.394697000	-0.439024000
H	-2.657618000	1.486593000	3.554447000
H	-1.148777000	1.012940000	2.713184000
H	-4.549951000	1.422738000	2.007816000
H	-4.864941000	-0.274359000	2.333664000
C	-6.155591000	0.079346000	-0.016380000
C	-5.641511000	0.183827000	-2.365341000
H	-3.510253000	0.440611000	-2.752767000
C	-2.497734000	3.822949000	2.231540000
C	-2.286625000	4.695192000	-0.005318000
H	-1.839089000	3.153716000	-1.478894000
H	-6.860857000	-0.024049000	0.803260000
C	-6.584073000	0.042580000	-1.343567000
H	-5.933934000	0.163425000	-3.409931000
H	-2.693226000	3.952666000	3.291531000
C	-2.519687000	4.911394000	1.353279000
H	-2.307372000	5.511784000	-0.719259000
H	-7.636012000	-0.094627000	-1.575935000
H	-2.729649000	5.909797000	1.725277000
H	-0.105416000	2.644181000	-2.769998000
H	1.731507000	1.240076000	-2.300694000
C	0.661085000	3.430907000	-2.788209000
H	0.244590000	4.271250000	-3.372393000
C	1.960687000	2.969321000	-3.386511000
H	2.036264000	2.506993000	-4.366738000
C	3.141936000	3.526017000	-2.638172000
H	3.854145000	4.046656000	-3.293639000
H	3.728927000	2.723576000	-2.150574000
C	1.077956000	3.910292000	-1.378956000
H	0.394726000	4.649864000	-0.951388000

H	1.096790000	3.044877000	-0.701569000
C	2.497863000	4.472912000	-1.592327000
H	2.427210000	5.480229000	-2.018737000
H	3.075911000	4.555394000	-0.664367000

$I^{-10}Int_{hs-is}$

Fe	1.702773000	-0.060103000	-0.213752000
O	1.468280000	0.559134000	-1.941461000
Fe	-1.586118000	0.109770000	-0.343361000
O	-1.226089000	0.007056000	-2.136652000
H	-0.258121000	0.170698000	-2.262112000
O	0.069041000	0.281454000	0.464823000
N	1.247288000	-2.149228000	-0.747268000
N	2.610334000	1.368877000	1.192213000
N	3.648939000	-0.671729000	-0.683178000
C	1.340078000	-3.051541000	0.241370000
C	1.308558000	-4.420895000	-0.008742000
H	1.395420000	-5.127957000	0.810639000
C	1.166207000	-4.855823000	-1.329815000
H	1.147410000	-5.917695000	-1.557279000
C	1.059682000	-3.909946000	-2.351198000
H	0.953353000	-4.209164000	-3.388786000
C	1.111837000	-2.555979000	-2.015475000
H	1.045944000	-1.765916000	-2.756298000
C	2.600937000	1.003978000	2.486793000
C	3.120438000	1.822976000	3.486405000
H	3.111821000	1.491377000	4.520382000
C	3.656989000	3.063169000	3.129004000
H	4.070766000	3.720752000	3.887595000
C	3.669492000	3.433645000	1.783491000
H	4.088497000	4.380588000	1.460300000
C	3.137683000	2.549652000	0.845659000
H	3.126353000	2.782743000	-0.2111710000
C	4.325948000	-1.425931000	0.203020000
C	5.566243000	-1.982784000	-0.108112000
H	6.081833000	-2.593560000	0.627004000
C	6.125812000	-1.740143000	-1.361942000
H	7.091946000	-2.161344000	-1.623099000
C	5.418657000	-0.954471000	-2.274646000
H	5.810885000	-0.744372000	-3.263961000
C	4.178495000	-0.447407000	-1.900812000
H	3.550501000	0.135317000	-2.565357000
C	1.420395000	-2.461715000	1.632256000
H	1.761200000	-3.211989000	2.359725000
C	1.986251000	-0.349322000	2.766606000
H	0.900030000	-0.233466000	2.799437000
H	2.337216000	-0.748803000	3.728639000
C	3.728602000	-1.603333000	1.580558000
H	3.897227000	-2.629742000	1.931577000
H	4.271919000	-0.945831000	2.269778000
N	2.283864000	-1.264705000	1.645663000
H	0.416101000	-2.136152000	1.913251000
H	-2.808803000	-5.553052000	1.469027000
C	-2.533595000	-4.556752000	1.135670000
C	-2.521305000	-3.489993000	2.039866000
C	-2.208600000	-4.319188000	-0.200698000
C	-2.175954000	-2.222186000	1.576818000
H	-2.789909000	-3.634205000	3.081998000
H	-2.221217000	-5.116973000	-0.935455000
C	-1.875224000	-3.020683000	-0.583750000
N	-1.847482000	-2.007604000	0.289651000
C	-2.126419000	-0.999131000	2.471352000
H	-1.622287000	-2.760592000	-1.605838000
H	-1.081428000	-0.775574000	2.707256000
H	-2.656528000	-1.193746000	3.415802000
N	-2.666424000	0.168882000	1.763015000
N	-3.774286000	-0.295543000	-0.762863000
N	-2.369569000	2.144624000	-0.034814000
C	-2.179666000	1.469952000	2.274196000
C	-4.140623000	0.112925000	1.626602000
C	-4.625725000	-0.369438000	0.269592000
C	-4.189445000	-0.635864000	-1.994623000
C	-2.510348000	2.533771000	1.247094000
C	-2.750380000	2.963079000	-1.023738000
H	-2.613383000	1.727114000	3.251436000

H	-1.091437000	1.384692000	2.368201000
H	-4.543261000	1.121044000	1.781528000
H	-4.574121000	-0.514932000	2.417038000
C	-5.941103000	-0.806498000	0.105236000
C	-5.490502000	-1.065426000	-2.245450000
H	-3.435988000	-0.555635000	-2.772372000
C	-2.990864000	3.797748000	1.577839000
C	-3.248094000	4.241690000	-0.776614000
H	-2.640522000	2.569247000	-2.027521000
H	-6.607264000	-0.863832000	0.961373000
C	-6.380202000	-1.157215000	-1.171946000
H	-5.793809000	-1.326143000	-3.254007000
H	-3.099521000	4.082716000	2.619788000
C	-3.352855000	4.671076000	0.547171000
H	-3.546645000	4.878145000	-1.602778000
H	-7.400052000	-1.497179000	-1.326012000
H	-3.734194000	5.661294000	0.778128000
H	-0.483510000	2.478734000	-2.420894000
H	1.444122000	1.524283000	-2.093844000
C	0.033730000	3.444338000	-2.359338000
H	-0.642546000	4.195240000	-2.809295000
C	1.361439000	3.442036000	-3.057979000
H	1.503855000	3.082585000	-4.073104000
C	2.364207000	4.293243000	-2.332711000
H	2.759879000	5.103941000	-2.962446000
H	3.253219000	3.708862000	-2.034964000
C	0.400473000	3.858830000	-0.915317000
H	-0.434862000	4.312657000	-0.373505000
H	0.710822000	2.967581000	-0.353882000
C	1.578178000	4.838351000	-1.108623000
H	1.184858000	5.832403000	-1.350878000
H	2.196106000	4.945580000	-0.210592000

I-⁸Int_{hs-is}

Fe	1.691123000	-0.052905000	-0.181473000
O	1.470444000	0.471138000	-1.933551000
Fe	-1.611260000	0.127571000	-0.342558000
O	-1.245409000	0.055003000	-2.138124000
H	-0.267378000	0.153954000	-2.250159000
O	0.041368000	0.257973000	0.465951000
N	1.314013000	-2.167945000	-0.677322000
N	2.497984000	1.441475000	1.218010000
N	3.668601000	-0.606205000	-0.577847000
C	1.405502000	-3.044671000	0.334025000
C	1.419263000	-4.420056000	0.116134000
H	1.503176000	-5.104837000	0.954568000
C	1.330522000	-4.889989000	-1.197411000
H	1.349265000	-5.956977000	-1.399415000
C	1.229401000	-3.971218000	-2.243627000
H	1.165350000	-4.296999000	-3.276706000
C	1.229932000	-2.609229000	-1.938886000
H	1.166723000	-1.838057000	-2.699666000
C	2.439622000	1.109094000	2.520093000
C	2.862283000	1.980237000	3.521612000
H	2.818042000	1.674246000	4.562587000
C	3.349238000	3.238751000	3.158253000
H	3.686001000	3.936954000	3.918660000
C	3.414443000	3.574911000	1.805319000
H	3.799732000	4.534716000	1.477912000
C	2.982407000	2.639441000	0.866402000
H	3.021319000	2.844373000	-0.195887000
C	4.341726000	-1.313107000	0.349498000
C	5.609511000	-1.834629000	0.092505000
H	6.121383000	-2.408252000	0.859442000
C	6.201239000	-1.604603000	-1.148890000
H	7.189167000	-1.998366000	-1.367910000
C	5.497864000	-0.868053000	-2.104450000
H	5.914635000	-0.670172000	-3.086221000
C	4.229386000	-0.395962000	-1.783813000
H	3.603153000	0.143537000	-2.485163000
C	1.433110000	-2.423656000	1.713282000
H	1.785827000	-3.145850000	2.463087000
C	1.878238000	-0.265122000	2.811725000
H	0.787460000	-0.197245000	2.810106000
H	2.216944000	-0.625957000	3.793345000

C	3.707644000	-1.473008000	1.712749000
H	3.907754000	-2.479641000	2.102432000
H	4.201020000	-0.771209000	2.395819000
N	2.248931000	-1.193055000	1.723535000
H	0.410260000	-2.135078000	1.966156000
H	-2.660709000	-5.651971000	1.163555000
C	-2.428388000	-4.628093000	0.885647000
C	-2.475673000	-3.610995000	1.843859000
C	-2.100017000	-4.307094000	-0.432699000
C	-2.184086000	-2.306078000	1.451385000
H	-2.749007000	-3.822024000	2.873401000
H	-2.067172000	-5.065788000	-1.207101000
C	-1.825831000	-2.976181000	-0.744596000
N	-1.854941000	-2.010848000	0.181767000
C	-2.187665000	-1.134540000	2.414510000
H	-1.578559000	-2.646460000	-1.748021000
H	-1.156712000	-0.919003000	2.712325000
H	-2.753749000	-1.389026000	3.323168000
N	-2.708867000	0.072876000	1.759763000
N	-3.797886000	-0.245118000	-0.796876000
N	-2.348913000	2.163464000	0.082811000
C	-2.220835000	1.338619000	2.350068000
C	-4.181735000	0.039623000	1.603904000
C	-4.652348000	-0.390695000	0.225955000
C	-4.200993000	-0.534476000	-2.045729000
C	-2.523326000	2.465955000	1.384731000
C	-2.679742000	3.061118000	-0.854594000
H	-2.665601000	1.543267000	3.334870000
H	-1.134729000	1.240269000	2.454610000
H	-4.571776000	1.048467000	1.784242000
H	-4.634015000	-0.606511000	2.368679000
C	-5.956329000	-0.849353000	0.034541000
C	-5.491658000	-0.979131000	-2.323618000
H	-3.445284000	-0.405169000	-2.814339000
C	-3.002359000	3.708465000	1.790105000
C	-3.168682000	4.326711000	-0.531366000
H	-2.543022000	2.744044000	-1.881788000
H	-6.623125000	-0.965494000	0.884130000
C	-6.383135000	-1.144771000	-1.260828000
H	-5.784722000	-1.196623000	-3.345364000
H	-3.141831000	3.918515000	2.846103000
C	-3.319463000	4.659450000	0.815051000
H	-3.427487000	5.026283000	-1.319085000
H	-7.394237000	-1.499986000	-1.436648000
H	-3.699163000	5.634801000	1.104480000
H	-0.555615000	2.420638000	-2.589060000
H	1.455923000	1.420674000	-2.188656000
C	0.054135000	3.330711000	-2.651517000
H	-0.531362000	4.073237000	-3.224393000
C	1.382336000	3.084000000	-3.306712000
H	1.490872000	2.594982000	-4.270547000
C	2.476756000	3.881375000	-2.654914000
H	3.022143000	4.515338000	-3.368535000
H	3.245283000	3.220435000	-2.211997000
C	0.451105000	3.909199000	-1.272600000
H	-0.332022000	4.526045000	-0.822126000
H	0.657946000	3.080151000	-0.581175000
C	1.733307000	4.712166000	-1.575701000
H	1.458529000	5.683960000	-2.001940000
H	2.339034000	4.910390000	-0.684488000

I-⁴Int_{hs-is}

Fe	1.607245000	-0.171069000	-0.181022000
O	1.381969000	0.473377000	-1.890310000
Fe	-1.610322000	0.137089000	-0.353992000
O	-1.257275000	0.011214000	-2.133917000
H	-0.281846000	0.172222000	-2.256652000
O	0.046031000	0.211383000	0.494827000
N	1.109507000	-2.298818000	-0.790000000
N	2.724291000	1.348939000	1.182972000
N	3.541830000	-0.829030000	-0.733785000
C	1.193436000	-3.135659000	0.257189000
C	1.159764000	-4.518890000	0.098063000
H	1.237573000	-5.173585000	0.960887000
C	1.026010000	-5.037926000	-1.194286000

H	1.004499000	-6.112344000	-1.352068000
C	0.930844000	-4.160963000	-2.276759000
H	0.831165000	-4.528707000	-3.292874000
C	0.984940000	-2.787517000	-2.026806000
H	0.926698000	-2.046737000	-2.819128000
C	2.667041000	0.946591000	2.467059000
C	3.237170000	1.683757000	3.503424000
H	3.184713000	1.319610000	4.525231000
C	3.880914000	2.886479000	3.198472000
H	4.334387000	3.481292000	3.985705000
C	3.946516000	3.297908000	1.867107000
H	4.447910000	4.216931000	1.582234000
C	3.356931000	2.491621000	0.892863000
H	3.386028000	2.766301000	-0.154380000
C	4.207531000	-1.589210000	0.153568000
C	5.421938000	-2.195440000	-0.163968000
H	5.930195000	-2.810552000	0.572503000
C	5.964975000	-1.993433000	-1.432918000
H	6.911573000	-2.451697000	-1.703253000
C	5.269185000	-1.201260000	-2.349486000
H	5.652470000	-1.024226000	-3.348712000
C	4.053490000	-0.645169000	-1.964508000
H	3.433786000	-0.054284000	-2.629607000
C	1.260423000	-2.458108000	1.610794000
H	1.558098000	-3.166797000	2.395457000
C	1.941101000	-0.360461000	2.715843000
H	0.865121000	-0.171343000	2.746509000
H	2.258374000	-0.809422000	3.667122000
C	3.606502000	-1.710471000	1.530699000
H	3.708237000	-2.737699000	1.902157000
H	4.181185000	-1.071697000	2.211020000
N	2.173574000	-1.287215000	1.579810000
H	0.266315000	-2.070219000	1.841993000
H	-3.058788000	-5.430479000	1.545038000
C	-2.753118000	-4.448920000	1.194922000
C	-2.717373000	-3.366074000	2.078870000
C	-2.409922000	-4.247319000	-0.143089000
C	-2.330793000	-2.117443000	1.596270000
H	-2.996248000	-3.483296000	3.121653000
H	-2.437362000	-5.058918000	-0.862062000
C	-2.038528000	-2.966437000	-0.548464000
N	-1.989686000	-1.937543000	0.306724000
C	-2.231287000	-0.887315000	2.478278000
H	-1.770074000	-2.733482000	-1.573143000
H	-1.179565000	-0.723919000	2.735273000
H	-2.788820000	-1.043167000	3.413957000
N	-2.688662000	0.305077000	1.752698000
N	-3.818357000	-0.113265000	-0.767018000
N	-2.212260000	2.221675000	-0.080256000
C	-2.115653000	1.577705000	2.245353000
C	-4.162567000	0.353222000	1.612080000
C	-4.675511000	-0.120396000	0.263296000
C	-4.249767000	-0.446484000	-1.995375000
C	-2.348450000	2.642822000	1.192396000
C	-2.502985000	3.049094000	-1.092166000
H	-2.544937000	1.886933000	3.209273000
H	-1.038715000	1.416492000	2.362785000
H	-4.489830000	1.391688000	1.742898000
H	-4.643254000	-0.223827000	2.413834000
C	-6.014334000	-0.479576000	0.100800000
C	-5.573589000	-0.800619000	-2.244225000
H	-3.490838000	-0.424182000	-2.771511000
C	-2.737119000	3.945838000	1.489988000
C	-2.906251000	4.366178000	-0.877393000
H	-2.398905000	2.628282000	-2.085580000
H	-6.684871000	-0.483754000	0.955349000
C	-6.470157000	-0.822395000	-1.172719000
H	-5.889167000	-1.058071000	-3.249829000
H	-2.844823000	4.258208000	2.524129000
C	-3.008724000	4.825134000	0.436490000
H	-3.134149000	5.009248000	-1.720681000
H	-7.508114000	-1.102863000	-1.325555000
H	-3.318226000	5.845467000	0.642428000
H	1.589997000	1.421638000	-1.993800000
H	-0.212875000	2.535636000	-2.423873000

C	0.336894000	3.481209000	-2.347907000
H	-0.301722000	4.258731000	-2.808100000
C	1.680334000	3.433815000	-3.014220000
H	1.836569000	3.060943000	-4.022602000
C	2.681322000	4.281024000	-2.280509000
H	3.088696000	5.087365000	-2.908784000
H	3.563653000	3.694104000	-1.969561000
C	0.688023000	3.879409000	-0.896097000
H	-0.146760000	4.342799000	-0.361316000
H	0.980893000	2.980348000	-0.338030000
C	1.885677000	4.838483000	-1.067404000
H	1.513964000	5.840201000	-1.312554000
H	2.491345000	4.930968000	-0.159367000

I-²Int_{hs-is}

Fe	1.641853000	-0.216586000	-0.320333000
O	1.318791000	0.570704000	-1.954118000
Fe	-1.538347000	-0.103654000	-0.407296000
O	-1.183067000	-0.512508000	-2.155068000
H	-0.258830000	-0.203078000	-2.337734000
O	0.104877000	0.154718000	0.438713000
N	1.002370000	-2.427659000	-0.698541000
N	2.918485000	1.318557000	0.732546000
N	3.412075000	-1.027761000	-1.085029000
C	1.219205000	-3.154415000	0.410386000
C	1.179133000	-4.547025000	0.403097000
H	1.363970000	-5.104833000	1.316237000
C	0.895586000	-5.200818000	-0.800263000
H	0.865576000	-6.285799000	-0.840874000
C	0.657575000	-4.440428000	-1.946713000
H	0.433935000	-4.910472000	-2.898930000
C	0.725387000	-3.048021000	-1.849513000
H	0.531615000	-2.403790000	-2.700907000
C	2.993027000	1.072262000	2.052119000
C	3.644428000	1.936700000	2.930183000
H	3.700305000	1.703502000	3.989209000
C	4.226604000	3.098396000	2.413651000
H	4.743152000	3.790262000	3.072275000
C	4.150014000	3.348342000	1.042685000
H	4.596838000	4.234383000	0.604664000
C	3.481357000	2.427331000	0.235694000
H	3.395078000	2.563482000	-0.837072000
C	4.145426000	-1.774022000	-0.238060000
C	5.235018000	-2.520417000	-0.680277000
H	5.805308000	-3.119677000	0.022931000
C	5.577532000	-2.474920000	-2.033068000
H	6.424190000	-3.046145000	-2.401941000
C	4.817932000	-1.688319000	-2.902207000
H	5.053199000	-1.626602000	-3.959325000
C	3.733422000	-0.982108000	-2.389134000
H	3.080980000	-0.363711000	-2.996853000
C	1.439355000	-2.348688000	1.673436000
H	1.802853000	-2.986388000	2.490674000
C	2.305481000	-0.199154000	2.510665000
H	1.243480000	0.007791000	2.675313000
H	2.747352000	-0.574352000	3.443958000
C	3.771981000	-1.693783000	1.222025000
H	3.922376000	-2.661617000	1.716323000
H	4.450942000	-0.981262000	1.704028000
N	2.370076000	-1.218442000	1.432843000
H	0.482546000	-1.905046000	1.961511000
H	-3.008850000	-4.951070000	2.944518000
C	-2.701498000	-4.109748000	2.330427000
C	-2.619395000	-2.827327000	2.881776000
C	-2.398262000	-4.288192000	0.980100000
C	-2.230486000	-1.767163000	2.066172000
H	-2.862284000	-2.648034000	3.924659000
H	-2.458101000	-5.264467000	0.511168000
C	-2.022050000	-3.175125000	0.229495000
N	-1.932750000	-1.950859000	0.764268000
C	-2.090537000	-0.346863000	2.575162000
H	-1.777820000	-3.249883000	-0.824807000
H	-1.025318000	-0.122792000	2.697667000
H	-2.588507000	-0.237857000	3.549979000
N	-2.612142000	0.599409000	1.577024000

N	-3.732658000	-0.406557000	-0.767006000
N	-2.062727000	1.997152000	-0.685939000
C	-2.098019000	1.977936000	1.724329000
C	-4.088009000	0.553294000	1.462124000
C	-4.599368000	-0.166706000	0.225980000
C	-4.165588000	-0.969994000	-1.908975000
C	-2.309778000	2.720310000	0.422851000
C	-2.218125000	2.548261000	-1.896775000
H	-2.570326000	2.512185000	2.561040000
H	-1.020793000	1.903187000	1.910034000
H	-4.468010000	1.581803000	1.426986000
H	-4.525561000	0.095974000	2.359617000
C	-5.950174000	-0.502082000	0.116603000
C	-5.498593000	-1.321928000	-2.101311000
H	-3.400871000	-1.126667000	-2.663260000
C	-2.725209000	4.045870000	0.349608000
C	-2.617310000	3.875587000	-2.053381000
H	-2.016184000	1.888499000	-2.735158000
H	-6.629482000	-0.299966000	0.939837000
C	-6.406084000	-1.087637000	-1.064301000
H	-5.814476000	-1.769957000	-3.037547000
H	-2.930927000	4.603230000	1.258097000
C	-2.870215000	4.635346000	-0.910481000
H	-2.730795000	4.296080000	-3.046944000
H	-7.452850000	-1.355114000	-1.174246000
H	-3.191226000	5.669178000	-0.996462000
H	1.080185000	1.505149000	-1.833867000
H	1.478822000	4.274274000	1.709976000
C	0.843783000	4.554148000	0.856187000
H	-0.150051000	4.796672000	1.276529000
C	0.739415000	3.477553000	-0.181964000
H	0.497571000	2.445716000	0.044588000
C	0.933921000	4.027171000	-1.566570000
H	0.199259000	3.654279000	-2.294860000
H	1.927121000	3.763168000	-1.978364000
C	1.397822000	5.763802000	0.066399000
H	1.117386000	6.728527000	0.500321000
H	2.494541000	5.711338000	0.046487000
C	0.846248000	5.558210000	-1.357884000
H	-0.207286000	5.864118000	-1.392017000
H	1.389169000	6.128028000	-2.118177000

I-⁸Int_{is-is}

Fe	1.524658000	-0.406700000	-0.213439000
O	1.431729000	0.813176000	-1.583864000
Fe	-1.647431000	0.116577000	-0.279919000
O	-1.133292000	-0.077033000	-1.987390000
H	-0.192147000	0.208471000	-2.078370000
O	-0.028472000	0.030006000	0.540852000
N	0.681886000	-2.427822000	-0.886830000
N	2.871570000	0.780102000	1.127313000
N	3.219665000	-1.243200000	-1.047011000
C	0.741098000	-3.355036000	0.081887000
C	0.486470000	-4.702176000	-0.165991000
H	0.552449000	-5.427653000	0.639172000
C	0.146154000	-5.089357000	-1.465199000
H	-0.048931000	-6.133181000	-1.693461000
C	0.065344000	-4.116985000	-2.464244000
H	-0.196607000	-4.377237000	-3.484595000
C	0.347980000	-2.790607000	-2.130245000
H	0.289906000	-1.989968000	-2.859054000
C	2.927765000	0.306683000	2.384666000
C	3.689237000	0.926207000	3.372217000
H	3.728227000	0.512319000	4.375375000
C	4.401225000	2.082468000	3.037892000
H	5.004530000	2.588339000	3.785795000
C	4.336992000	2.569240000	1.731262000
H	4.878630000	3.460165000	1.433920000
C	3.559980000	1.880466000	0.798887000
H	3.465445000	2.207656000	-0.232098000
C	3.847217000	-2.190475000	-0.325037000
C	4.892698000	-2.938986000	-0.862245000
H	5.379289000	-3.701716000	-0.261831000
C	5.301872000	-2.683579000	-2.172257000
H	6.115411000	-3.253284000	-2.611328000

C	4.653685000	-1.687789000	-2.907355000
H	4.945713000	-1.457670000	-3.926365000
C	3.609179000	-0.989791000	-2.308566000
H	3.051203000	-0.206261000	-2.811141000
C	1.029278000	-2.812492000	1.463097000
H	1.306597000	-3.618839000	2.156276000
C	2.094695000	-0.934098000	2.631594000
H	1.056912000	-0.635513000	2.813413000
H	2.464238000	-1.493285000	3.502477000
C	3.424048000	-2.350931000	1.118807000
H	3.452878000	-3.408573000	1.409687000
H	4.162921000	-1.832872000	1.741209000
N	2.078684000	-1.770792000	1.409077000
H	0.119571000	-2.325699000	1.827553000
H	-3.619900000	-4.871541000	2.679434000
C	-3.232476000	-4.023333000	2.122798000
C	-3.031070000	-2.794831000	2.760360000
C	-2.939785000	-4.139856000	0.762980000
C	-2.540846000	-1.727335000	2.011038000
H	-3.255740000	-2.665477000	3.814844000
H	-3.085835000	-5.074853000	0.232549000
C	-2.459351000	-3.018028000	0.086391000
N	-2.265488000	-1.845987000	0.700034000
C	-2.240048000	-0.366865000	2.600972000
H	-2.210478000	-3.048236000	-0.970114000
H	-1.160778000	-0.286496000	2.766780000
H	-2.760487000	-0.226262000	3.558483000
N	-2.591956000	0.691894000	1.631305000
N	-3.629943000	0.095356000	-0.867154000
N	-1.847663000	2.359266000	-0.377718000
C	-1.974697000	1.995195000	1.985710000
C	-4.070476000	0.802026000	1.445235000
C	-4.551078000	0.391797000	0.067234000
C	-4.017075000	-0.227600000	-2.114494000
C	-2.098678000	2.936359000	0.809497000
C	-1.912866000	3.084972000	-1.498542000
H	-2.426201000	2.421342000	2.892049000
H	-0.912985000	1.793834000	2.164523000
H	-4.375918000	1.840423000	1.620918000
H	-4.583974000	0.196498000	2.202070000
C	-5.915177000	0.356673000	-0.222978000
C	-5.358591000	-0.279575000	-2.477375000
H	-3.203182000	-0.427099000	-2.803840000
C	-2.442112000	4.281076000	0.916724000
C	-2.233991000	4.443716000	-1.481035000
H	-1.707541000	2.542910000	-2.416939000
H	-6.639919000	0.599370000	0.548609000
C	-6.325087000	0.014882000	-1.511446000
H	-5.636384000	-0.542241000	-3.492538000
H	-2.652855000	4.718078000	1.888065000
C	-2.507493000	5.047429000	-0.252848000
H	-2.275886000	5.006174000	-2.407677000
H	-7.381975000	-0.016837000	-1.758776000
H	-2.773076000	6.099187000	-0.202596000
H	0.822384000	3.355607000	-2.296230000
H	1.028040000	1.626746000	-1.236837000
C	1.240709000	4.226952000	-1.773101000
H	0.656536000	5.096435000	-2.129946000
C	2.704825000	4.419478000	-2.019517000
H	3.165219000	4.359456000	-3.000633000
C	3.396764000	4.971421000	-0.807205000
H	3.877451000	5.942448000	-1.000517000
H	4.212747000	4.310404000	-0.469296000
C	1.144793000	4.150001000	-0.230782000
H	0.162418000	4.442136000	0.149472000
H	1.339504000	3.125649000	0.113120000
C	2.270108000	5.089921000	0.256424000
H	1.897979000	6.120882000	0.276427000
H	2.612296000	4.845148000	1.268113000

I-⁶Int_{is-is}

Fe	1.526038000	-0.402274000	-0.212905000
O	1.430826000	0.818427000	-1.582079000
Fe	-1.647036000	0.113266000	-0.279808000
O	-1.132117000	-0.078593000	-1.987343000

H	-0.191909000	0.209884000	-2.078087000
O	-0.028378000	0.030166000	0.541707000
N	0.689060000	-2.425579000	-0.886535000
N	2.867770000	0.789210000	1.128333000
N	3.223527000	-1.233706000	-1.046522000
C	0.751516000	-3.352942000	0.081862000
C	0.501382000	-4.700833000	-0.166441000
H	0.569906000	-5.426354000	0.638472000
C	0.162208000	-5.088721000	-1.465746000
H	-0.029399000	-6.133119000	-1.694330000
C	0.077974000	-4.116278000	-2.464438000
H	-0.183266000	-4.377043000	-3.484841000
C	0.356194000	-2.789067000	-2.130017000
H	0.295294000	-1.988353000	-2.858516000
C	2.926453000	0.315266000	2.385351000
C	3.686561000	0.936875000	3.372615000
H	3.727735000	0.522698000	4.375567000
C	4.394381000	2.095689000	3.038225000
H	4.996637000	2.603181000	3.785878000
C	4.327377000	2.583017000	1.731941000
H	4.865879000	3.475914000	1.434911000
C	3.551873000	1.892148000	0.799774000
H	3.454777000	2.219527000	-0.231012000
C	3.853933000	-2.179163000	-0.324654000
C	4.901622000	-2.924496000	-0.861967000
H	5.390542000	-3.685807000	-0.261646000
C	5.309985000	-2.667728000	-2.171966000
H	6.125200000	-3.234974000	-2.611113000
C	4.658851000	-1.673767000	-2.906930000
H	4.950194000	-1.442658000	-3.925911000
C	3.612289000	-0.978940000	-2.308031000
H	3.052049000	-0.196929000	-2.810449000
C	1.038002000	-2.809843000	1.463210000
H	1.317804000	-3.615447000	2.156248000
C	2.097588000	-0.928360000	2.632140000
H	1.058853000	-0.633218000	2.814099000
H	2.469070000	-1.486498000	3.502864000
C	3.431373000	-2.340766000	1.119218000
H	3.463698000	-3.398243000	1.410352000
H	4.168589000	-1.820125000	1.741437000
N	2.084190000	-1.764876000	1.409435000
H	0.126783000	-2.325941000	1.827744000
H	-3.602161000	-4.882755000	2.678353000
C	-3.218047000	-4.032958000	2.121847000
C	-3.020714000	-2.803989000	2.759772000
C	-2.925613000	-4.147913000	0.761837000
C	-2.534672000	-1.734451000	2.010620000
H	-3.245314000	-2.675839000	3.814417000
H	-3.068541000	-5.083229000	0.231120000
C	-2.449562000	-3.024093000	0.085449000
N	-2.259601000	-1.851605000	0.699439000
C	-2.238372000	-0.373194000	2.601076000
H	-2.201110000	-3.052992000	-0.971196000
H	-1.159392000	-0.289389000	2.767016000
H	-2.759395000	-0.234681000	3.558578000
N	-2.593636000	0.684719000	1.631788000
N	-3.629617000	0.086493000	-0.867159000
N	-1.855085000	2.355158000	-0.376941000
C	-1.980367000	1.989882000	1.986321000
C	-4.072470000	0.790224000	1.445724000
C	-4.551694000	0.379602000	0.067350000
C	-4.015703000	-0.236699000	-2.114761000
C	-2.108217000	2.930955000	0.810462000
C	-1.924082000	3.080671000	-1.497644000
H	-2.432688000	2.414294000	2.893066000
H	-0.917899000	1.791833000	2.164362000
H	-4.381324000	1.827458000	1.622312000
H	-4.584026000	0.182352000	2.201993000
C	-5.915662000	0.340677000	-0.223016000
C	-5.357030000	-0.292356000	-2.477807000
H	-3.201175000	-0.433323000	-2.804191000
C	-2.457459000	4.274153000	0.917994000
C	-2.251219000	4.437974000	-1.479864000
H	-1.716834000	2.539585000	-2.416182000
H	-6.641181000	0.580717000	0.548674000

C	-6.324466000	-0.001424000	-1.511753000
H	-5.633959000	-0.555116000	-3.493181000
H	-2.669782000	4.710096000	1.889465000
C	-2.526765000	5.040341000	-0.251459000
H	-2.296145000	5.000309000	-2.406441000
H	-7.381236000	-0.036075000	-1.759190000
H	-2.796986000	6.090906000	-0.200951000
H	0.805981000	3.351362000	-2.294710000
H	1.025115000	1.630508000	-1.234081000
C	1.227069000	4.223169000	-1.774688000
H	0.646814000	5.093436000	-2.136089000
C	2.692115000	4.409017000	-2.019835000
H	3.153862000	4.341222000	-2.999842000
C	3.381766000	4.973962000	-0.812153000
H	3.856530000	5.946264000	-1.013926000
H	4.202038000	4.320801000	-0.469961000
C	1.129380000	4.153985000	-0.232154000
H	0.146893000	4.448855000	0.145700000
H	1.322923000	3.131103000	0.116872000
C	2.255070000	5.095545000	0.251428000
H	1.882898000	6.126504000	0.268687000
H	2.597622000	4.853810000	1.263702000

$I^{-2}Int_{is-is}$

Fe	1.557814000	-0.225665000	-0.236070000
O	1.460669000	0.993185000	-1.604301000
Fe	-1.605223000	0.060172000	-0.260790000
O	-1.079989000	-0.047000000	-1.982830000
H	-0.169894000	0.318574000	-2.076015000
O	0.001062000	0.172726000	0.544228000
N	0.868353000	-2.282295000	-0.878579000
N	2.837530000	0.990604000	1.160557000
N	3.338936000	-0.975447000	-1.021611000
C	1.005615000	-3.235738000	0.056420000
C	0.873808000	-4.589638000	-0.242807000
H	0.999921000	-5.334607000	0.536921000
C	0.577372000	-4.957959000	-1.557988000
H	0.478024000	-6.005923000	-1.825536000
C	0.415705000	-3.960322000	-2.521967000
H	0.184642000	-4.204788000	-3.553569000
C	0.576372000	-2.627312000	-2.138673000
H	0.450894000	-1.808490000	-2.837519000
C	2.914692000	0.513928000	2.415521000
C	3.664474000	1.148054000	3.402522000
H	3.718528000	0.728868000	4.402785000
C	4.349201000	2.322235000	3.071706000
H	4.942241000	2.839459000	3.820008000
C	4.272867000	2.807263000	1.766032000
H	4.792839000	3.710670000	1.465696000
C	3.504841000	2.103719000	0.836958000
H	3.409698000	2.429987000	-0.192279000
C	4.021999000	-1.875069000	-0.290722000
C	5.126450000	-2.547863000	-0.811877000
H	5.656217000	-3.273622000	-0.202122000
C	5.537608000	-2.265431000	-2.115010000
H	6.396206000	-2.776085000	-2.540704000
C	4.830667000	-1.318633000	-2.860450000
H	5.120126000	-1.067857000	-3.875363000
C	3.729862000	-0.697708000	-2.277885000
H	3.125868000	0.044432000	-2.790044000
C	1.247103000	-2.717230000	1.454813000
H	1.583391000	-3.522107000	2.123729000
C	2.144197000	-0.767519000	2.648239000
H	1.087017000	-0.529137000	2.802745000
H	2.524138000	-1.302683000	3.530058000
C	3.596489000	-2.071581000	1.148011000
H	3.706167000	-3.125545000	1.434563000
H	4.289504000	-1.502866000	1.778831000
N	2.210515000	-1.600486000	1.427119000
H	0.301918000	-2.316857000	1.833112000
H	-3.217603000	-5.124416000	2.614210000
C	-2.878792000	-4.246086000	2.072791000
C	-2.755946000	-3.016964000	2.728894000
C	-2.573508000	-4.322608000	0.713303000
C	-2.327428000	-1.910265000	1.999336000

H	-2.996495000	-2.916219000	3.782948000	C	3.930500000	2.418581000	1.721254000
H	-2.662485000	-5.255373000	0.166483000	H	4.517471000	3.264584000	1.380304000
C	-2.153452000	-3.164026000	0.058222000	C	3.275635000	1.616357000	0.787820000
N	-2.029987000	-1.991700000	0.689122000	H	3.348412000	1.814619000	-0.274549000
C	-2.146237000	-0.536991000	2.608220000	C	3.640276000	-2.679378000	0.356821000
H	-1.897935000	-3.165711000	-0.997038000	C	4.669455000	-3.576928000	0.080657000
H	-1.078311000	-0.348564000	2.759420000	H	4.951192000	-4.325529000	0.815010000
H	-2.663680000	-0.464176000	3.575087000	C	5.325677000	-3.485496000	-1.147702000
N	-2.619494000	0.490747000	1.659118000	H	6.133173000	-4.169807000	-1.389921000
N	-3.584175000	-0.202069000	-0.850384000	C	4.925384000	-2.504834000	-2.058596000
N	-2.133384000	2.239050000	-0.330007000	H	5.408943000	-2.401849000	-3.024216000
C	-2.161991000	1.853093000	2.031855000	C	3.876227000	-1.656880000	-1.714344000
C	-4.099808000	0.427584000	1.468958000	H	3.485128000	-0.889867000	-2.373672000
C	-4.528255000	-0.052970000	0.095764000	C	0.478475000	-2.817530000	1.473572000
C	-3.932145000	-0.569705000	-2.096222000	H	0.559025000	-3.690761000	2.133162000
C	-2.422351000	2.780050000	0.865654000	C	1.530261000	-0.944099000	2.758969000
C	-2.345328000	2.938040000	-1.449803000	H	0.493181000	-0.608890000	2.786840000
H	-2.654223000	2.209912000	2.946947000	H	1.796238000	-1.408103000	3.717304000
H	-1.082131000	1.779600000	2.200407000	C	2.941622000	-2.640822000	1.692195000
H	-4.520515000	1.427979000	1.625127000	H	2.786481000	-3.651444000	2.088823000
H	-4.545983000	-0.217550000	2.235734000	H	3.593259000	-2.117066000	2.401306000
C	-5.875075000	-0.289666000	-0.180574000	N	1.642750000	-1.904944000	1.629366000
C	-5.255188000	-0.818156000	-2.446861000	H	-0.410414000	-2.241655000	1.740034000
H	-3.103975000	-0.645614000	-2.793689000	H	-4.886480000	-4.444256000	1.617244000
C	-2.942552000	0.466413000	0.983578000	C	-4.221363000	-3.659476000	1.269196000
C	-2.859301000	4.234962000	-1.421616000	C	-3.889966000	-2.591528000	2.109748000
H	-2.097847000	2.421190000	-2.372173000	C	-3.696984000	-3.693810000	-0.023693000
H	-6.619684000	-0.164108000	0.600008000	C	-3.043466000	-1.597888000	1.623619000
C	-6.243375000	-0.679357000	-1.468292000	H	-4.288252000	-2.525614000	3.117774000
H	-5.502794000	-1.111865000	-3.461377000	H	-3.937833000	-4.500415000	-0.708362000
H	-3.176500000	4.476340000	1.961351000	C	-2.858131000	-2.654655000	-0.429871000
C	-3.161562000	4.805450000	-0.183978000	N	-2.537268000	-1.639100000	0.378206000
H	-3.021804000	4.778183000	-2.346575000	C	-2.603184000	-0.407463000	2.448979000
H	-7.286329000	-0.867571000	-1.705138000	H	-2.425615000	-2.622570000	-1.425321000
H	-3.569358000	5.810170000	-0.125613000	H	-1.567754000	-0.561471000	2.768285000
H	1.040925000	1.841487000	-1.349794000	H	-3.228991000	-0.301324000	3.346737000
H	-0.364865000	4.309859000	0.043854000	N	-2.617350000	0.818329000	1.629565000
C	0.410452000	4.796523000	-0.558957000	N	-3.533107000	0.581492000	-0.982767000
H	-0.000428000	5.780003000	-0.852447000	N	-1.535813000	2.573452000	-0.070469000
C	0.812707000	4.013930000	-1.773045000	C	-1.805756000	1.906629000	2.223090000
H	0.105815000	3.672120000	-2.524203000	C	-4.009659000	1.255354000	1.322057000
C	2.284982000	4.144609000	-2.046744000	C	-4.475224000	0.876660000	-0.068793000
H	2.487158000	4.569648000	-3.041178000	C	-3.887078000	0.330409000	-2.254598000
H	2.772933000	3.155828000	-2.049954000	C	-1.631109000	3.007020000	1.197360000
C	1.738910000	4.982480000	0.205338000	C	-1.400672000	3.453153000	-1.068362000
H	1.739222000	5.864473000	0.854163000	H	-2.253190000	2.295006000	3.149142000
H	1.912513000	4.103595000	0.837016000	H	-0.825203000	1.471125000	2.443177000
C	2.806959000	5.063353000	-0.907365000	H	-4.053702000	2.347849000	1.399006000
H	2.874047000	6.093650000	-1.274478000	H	-4.707725000	0.861650000	2.072296000
H	3.807311000	4.781081000	-0.557962000	C	-5.828332000	0.908167000	-0.404135000

$I-^{6}\text{Int}_{\text{is-is}}$

Fe	1.513942000	-0.683906000	-0.061975000
O	1.658179000	0.205048000	-1.654189000
Fe	-1.578719000	0.337866000	-0.295698000
O	-1.006027000	0.254073000	-1.987518000
H	-0.017743000	0.314868000	-1.993024000
O	-0.036276000	0.018727000	0.584617000
N	0.587865000	-2.254642000	-0.875248000
N	2.522733000	0.568572000	1.146434000
N	3.253116000	-1.744353000	-0.526398000
C	0.325564000	-3.226769000	0.025031000
C	-0.119095000	-4.483623000	-0.371186000
H	-0.308149000	-5.251477000	0.372282000
C	-0.315746000	-4.728927000	-1.733680000
H	-0.652760000	-5.704649000	-2.071064000
C	-0.069300000	-3.707008000	-2.651440000
H	-0.210911000	-3.858345000	-3.716290000
C	0.392235000	-2.476703000	-2.181211000
H	0.622975000	-1.645072000	-2.834980000
C	2.408675000	0.251445000	2.457464000
C	3.049807000	0.991418000	3.445834000
H	2.954337000	0.700079000	4.487343000
C	3.815214000	2.101401000	3.074023000
H	4.321591000	2.695658000	3.828602000

C	3.930500000	2.418581000	1.721254000
H	4.517471000	3.264584000	1.380304000
C	3.275635000	1.616357000	0.787820000
H	3.348412000	1.814619000	-0.274549000
C	3.640276000	-2.679378000	0.356821000
C	4.669455000	-3.576928000	0.080657000
H	4.951192000	-4.325529000	0.815010000
C	5.325677000	-3.485496000	-1.147702000
H	6.133173000	-4.169807000	-1.389921000
C	4.925384000	-2.504834000	-2.058596000
H	5.408943000	-2.401849000	-3.024216000
C	3.876227000	-1.656880000	-1.714344000
H	3.485128000	-0.889867000	-2.373672000
C	0.478475000	-2.817530000	1.473572000
H	0.559025000	-3.690761000	2.133162000
C	1.530261000	-0.944099000	2.758969000
H	0.493181000	-0.608890000	2.786840000
H	1.796238000	-1.408103000	3.717304000
C	2.941622000	-2.640822000	1.692195000
H	2.786481000	-3.651444000	2.088823000
H	3.593259000	-2.117066000	2.401306000
N	1.642750000	-1.904944000	1.629366000
H	-0.410414000	-2.241655000	1.740034000
H	-4.886480000	-4.444256000	1.617244000
C	-4.221363000	-3.659476000	1.269196000
C	-3.889966000	-2.591528000	2.109748000
C	-3.696984000	-3.693810000	-0.023693000
C	-3.043466000	-1.597888000	1.623619000
H	-4.288252000	-2.525614000	3.117774000
H	-3.937833000	-4.500415000	-0.708362000
C	-2.858131000	-2.654655000	-0.429871000
N	-2.537268000	-1.639100000	0.378206000
C	-2.603184000	-0.407463000	2.448979000
H	-2.425615000	-2.622570000	-1.425321000
H	-1.567754000	-0.561471000	2.768285000
H	-3.228991000	-0.301324000	3.346737000
N	-2.617350000	0.818329000	1.629565000
N	-3.533107000	0.581492000	-0.982767000
N	-1.535813000	2.573452000	-0.070469000
C	-1.805756000	1.906629000	2.223090000
C	-4.009659000	1.255354000	1.322057000
C	-4.475224000	0.876660000	-0.068793000
C	-3.887078000	0.330409000	-2.254598000
C	-1.631109000	3.007020000	1.197360000
C	-1.400672000	3.453153000	-1.068362000
H	-2.253190000	2.295006000	3.149142000
H	-0.825203000	1.471125000	2.443177000
H	-4.053702000	2.347849000	1.399006000
H	-4.707725000	0.861650000	2.072296000
C	-5.828332000	0.908167000	-0.404135000
C	-5.216266000	0.356211000	-2.667060000
H	-3.056955000	0.114157000	-2.919780000
C	-1.586192000	4.362080000	1.516214000
C	-1.343219000	4.828339000	-0.837541000
H	-1.337266000	3.022082000	-2.062914000
H	-6.570354000	1.143097000	0.353151000
C	-6.204202000	0.644165000	-1.722016000
H	-5.467974000	0.152712000	-3.702488000
H	-1.680442000	4.686565000	2.548208000
C	-1.433215000	5.286662000	0.477907000
H	-1.234840000	5.517250000	-1.668548000
H	-7.252063000	0.665548000	-2.006371000
H	-1.399329000	6.350291000	0.694612000
H	1.021912000	2.975103000	-1.849603000
H	1.939531000	1.128347000	-1.546843000
C	1.832393000	3.690740000	-2.042971000
H	1.484950000	4.318240000	-2.884735000
C	3.146730000	3.045022000	-2.378165000
H	3.264578000	2.310269000	-3.170281000
C	4.297248000	3.796859000	-1.767114000
H	5.039751000	4.105650000	-2.516584000
H	4.859267000	3.178546000	-1.044098000
C	2.166893000	4.576168000	-0.821231000
H	1.486810000	5.426181000	-0.711979000
H	2.096198000	3.977137000	0.096068000

C	3.627144000	5.011096000	-1.068888000
H	3.640003000	5.869905000	-1.749768000
H	4.142667000	5.315531000	-0.151203000

I-⁴Int_{is-is}

Fe	1.511490000	-0.688112000	-0.061931000
O	1.657272000	0.202555000	-1.653141000
Fe	-1.578870000	0.340758000	-0.296123000
O	-1.006655000	0.253652000	-1.987979000
H	-0.018251000	0.311914000	-1.993625000
O	-0.037777000	0.017202000	0.584868000
N	0.582387000	-2.256638000	-0.876225000
N	2.522250000	0.561733000	1.147097000
N	3.247877000	-1.751979000	-0.526826000
C	0.317360000	-3.228204000	0.023885000
C	-0.130555000	-4.483819000	-0.372601000
H	-0.321827000	-5.251264000	0.370720000
C	-0.327606000	-4.728416000	-1.735164000
H	-0.667195000	-5.703181000	-2.072736000
C	-0.078157000	-3.707072000	-2.652746000
H	-0.219885000	-3.857893000	-3.717652000
C	0.386578000	-2.478079000	-2.182249000
H	0.619717000	-1.647076000	-2.835959000
C	2.407312000	0.244634000	2.458053000
C	3.049750000	0.983196000	3.446613000
H	2.953471000	0.691974000	4.488081000
C	3.817598000	2.091562000	3.075019000
H	4.325037000	2.684719000	3.829751000
C	3.934008000	2.408503000	1.722292000
H	4.523016000	3.253170000	1.381576000
C	3.277614000	1.607812000	0.788593000
H	3.351230000	1.805757000	-0.273836000
C	3.633100000	-2.688078000	0.356106000
C	4.660625000	-3.587438000	0.079673000
H	4.940887000	-4.336880000	0.813732000
C	5.317168000	-3.496693000	-1.148573000
H	6.123396000	-4.182428000	-1.390986000
C	4.918936000	-2.514823000	-2.059080000
H	5.402908000	-2.412304000	-3.024542000
C	3.871368000	-1.665001000	-1.714606000
H	3.482055000	-0.896650000	-2.373454000
C	0.470830000	-2.819632000	1.472551000
H	0.549073000	-3.693216000	2.131957000
C	1.526611000	-0.949332000	2.759087000
H	0.490167000	-0.612180000	2.787139000
C	1.791719000	-1.414277000	3.717211000
C	2.934384000	-2.648728000	1.691481000
H	2.776897000	-3.659242000	2.087466000
H	3.587172000	-2.126908000	2.400961000
N	1.637218000	-1.909854000	1.629024000
H	-0.416786000	-2.241665000	1.738770000
H	-4.897735000	-4.431951000	1.620870000
C	-4.231007000	-3.648841000	1.272138000
C	-3.897400000	-2.580874000	2.111788000
C	-3.706728000	-3.685390000	-0.020742000
C	-3.048829000	-1.589411000	1.624816000
H	-4.295527000	-2.513309000	3.119767000
H	-3.949281000	-4.492081000	-0.704706000
C	-2.865776000	-2.648291000	-0.427836000
N	-2.542793000	-1.632760000	0.379433000
C	-2.605754000	-0.399351000	2.449250000
H	-2.433293000	-2.617819000	-1.423361000
H	-1.570826000	-0.555868000	2.768998000
H	-3.231547000	-0.290799000	3.346726000
N	-2.616394000	0.825798000	1.628809000
N	-3.532755000	0.589514000	-0.983413000
N	-1.528154000	2.575790000	-0.072675000
C	-1.801674000	1.912252000	2.221432000
C	-4.007360000	1.266622000	1.320823000
C	-4.474068000	0.887700000	-0.069584000
C	-3.887487000	0.338204000	-2.254983000
C	-1.623054000	3.010999000	1.194605000
C	-1.389229000	3.453924000	-1.071449000
H	-2.248227000	2.303057000	3.146886000
H	-0.822560000	1.473957000	2.442372000

H	-4.048069000	2.359347000	1.396408000
H	-4.706624000	0.875984000	2.071552000
C	-5.827138000	0.922151000	-0.404779000
C	-5.216661000	0.366858000	-2.667317000
H	-3.057989000	0.119290000	-2.920077000
C	-1.573998000	4.366276000	1.512001000
C	-1.327492000	4.829151000	-0.842077000
H	-1.326288000	3.021439000	-2.065430000
H	-6.568503000	1.159461000	0.352406000
C	-6.203793000	0.657954000	-1.722401000
H	-5.468979000	0.163099000	-3.702545000
H	-1.668008000	4.692200000	2.543563000
C	-1.417173000	5.289205000	0.472808000
H	-1.216126000	5.516820000	-1.673718000
H	-7.251634000	0.681585000	-2.006651000
H	-1.380023000	6.352958000	0.688366000
H	1.036681000	2.975038000	-1.849054000
H	1.934046000	1.126768000	-1.543680000
C	1.849179000	3.688967000	-2.041240000
H	1.503936000	4.316534000	-2.883839000
C	3.163093000	3.041162000	-2.373908000
H	3.281209000	2.305170000	-3.164794000
C	4.313594000	3.789840000	-1.759122000
H	5.059746000	4.096404000	-2.505852000
H	4.871031000	3.169970000	-1.033872000
C	2.182703000	4.574167000	-0.819037000
H	1.504089000	5.425584000	-0.711574000
H	2.108693000	3.975505000	0.098242000
C	3.644409000	5.005962000	-1.063389000
H	3.660710000	5.864245000	-1.744864000
H	4.158321000	5.309957000	-0.144656000

I-⁴Int_{is-is}

Fe	-1.631284000	-0.298036000	-0.148310000
O	-1.692030000	0.759900000	1.348125000
Fe	1.586247000	0.178573000	0.189816000
O	0.929014000	0.276965000	1.856652000
H	-0.042486000	0.449176000	1.805588000
O	0.052747000	0.018275000	-0.719958000
N	-1.096754000	-1.927669000	0.877378000
N	-2.270620000	1.005368000	-1.527642000
N	-3.572156000	-0.940124000	0.267326000
C	-0.944769000	-3.010000000	0.084611000
C	-0.750346000	-4.279878000	0.618064000
H	-0.642746000	-5.135163000	-0.041441000
C	-0.698594000	-4.424627000	2.007654000
H	-0.556932000	-5.406032000	2.450596000
C	-0.841849000	-3.295826000	2.815737000
H	-0.813127000	-3.368797000	3.897723000
C	-1.048799000	-2.056737000	2.209142000
H	-1.194130000	-1.141787000	2.770130000
C	-2.167619000	0.537200000	-2.793088000
C	-2.589257000	1.289423000	-3.884758000
H	-2.511569000	0.879892000	-4.887261000
C	-3.115719000	2.566120000	-3.665106000
H	-3.452630000	3.171227000	-4.501344000
C	-3.215997000	3.040795000	-2.357589000
H	-3.628060000	4.020678000	-2.141451000
C	-2.788242000	2.222665000	-1.312530000
H	-2.858025000	2.532302000	-0.277436000
C	-4.081627000	-1.875156000	-0.551030000
C	-5.290299000	-2.513679000	-0.281381000
H	-5.670419000	-3.271449000	-0.959941000
C	-5.996055000	-2.153157000	0.867448000
H	-6.941791000	-2.632244000	1.102187000
C	-5.467193000	-1.170741000	1.708258000
H	-5.985698000	-0.862258000	2.609852000
C	-4.245081000	-0.591599000	1.377687000
H	-3.752801000	0.159211000	1.986364000
C	-0.929005000	-2.723138000	-1.401528000
H	-1.126322000	-3.629645000	-1.987750000
C	-1.540245000	-0.835014000	-2.928420000
H	-0.455709000	-0.716891000	-2.921989000
H	-1.850508000	-1.328893000	-3.858125000
C	-3.302324000	-2.131375000	-1.817604000

H	-3.316089000	-3.195588000	-2.082421000
H	-3.798337000	-1.594337000	-2.634640000
N	-1.894828000	-1.638728000	-1.729256000
H	0.065447000	-2.342217000	-1.644485000
H	4.049073000	-5.324841000	-0.716590000
C	3.528972000	-4.386755000	-0.546541000
C	3.456565000	-3.427551000	-1.562208000
C	2.936988000	-4.116806000	0.688429000
C	2.790664000	-2.231875000	-1.302847000
H	3.914726000	-3.600299000	-2.531460000
H	2.980456000	-4.833114000	1.502290000
C	2.293415000	-2.890942000	0.864600000
N	2.220867000	-1.980184000	-0.111638000
C	2.617178000	-1.137737000	-2.335622000
H	1.820726000	-2.613776000	1.802099000
H	1.601466000	-1.193939000	-2.741673000
H	3.321726000	-1.272568000	-3.168859000
N	2.759846000	0.194381000	-1.716304000
N	3.519124000	0.277910000	0.961188000
N	1.853331000	2.345761000	-0.394594000
C	2.139908000	1.263124000	-2.531273000
C	4.181967000	0.496801000	-1.384100000
C	4.530340000	0.274240000	0.072873000
C	3.780993000	0.181965000	2.275820000
C	2.043779000	2.532528000	-1.712096000
C	1.752691000	3.406384000	0.415154000
H	2.689800000	1.438237000	-3.467018000
H	1.124698000	0.925097000	-2.762673000
H	4.369169000	1.553118000	-1.608970000
H	4.856962000	-0.083584000	-2.026522000
C	5.857231000	0.152241000	0.482381000
C	5.081423000	0.074834000	2.761124000
H	2.901661000	0.192673000	2.912220000
C	2.137952000	3.805092000	-2.271083000
C	1.823115000	4.715609000	-0.063030000
H	1.608060000	3.186690000	1.466718000
H	6.654658000	0.143913000	-0.254668000
C	6.136937000	0.052662000	1.846392000
H	5.258551000	0.004918000	3.829111000
H	2.310717000	3.922660000	-3.336750000
C	2.016638000	4.915887000	-1.430918000
H	1.737007000	5.551246000	0.623609000
H	7.163469000	-0.039779000	2.188470000
H	2.087731000	5.920304000	-1.837716000
H	-1.542447000	1.709279000	1.162447000
H	0.083474000	2.473256000	2.766149000
C	-1.407698000	3.707471000	1.736807000
H	-0.943568000	4.086595000	0.829543000
C	-0.624652000	3.291214000	2.954613000
H	-0.038042000	4.143732000	3.343099000
C	-1.724181000	2.891714000	3.964048000
H	-1.399355000	2.974032000	5.005849000
H	-2.013646000	1.851146000	3.769961000
C	-2.864564000	3.898167000	2.071482000
H	-3.282458000	4.830431000	1.667850000
H	-3.483836000	3.076188000	1.665318000
C	-2.893352000	3.832479000	3.618907000
H	-2.696913000	4.831457000	4.027151000
H	-3.856227000	3.491521000	4.013080000

$I^{-2}Int_{ls-is}$

Fe	1.492507000	-0.703498000	-0.060315000
O	1.662117000	0.186363000	-1.662430000
Fe	-1.580001000	0.347132000	-0.292833000
O	-1.013733000	0.214857000	-1.985381000
H	-0.024590000	0.260044000	-1.993600000
O	-0.033459000	0.035613000	0.564197000
N	0.541340000	-2.262609000	-0.880609000
N	2.526665000	0.520551000	1.145979000
N	3.207731000	-1.804519000	-0.531667000
C	0.258125000	-3.226318000	0.022552000
C	-0.206804000	-4.476951000	-0.370392000
H	-0.413362000	-5.237979000	0.375438000
C	-0.399503000	-4.725221000	-1.732857000
H	-0.752240000	-5.696252000	-2.067730000

C	-0.126635000	-3.713195000	-2.654188000
H	-0.262025000	-3.868033000	-3.719331000
C	0.353582000	-2.489067000	-2.186898000
H	0.607290000	-1.666723000	-2.843832000
C	2.407796000	0.208874000	2.457813000
C	3.067532000	0.936919000	3.442498000
H	2.968000000	0.651231000	4.485177000
C	3.857495000	2.027867000	3.064966000
H	4.379013000	2.612691000	3.816606000
C	3.977386000	2.338561000	1.711099000
H	4.582506000	3.170146000	1.366712000
C	3.302262000	1.549361000	0.780796000
H	3.374947000	1.740333000	-0.283182000
C	3.575171000	-2.747214000	0.351463000
C	4.583512000	-3.667600000	0.073770000
H	4.850146000	-4.422349000	0.807486000
C	5.239249000	-3.590491000	-1.156072000
H	6.030780000	-4.292732000	-1.399751000
C	4.860252000	-2.600570000	-2.066136000
H	5.345468000	-2.507999000	-3.031996000
C	3.830874000	-1.729195000	-1.720057000
H	3.456705000	-0.950211000	-2.375641000
C	0.414767000	-2.816988000	1.470995000
H	0.474905000	-3.691384000	2.131405000
C	1.504277000	-0.967678000	2.759889000
H	0.473957000	-0.611614000	2.788750000
H	1.760297000	-1.437183000	3.718323000
C	2.880441000	-2.691727000	1.689095000
H	2.705413000	-3.698208000	2.088100000
H	3.545069000	-2.180307000	2.395143000
N	1.597245000	-1.928969000	1.629354000
H	-0.462903000	-2.223093000	1.735415000
H	-4.991093000	-4.342327000	1.636430000
C	-4.308167000	-3.573721000	1.286771000
C	-3.955851000	-2.509749000	2.124021000
C	-3.781670000	-3.625344000	-0.004758000
C	-3.086570000	-1.537063000	1.636167000
H	-4.355276000	-2.431196000	3.130669000
H	-4.038899000	-4.429352000	-0.686489000
C	-2.919126000	-2.606781000	-0.413336000
N	-2.578208000	-1.595485000	0.392153000
C	-2.622164000	-0.351899000	2.456549000
H	-2.483487000	-2.586525000	-1.407771000
H	-1.591991000	-0.527663000	2.782562000
H	-3.248883000	-0.226220000	3.351117000
N	-2.605216000	0.868486000	1.628755000
N	-3.527699000	0.649012000	-0.986145000
N	-1.478070000	2.578661000	-0.087044000
C	-1.767438000	1.941602000	2.213424000
C	-3.986529000	1.338474000	1.318095000
C	-4.461668000	0.968502000	-0.072084000
C	-3.888653000	0.404315000	-2.257244000
C	-1.562395000	3.026599000	1.176596000
C	-1.317007000	3.444086000	-1.093462000
H	-2.206900000	2.351107000	3.134121000
H	-0.798557000	1.484595000	2.441227000
H	-4.003880000	2.431897000	1.392673000
H	-4.694458000	0.964027000	2.068897000
C	-5.813867000	1.033016000	-0.406406000
C	-5.217095000	0.462730000	-2.668986000
H	-3.064517000	0.164420000	-2.921921000
C	-1.480246000	4.383009000	1.482035000
C	-1.221439000	4.819257000	-0.875861000
H	-1.264416000	3.001340000	-2.083581000
H	-6.549444000	1.287160000	0.350973000
C	-6.196893000	0.776652000	-1.723782000
H	-5.474638000	0.263678000	-3.703850000
H	-1.566405000	4.720136000	2.510671000
C	-1.300370000	5.292731000	0.434887000
H	-1.091623000	5.496498000	-1.713332000
H	-7.244096000	0.823493000	-2.007521000
H	-1.236893000	6.357051000	0.641233000
H	1.891251000	1.121885000	-1.543759000
H	1.110735000	3.008746000	-1.872673000
C	1.947668000	3.701533000	-2.036149000

H	1.636030000	4.355401000	-2.871906000
C	3.247987000	3.021951000	-2.356278000
H	3.357522000	2.284269000	-3.146524000
C	4.408601000	3.730290000	-1.713908000
H	5.168956000	4.036628000	-2.446514000
H	4.944896000	3.081351000	-0.998453000
C	2.282844000	4.552952000	-0.790622000
H	1.626910000	5.421465000	-0.678716000
H	2.174331000	3.938742000	0.112784000
C	3.760873000	4.947283000	-0.998774000
H	3.814896000	5.822238000	-1.656638000
H	4.265902000	5.212967000	-0.063250000

I-⁴Int_{ls-ls}

Fe	-1.163777000	0.778172000	0.118339000
O	-1.360598000	-0.230738000	-1.438215000
Fe	1.801437000	-0.513093000	-0.246290000
O	1.281151000	-0.067302000	-1.896881000
H	0.298809000	-0.209940000	-1.904811000
O	0.372551000	0.111339000	0.735316000
N	-0.261785000	2.295424000	-0.830298000
N	-2.141478000	-0.386154000	1.432559000
N	-2.886396000	1.837744000	-0.367867000
C	0.108235000	3.282817000	0.011974000
C	0.615994000	4.489987000	-0.458678000
H	0.897259000	5.270435000	0.241387000
C	0.748279000	4.670987000	-1.838398000
H	1.133876000	5.606268000	-2.233508000
C	0.362613000	3.642253000	-2.699180000
H	0.438867000	3.749153000	-3.776020000
C	-0.148928000	2.465214000	-2.153313000
H	-0.485732000	1.634719000	-2.760037000
C	-1.967359000	0.004075000	2.716664000
C	-2.541295000	-0.692820000	3.775694000
H	-2.399012000	-0.343846000	4.793942000
C	-3.299914000	-1.835004000	3.503339000
H	-3.755395000	-2.396832000	4.313280000
C	-3.477019000	-2.227481000	2.176818000
H	-4.069222000	-3.097510000	1.916402000
C	-2.889713000	-1.466280000	1.166945000
H	-3.015782000	-1.716999000	0.119184000
C	-3.226500000	2.831891000	0.468440000
C	-4.252248000	3.727200000	0.170299000
H	-4.498502000	4.525356000	0.864172000
C	-4.949397000	3.571358000	-1.028981000
H	-5.754828000	4.252737000	-1.286113000
C	-4.590955000	2.533838000	-1.893467000
H	-5.105178000	2.383928000	-2.836892000
C	-3.543399000	1.691582000	-1.531034000
H	-3.178023000	0.880442000	-2.151204000
C	-0.005681000	2.953173000	1.484308000
H	-0.024364000	3.862861000	2.098413000
C	-1.078491000	1.213779000	2.916222000
H	-0.042735000	0.872444000	2.951108000
H	-1.320101000	1.739860000	3.849021000
C	-2.472945000	2.879452000	1.776854000
H	-2.274428000	3.915328000	2.078076000
H	-3.110916000	2.440526000	2.552986000
N	-1.199655000	2.100322000	1.731318000
H	0.866547000	2.350363000	1.750102000
H	5.259966000	3.965217000	1.103345000
C	4.576398000	3.166988000	0.829974000
C	4.288505000	2.146081000	1.742093000
C	3.984331000	3.140998000	-0.433886000
C	3.415142000	1.131800000	1.359849000
H	4.737271000	2.134448000	2.730654000
H	4.187024000	3.914500000	-1.166820000
C	3.128419000	2.087538000	-0.751778000
N	2.857987000	1.117158000	0.129783000
C	2.961508000	0.028894000	2.298625000
H	2.631040000	1.978924000	-1.709592000
H	2.029529000	0.353627000	2.768872000
H	3.703475000	-0.145263000	3.088595000
N	2.653440000	-1.218578000	1.552871000
N	3.577229000	-1.260139000	-0.993620000

N	0.936513000	-2.316503000	-0.179348000
C	1.568098000	-2.046797000	2.145686000
C	3.869224000	-2.037702000	1.276120000
C	4.436905000	-1.775995000	-0.098540000
C	3.967453000	-1.085293000	-2.267728000
C	0.946003000	-2.884138000	1.046719000
C	0.390403000	-2.966627000	-1.215817000
H	1.934101000	-2.674005000	2.969004000
H	0.804614000	-1.357938000	2.512627000
H	3.578963000	-3.093950000	1.323862000
H	4.625851000	-1.880271000	2.054808000
C	5.740478000	-2.124465000	-0.445137000
C	5.248169000	-1.425912000	-2.695834000
H	3.211142000	-0.657682000	-2.917500000
C	0.393760000	-4.142719000	1.266285000
C	-0.194898000	-4.223100000	-1.068169000
H	0.442531000	-2.442912000	-2.164053000
H	6.413131000	-2.532587000	0.303231000
C	6.152145000	-1.947249000	-1.767302000
H	5.529403000	-1.276907000	-3.732961000
H	0.430144000	-4.585414000	2.256901000
C	-0.194450000	-4.819036000	0.193452000
H	-0.637832000	-4.718504000	-1.924796000
H	7.161727000	-2.212374000	-2.066490000
H	-0.631231000	-5.802457000	0.338866000
H	-3.003576000	-4.123144000	-0.318107000
H	-1.552471000	-1.160948000	-1.239981000
C	-3.625552000	-3.961611000	-1.212549000
H	-3.605521000	-4.914521000	-1.770059000
C	-3.149174000	-2.826776000	-2.077116000
H	-2.183721000	-2.815011000	-2.573639000
C	-4.290972000	-1.937981000	-2.483657000
H	-4.256551000	-1.652118000	-3.543167000
H	-4.282340000	-0.995474000	-1.907173000
C	-5.086843000	-3.572859000	-0.878008000
H	-5.721666000	-4.439259000	-0.668773000
H	-5.108024000	-2.920028000	0.005226000
C	-5.543312000	-2.767360000	-2.109600000
H	-5.784558000	-3.454171000	-2.929732000
H	-6.426635000	-2.150640000	-1.914585000

I-²Int_{ls-ls}

Fe	-1.164299000	0.777880000	0.118230000
O	-1.360822000	-0.229840000	-1.439380000
Fe	1.801265000	-0.512785000	-0.246484000
O	1.280984000	-0.066791000	-1.896993000
H	0.298611000	-0.209410000	-1.905006000
O	0.372096000	0.111152000	0.734987000
N	-0.262478000	2.295780000	-0.829490000
N	-2.141537000	-0.387450000	1.431798000
N	-2.887038000	1.837898000	-0.367748000
C	0.107160000	3.282881000	0.013291000
C	0.614823000	4.490327000	-0.456752000
H	0.895781000	5.270544000	0.243693000
C	0.747407000	4.671909000	-1.836368000
H	1.132929000	5.607422000	-2.231001000
C	0.362161000	3.643450000	-2.697664000
H	0.438681000	3.750796000	-3.774441000
C	-0.149306000	2.466095000	-2.152409000
H	-0.485787000	1.635751000	-2.759520000
C	-1.967487000	0.002090000	2.716127000
C	-2.540574000	-0.696019000	3.774814000
H	-2.398420000	-0.347561000	4.793256000
C	-3.298095000	-1.838792000	3.501879000
H	-3.752902000	-2.401564000	4.311544000
C	-3.474897000	-2.230703000	2.175157000
H	-4.066148000	-3.101250000	1.914326000
C	-2.888571000	-1.468260000	1.165647000
H	-3.014330000	-1.718772000	0.117780000
C	-3.227224000	2.831533000	0.469145000
C	-4.252532000	3.727405000	0.171227000
H	-4.498840000	4.525107000	0.865602000
C	-4.949168000	3.572726000	-1.028510000
H	-5.754259000	4.254563000	-1.285491000
C	-4.590594000	2.535819000	-1.893662000

H	-5.104363000	2.386860000	-2.837485000	O	0.351746000	0.172609000	0.824627000
C	-3.543463000	1.692947000	-1.531390000	N	-0.770498000	2.054018000	-0.847355000
H	-3.177952000	0.882306000	-2.152119000	N	-1.959155000	-0.737250000	1.735903000
C	-0.006941000	2.952605000	1.485475000	N	-3.237036000	1.141367000	-0.166445000
H	-0.026000000	3.862053000	2.099927000	C	-0.535494000	3.157553000	-0.107452000
C	-1.079311000	1.212177000	2.916443000	C	-0.271987000	4.389277000	-0.699180000
H	-0.043405000	0.871304000	2.951445000	H	-0.096468000	5.262778000	-0.079085000
H	-1.321376000	1.737638000	3.849475000	C	-0.245719000	4.472751000	-2.094114000
C	-2.474209000	2.877893000	1.777904000	H	-0.050515000	5.423012000	-2.582395000
H	-2.276183000	3.913501000	2.080380000	C	-0.491597000	3.324529000	-2.848610000
H	-3.112321000	2.437841000	2.553282000	H	-0.492348000	3.351338000	-3.933073000
N	-1.200647000	2.099259000	1.732004000	C	-0.759811000	2.128260000	-2.183995000
H	0.865469000	2.350006000	1.751171000	H	-0.981052000	1.204767000	-2.703065000
H	5.258785000	3.966182000	1.103680000	C	-1.829595000	-0.194896000	2.969427000
C	4.575387000	3.167835000	0.830229000	C	-2.236021000	-0.875480000	4.113067000
C	4.287631000	2.146830000	1.742280000	H	-2.137739000	-0.404606000	5.086419000
C	3.983410000	3.141784000	-0.433672000	C	-2.772131000	-2.160388000	3.983712000
C	3.414490000	1.132397000	1.359929000	H	-3.099828000	-2.708891000	4.861677000
H	4.736338000	2.135232000	2.730868000	C	-2.888554000	-2.717301000	2.710658000
H	4.186015000	3.915350000	-1.166564000	H	-3.304250000	-3.708298000	2.562486000
C	3.127720000	2.088177000	-0.751669000	C	-2.475369000	-1.967594000	1.609796000
N	2.857408000	1.117708000	0.129832000	H	-2.555029000	-2.352385000	0.600468000
C	2.961050000	0.029323000	2.298596000	C	-3.713253000	2.127778000	0.610681000
H	2.630425000	1.979506000	-1.709517000	C	-4.912301000	2.778833000	0.325698000
H	2.028953000	0.353787000	2.768796000	H	-5.265675000	3.578052000	0.970349000
H	3.702996000	-0.144699000	3.088616000	C	-5.641598000	2.380372000	-0.795536000
N	2.653360000	-1.218169000	1.552727000	H	-6.580232000	2.868459000	-1.040128000
N	3.577278000	-1.259272000	-0.993759000	C	-5.142144000	1.352073000	-1.598398000
N	0.936888000	-2.316479000	-0.179689000	H	-5.675506000	1.014709000	-2.480834000
C	1.568218000	-2.046718000	2.145422000	C	-3.928754000	0.763062000	-1.255436000
C	3.869380000	-2.036936000	1.275947000	H	-3.460678000	-0.019939000	-1.838514000
C	4.437044000	-1.774978000	-0.098678000	C	-0.512591000	2.941511000	1.389793000
C	3.967508000	-1.84221000	-2.267835000	H	-0.674190000	3.881819000	1.932530000
C	0.946445000	-2.884176000	1.046361000	C	-1.171542000	1.167605000	3.015527000
C	0.391100000	-2.966732000	-1.216227000	H	-0.089914000	1.021805000	3.008534000
H	1.934338000	-2.673877000	2.968727000	H	-1.458792000	1.722817000	3.917938000
H	0.804531000	-1.358095000	2.512381000	C	-2.904881000	2.446459000	1.846028000
H	3.579410000	-3.093267000	1.323604000	H	-2.885722000	3.526977000	2.033377000
H	4.625943000	-1.879355000	2.054668000	H	-3.403894000	1.985369000	2.706572000
C	5.740721000	-2.123085000	-0.445249000	N	-1.512685000	1.908799000	1.775885000
C	5.248329000	-1.424478000	-2.695914000	H	0.470379000	2.537265000	1.646599000
H	3.211108000	-0.656738000	-2.917591000	H	4.529408000	4.768192000	0.679873000
C	0.394621000	-4.142950000	1.265817000	C	3.979016000	3.851010000	0.492739000
C	-0.193717000	-4.223461000	-1.068704000	C	3.913715000	2.858186000	1.475997000
H	0.443068000	-2.442913000	-2.164416000	C	3.338098000	3.644433000	-0.730022000
H	6.413451000	-2.531091000	0.303113000	C	3.207410000	1.689777000	1.204298000
C	6.152396000	-1.945658000	-1.767383000	H	4.405065000	2.986652000	2.435610000
H	5.529570000	-1.275318000	-3.733017000	H	3.369463000	4.391555000	-1.515796000
H	0.431063000	-4.585670000	2.256419000	C	2.660785000	2.443913000	-0.937904000
C	-0.193199000	-4.819454000	0.192879000	N	2.603857000	1.500791000	0.010986000
H	-0.636321000	-4.719026000	-1.925408000	C	2.990046000	0.595757000	2.233925000
H	7.162059000	-2.210500000	-2.066550000	H	2.144488000	2.192524000	-1.858194000
H	-0.629587000	-5.803066000	0.338190000	H	2.047052000	0.805172000	2.746140000
H	-3.005247000	-4.129502000	-0.320168000	H	3.794176000	0.594689000	2.980902000
H	-1.553553000	-1.160085000	-1.242149000	N	2.841976000	-0.733850000	1.587200000
C	-3.626489000	-3.964824000	-1.214560000	N	3.648062000	-0.808265000	-0.999480000
H	-3.608112000	-4.916566000	-1.774094000	N	1.241536000	-2.198656000	0.026401000
C	-3.147353000	-2.829115000	-2.076399000	C	1.923731000	-1.669543000	2.291906000
H	-2.181589000	-2.818134000	-2.572320000	C	4.153101000	-1.381521000	1.294082000
C	-4.286884000	-1.936640000	-2.481064000	C	4.614738000	-1.127136000	-0.121404000
H	-4.251393000	-1.648141000	-3.539825000	C	3.952011000	-0.658756000	-2.299793000
H	-4.276119000	-0.995563000	-1.902246000	C	1.383863000	-2.665847000	1.286233000
C	-5.087151000	-3.573769000	-0.879820000	C	0.748580000	-2.994424000	-0.931284000
H	-5.723958000	-4.439344000	-0.673249000	H	2.419024000	-2.175699000	3.130864000
H	-5.107455000	-2.923272000	0.005141000	H	1.082196000	-1.077705000	2.657135000
C	-5.541276000	-2.764013000	-2.109514000	H	4.025845000	-2.463685000	1.416211000
H	-5.783871000	-3.448124000	-2.931499000	H	4.910791000	-1.065803000	2.021994000
H	-6.423213000	-2.145722000	-1.913183000	C	5.940681000	-1.294487000	-0.514366000
				C	5.250925000	-0.826845000	-2.773265000
				H	3.110928000	-0.395425000	-2.932354000
				C	1.025749000	-3.968699000	1.620338000
				C	0.352682000	-4.304712000	-0.668032000
				H	0.678610000	-2.542981000	-1.914318000
				H	6.699896000	-1.544996000	0.220424000
				C	6.263334000	-1.142868000	-1.864226000

I-²Int_{ls-ls}

Fe	-1.311351000	0.478826000	0.269031000
O	-1.388999000	-0.655131000	-1.211899000
Fe	1.813841000	-0.294325000	-0.203782000
O	1.151919000	-0.053678000	-1.847791000
H	0.212559000	-0.366291000	-1.788493000

H	5.461663000	-0.704063000	-3.830344000
H	1.167622000	-4.326302000	2.635561000
C	0.495018000	-4.799579000	0.628882000
H	-0.050028000	-4.915901000	-1.467839000
H	7.288328000	-1.269353000	-2.199551000
H	0.212186000	-5.821227000	0.864615000
H	-1.445311000	-1.596115000	-0.980228000
H	-1.161170000	-3.302257000	-2.954740000
C	-2.858283000	-3.539312000	-1.587255000
H	-2.562885000	-4.291988000	-0.860000000
C	-2.251079000	-3.441693000	-2.957813000
H	-2.440697000	-4.369574000	-3.526795000
C	-3.001200000	-2.254639000	-3.602861000
H	-3.018935000	-2.305887000	-4.695917000
H	-2.502906000	-1.326478000	-3.301776000
C	-4.166251000	-2.797515000	-1.518450000
H	-4.985764000	-3.418508000	-1.129745000
H	-4.103298000	-1.923227000	-0.847820000
C	-4.409669000	-2.335585000	-2.978696000
H	-5.002665000	-3.092741000	-3.504710000
H	-4.960608000	-1.389663000	-3.036361000

Ia-²TS_{Rebbs-hs}

Fe	1.521386000	0.073958000	-0.046105000
O	1.490266000	0.197427000	1.801486000
Fe	-1.664374000	0.319841000	0.293587000
O	-1.130420000	-0.663808000	1.816297000
H	-1.678619000	-0.690377000	2.613970000
O	-0.162712000	0.572340000	-0.636295000
N	2.456718000	1.998118000	-0.524684000
N	1.071119000	-2.006875000	-0.639544000
N	3.697331000	-0.493388000	-0.004122000
C	2.723237000	2.235267000	-1.821975000
C	3.471114000	3.341206000	-2.219333000
H	3.682112000	3.505841000	-3.271636000
C	3.942940000	4.222060000	-1.241296000
H	4.532357000	5.088894000	-1.525245000
C	3.656184000	3.968487000	0.101464000
H	4.011217000	4.626408000	0.887776000
C	2.910150000	2.833654000	0.419356000
H	2.662301000	2.556464000	1.439933000
C	0.973255000	-2.229341000	-1.964159000
C	0.679210000	-3.494462000	-2.469891000
H	0.626712000	-3.649719000	-3.543241000
C	0.465836000	-4.548090000	-1.576519000
H	0.248236000	-5.545295000	-1.948090000
C	0.546356000	-4.302188000	-0.204933000
H	0.390231000	-5.091139000	0.523544000
C	0.853742000	-3.009966000	0.221483000
H	0.924333000	-2.753470000	1.269381000
C	4.367702000	-0.587731000	-1.162321000
C	5.760908000	-0.648469000	-1.203261000
H	6.274561000	-0.717642000	-2.157734000
C	6.472106000	-0.623448000	-0.002732000
H	7.557041000	-0.671452000	-0.007553000
C	5.768668000	-0.529643000	1.200392000
H	6.284179000	-0.503775000	2.154748000
C	4.378744000	-0.456506000	1.153756000
H	3.765611000	-0.355269000	2.041715000
C	2.108410000	1.259559000	-2.807288000
H	2.573296000	1.372172000	-3.798276000
C	1.151124000	-1.017427000	-2.858230000
H	0.210082000	-0.458245000	-2.842348000
H	1.365964000	-1.330901000	-3.890778000
C	3.543944000	-0.704744000	-2.430104000
H	4.088617000	-0.258965000	-3.274420000
H	3.440240000	-1.773228000	-2.656255000
N	2.190358000	-0.125006000	-2.314063000
H	1.043591000	1.503386000	-2.894033000
H	-1.310593000	5.963816000	2.409356000
C	-1.391354000	4.937520000	2.063721000
C	-1.717449000	4.667015000	0.731677000
C	-1.177653000	3.784204000	2.943093000
C	-1.817480000	3.339597000	0.322724000
H	-1.891713000	5.469642000	0.021612000

H	-0.921572000	4.044104000	3.983459000
C	-1.308687000	2.574252000	2.457764000
N	-1.630736000	2.320084000	1.182102000
C	-2.085737000	2.935446000	-1.111596000
H	-1.146010000	1.703198000	3.083686000
H	-1.120456000	2.720567000	-1.581667000
H	-2.585922000	3.744882000	-1.662076000
N	-2.864172000	1.676705000	-1.139800000
N	-3.893645000	0.046493000	0.880484000
N	-2.427655000	-1.082567000	-1.222261000
C	-2.801239000	0.985149000	-2.442631000
C	-4.251720000	1.885613000	-0.666465000
C	-4.786539000	0.720738000	0.137066000
C	-4.324890000	-0.966149000	1.647646000
C	-2.983050000	-0.514456000	-2.308137000
C	-2.462466000	-2.412288000	-1.070923000
H	-3.530821000	1.398298000	-3.153905000
H	-1.797751000	1.156989000	-2.847594000
H	-4.920258000	2.109146000	-1.509500000
H	-4.253907000	2.766135000	-0.013420000
C	-6.146660000	0.411594000	0.148830000
C	-5.666162000	-1.331996000	1.733264000
H	-3.557417000	-1.510323000	2.189192000
C	-3.613635000	-1.280472000	-3.286680000
C	-3.059864000	-3.249049000	-2.012212000
H	-1.991955000	-2.796182000	-0.171329000
H	-6.837482000	0.976861000	-0.469587000
C	-6.595846000	-0.626361000	0.966738000
H	-5.968400000	-2.152613000	2.375384000
H	-4.064938000	-0.797681000	-4.148119000
C	-3.652475000	-2.669543000	-3.135535000
H	-3.067508000	-4.322992000	-1.859661000
H	-7.650120000	-0.884543000	0.998119000
H	-4.141894000	-3.287149000	-3.882787000
H	0.573739000	-0.036693000	2.079960000
H	0.069699000	-0.619649000	4.289752000
C	0.748850000	-1.456103000	4.512221000
H	0.817064000	-1.512409000	5.613471000
C	2.107892000	-1.276604000	3.914905000
H	2.713314000	-0.393760000	4.081403000
C	2.641134000	-2.556849000	3.352002000
H	3.629071000	-2.819327000	3.759252000
H	2.784654000	-2.478689000	2.260962000
C	0.261404000	-2.802521000	3.929594000
H	-0.444048000	-3.320163000	4.588568000
H	-0.243728000	-2.606012000	2.977348000
C	1.560783000	-3.611730000	3.714323000
H	1.840197000	-4.110649000	4.648965000
H	1.457349000	-4.391237000	2.949660000

Ia-¹⁰TS_{Rebbs-hs}

Fe	-1.496750000	-0.087267000	0.254599000
O	-1.550441000	1.483289000	-0.841170000
Fe	1.640634000	0.223761000	-0.077459000
O	0.991449000	0.476316000	-1.796347000
H	0.055655000	0.760276000	-1.762627000
O	0.207093000	-0.093603000	1.043910000
N	-2.546303000	0.749141000	1.997710000
N	-1.029634000	-1.877651000	-1.005315000
N	-3.544939000	-0.678072000	-0.433614000
C	-2.608167000	-0.052143000	3.078543000
C	-3.283665000	0.334536000	4.233734000
H	-3.330570000	-0.335537000	5.086774000
C	-3.899344000	1.589388000	4.265990000
H	-4.434150000	1.913307000	5.153894000
C	-3.830547000	2.412552000	3.140089000
H	-4.305672000	3.387814000	3.124647000
C	-3.144047000	1.947895000	2.018851000
H	-3.062140000	2.523040000	1.101162000
C	-0.991596000	-3.035397000	-0.318720000
C	-0.834167000	-4.262452000	-0.960692000
H	-0.817735000	-5.179032000	-0.379077000
C	-0.706084000	-4.286072000	-2.351763000
H	-0.592415000	-5.230114000	-2.876720000
C	-0.736602000	-3.080736000	-3.055578000

H	-0.645961000	-3.054104000	-4.136430000
C	-0.905444000	-1.896117000	-2.338651000
H	-0.928983000	-0.932188000	-2.833968000
C	-4.099040000	-1.781542000	0.089965000
C	-5.259383000	-2.343530000	-0.445600000
H	-5.681694000	-3.241786000	-0.004476000
C	-5.863559000	-1.729535000	-1.542475000
H	-6.767517000	-2.147728000	-1.975270000
C	-5.290083000	-0.570640000	-2.072620000
H	-5.731322000	-0.058822000	-2.921405000
C	-4.125133000	-0.081820000	-1.488951000
H	-3.620094000	0.805459000	-1.851809000
C	-1.883112000	-1.376144000	2.944074000
H	-2.211510000	-2.081292000	3.721302000
C	-1.072116000	-2.911806000	1.188067000
H	-0.104159000	-2.537341000	1.537179000
H	-1.268968000	-3.893331000	1.644458000
C	-3.468407000	-2.361966000	1.343383000
H	-4.085865000	-2.049665000	2.194928000
H	-3.519222000	-3.458864000	1.310914000
N	-2.080531000	-1.911971000	1.581579000
H	-0.809771000	-1.190959000	3.054070000
H	2.147461000	5.915176000	1.878635000
C	2.054823000	4.901687000	1.499776000
C	2.338574000	3.812404000	2.328611000
C	1.664413000	4.671383000	0.178444000
C	2.210348000	2.523557000	1.814148000
H	2.654651000	3.957691000	3.357090000
H	1.442503000	5.490963000	-0.496818000
C	1.577893000	3.353542000	-0.267248000
N	1.840889000	2.313485000	0.536804000
C	2.431933000	1.273037000	2.640618000
H	1.299833000	3.096675000	-1.284540000
H	1.449382000	0.898649000	2.945681000
H	3.030079000	1.498324000	3.535292000
N	3.047141000	0.221531000	1.803955000
N	3.746941000	0.415421000	-0.879640000
N	2.354403000	-1.852976000	0.075979000
C	2.865089000	-1.139649000	2.337708000
C	4.451700000	0.523303000	1.454199000
C	4.769707000	0.329894000	-0.016473000
C	3.985033000	0.344556000	-2.199935000
C	2.954904000	-2.177970000	1.237310000
C	2.332070000	-2.731430000	-0.934477000
H	3.584317000	-1.365540000	3.138737000
H	1.851795000	-1.182872000	2.751376000
H	5.142148000	-0.069169000	2.070409000
H	4.645554000	1.575883000	1.695023000
C	6.084189000	0.153002000	-0.449325000
C	5.269612000	0.185259000	-2.714500000
H	3.103648000	0.415461000	-2.829585000
C	3.565397000	-3.417308000	1.416912000
C	2.909879000	-3.995812000	-0.828484000
H	1.836194000	-2.396073000	-1.839961000
H	6.890685000	0.080186000	0.274499000
C	6.337698000	0.081256000	-1.819815000
H	5.425567000	0.137951000	-3.787172000
H	4.052598000	-3.650832000	2.358617000
C	3.541332000	-4.340837000	0.367607000
H	2.873487000	-4.683242000	-1.666884000
H	7.352307000	-0.053708000	-2.182805000
H	4.015220000	-5.311248000	0.482301000
H	-0.957535000	2.171303000	-0.501487000
H	-2.982274000	5.283485000	-2.228320000
C	-2.499912000	4.597022000	-2.930811000
C	-3.282367000	3.283928000	-3.130245000
C	-1.103609000	4.125220000	-2.449223000
H	-2.397189000	5.116251000	-3.891065000
C	-2.219604000	2.328721000	-3.717511000
H	-4.158410000	3.402226000	-3.775304000
H	-3.610885000	2.905715000	-2.154703000
C	-0.959866000	2.757515000	-3.041708000
H	-1.076960000	4.087436000	-1.345064000
H	-0.288502000	4.801706000	-2.746339000
H	-2.131363000	2.491203000	-4.807403000

H	-2.438952000	1.261692000	-3.581125000
H	-0.007240000	2.255854000	-3.174975000

Ia-¹²TS_{Rebhs-hs}

Fe	-1.735513000	0.456632000	0.263956000
O	-1.444465000	0.372949000	2.142786000
Fe	1.486946000	0.345412000	0.091777000
O	1.037738000	-0.683803000	1.646101000
H	0.116159000	-0.441519000	1.926546000
O	-0.106203000	1.120711000	-0.395066000
N	-1.373989000	-1.591084000	-0.274913000
N	-2.766261000	2.341350000	-0.094830000
N	-3.765543000	-0.440822000	0.538243000
C	-1.602136000	-1.902446000	-1.585872000
C	-1.676086000	-3.215706000	-2.025615000
H	-1.869879000	-3.412938000	-3.075982000
C	-1.497889000	-4.265967000	-1.112601000
H	-1.557743000	-5.299999000	-1.434552000
C	-1.253347000	-3.937583000	0.235102000
H	-1.123075000	-4.708592000	0.988002000
C	-1.214902000	-2.605261000	0.612663000
H	-1.072393000	-2.313844000	1.644003000
C	-2.938038000	2.675115000	-1.391201000
C	-3.572491000	3.860348000	-1.756048000
H	-3.712886000	4.098476000	-2.805970000
C	-4.029197000	4.719987000	-0.753609000
H	-4.528959000	5.648017000	-1.014569000
C	-3.851393000	4.362711000	0.585448000
H	-4.205865000	4.996213000	1.391516000
C	-3.216136000	3.156405000	0.870804000
H	-3.063642000	2.811465000	1.889300000
C	-4.436783000	-0.776225000	-0.577813000
C	-5.514375000	-1.659086000	-0.548324000
H	-6.030291000	-1.915927000	-1.468672000
C	-5.916226000	-2.194353000	0.676924000
H	-6.755495000	-2.881551000	0.726096000
C	-5.219664000	-1.836119000	1.834119000
H	-5.499004000	-2.229950000	2.805685000
C	-4.142624000	-0.961784000	1.719002000
H	-3.539869000	-0.660367000	2.569289000
C	-1.720199000	-0.709945000	-2.495712000
H	-2.086751000	-1.002079000	-3.489774000
C	-2.395224000	1.679519000	-2.394372000
H	-1.313309000	1.827064000	-2.484611000
H	-2.862216000	1.823946000	-3.378986000
C	-4.021229000	-0.082401000	-1.857349000
H	-4.255299000	-0.713638000	-2.724730000
H	-4.625394000	0.828522000	-1.952461000
N	-2.593214000	0.312611000	-1.872651000
H	-0.730330000	-0.249572000	-2.593954000
H	2.332227000	-2.704312000	-5.061372000
C	2.122152000	-2.180378000	-4.134281000
C	2.326550000	-0.796631000	-4.038300000
C	1.645922000	-2.868029000	-3.015184000
C	2.048058000	-0.153670000	-2.839720000
H	2.694211000	-0.224760000	-4.885029000
H	1.464177000	-3.937052000	-3.042228000
C	1.407850000	-2.159494000	-1.840610000
N	1.599532000	-0.831090000	-1.753257000
C	2.133112000	1.345289000	-2.680654000
H	1.050468000	-2.651190000	-0.941885000
H	1.116570000	1.752125000	-2.751691000
H	2.743119000	1.789570000	-3.479934000
N	2.640462000	1.718515000	-1.344110000
N	3.596295000	-0.498828000	0.059911000
N	2.173008000	2.063177000	1.268200000
C	2.228198000	3.075640000	-0.921723000
C	4.102315000	1.518885000	-1.206851000
C	4.467657000	0.122479000	-0.756228000
C	3.887010000	-1.734971000	0.498704000
C	2.400751000	3.197175000	0.575335000
C	2.289821000	2.065252000	2.605440000
H	2.788896000	3.860336000	-1.448881000
H	1.163248000	3.170028000	-1.159585000
H	4.468248000	2.224425000	-0.451512000

H	4.614546000	1.761451000	-2.147946000
C	5.674428000	-0.465908000	-1.133199000
C	5.073517000	-2.388194000	0.179154000
H	3.126035000	-2.210438000	1.105229000
C	2.759038000	4.382663000	1.212380000
C	2.636288000	3.212055000	3.315800000
H	2.097264000	1.115041000	3.090405000
H	6.351261000	0.065626000	-1.795416000
C	5.989778000	-1.736626000	-0.650737000
H	5.267245000	-3.384488000	0.562547000
C	2.951046000	5.276566000	0.626890000
C	2.872569000	4.392367000	2.605121000
H	2.727092000	3.177133000	4.396381000
H	6.924855000	-2.213745000	-0.927928000
H	3.152919000	5.303261000	3.125368000
H	-1.034318000	1.165374000	2.526088000
H	2.203207000	-3.772833000	3.002053000
C	1.357028000	-3.081658000	2.887818000
H	1.023846000	-3.159251000	1.838194000
C	1.748480000	-1.666594000	3.199259000
H	2.762567000	-1.314140000	3.045589000
C	0.929845000	-1.145424000	4.343544000
H	0.719952000	-0.069818000	4.282439000
H	1.498323000	-1.306926000	5.275209000
C	0.187258000	-3.401117000	3.859904000
H	-0.590405000	-4.009814000	3.385797000
H	0.565128000	-3.965852000	4.719185000
C	-0.335569000	-2.025819000	4.329625000
H	-1.054540000	-1.600847000	3.620551000
H	-0.821469000	-2.074997000	5.308676000

Ia-¹⁰TS_{Rebhs-is}

Fe	-1.474300000	-0.214613000	0.122498000
O	-1.542445000	1.438304000	-0.823898000
Fe	1.666128000	0.252494000	-0.018507000
O	1.102555000	0.621300000	-1.745343000
H	0.152468000	0.851615000	-1.749509000
O	0.190536000	-0.230707000	0.985943000
N	-2.629876000	0.377589000	1.904792000
N	-0.903228000	-1.821134000	-1.303595000
N	-3.562193000	-0.706710000	-0.555585000
C	-2.770281000	-0.575843000	2.844810000
C	-3.580430000	-0.383783000	3.961374000
H	-3.684612000	-1.172739000	4.699910000
C	-4.253111000	0.833542000	4.104171000
H	-4.892344000	1.007421000	4.964672000
C	-4.103169000	1.815168000	3.122518000
H	-4.617406000	2.767834000	3.194098000
C	-3.282269000	1.540545000	2.029369000
H	-3.137477000	2.245119000	1.215647000
C	-0.733583000	-3.031890000	-0.737434000
C	-0.415514000	-4.156230000	-1.496843000
H	-0.299805000	-5.120846000	-1.012493000
C	-0.257734000	-4.016121000	-2.877899000
H	-0.019649000	-4.878716000	-3.493511000
C	-0.423361000	-2.755898000	-3.455583000
H	-0.317273000	-2.605291000	-4.524713000
C	-0.751010000	-1.682655000	-2.627272000
H	-0.894578000	-0.683197000	-3.022491000
C	-4.170409000	-1.771121000	-0.011788000
C	-5.534328000	-2.008799000	-0.192892000
H	-6.000273000	-2.875362000	0.267317000
C	-6.277718000	-1.121622000	-0.970691000
H	-7.339608000	-1.286844000	-1.127049000
C	-5.636915000	-0.017108000	-1.538451000
H	-6.178485000	0.699877000	-2.146511000
C	-4.277619000	0.156822000	-1.296863000
H	-3.723676000	1.005053000	-1.680811000
C	-1.963094000	-1.836903000	2.612090000
H	-2.313267000	-2.648540000	3.266584000
C	-0.881128000	-3.079061000	0.769012000
H	0.025637000	-2.649132000	1.206404000
H	-0.999103000	-4.116767000	1.113831000
C	-3.318106000	-2.756369000	0.768676000
H	-3.880777000	-3.117290000	1.640101000

H	-3.150057000	-3.630968000	0.127739000
N	-2.005410000	-2.219492000	1.187876000
H	-0.916488000	-1.612797000	2.844085000
H	1.749005000	5.755189000	2.449329000
C	1.736753000	4.776347000	1.979232000
C	2.026053000	3.632659000	2.729354000
C	1.447153000	4.646850000	0.618695000
C	2.002738000	2.390052000	2.098719000
H	2.267694000	3.701310000	3.785600000
H	1.226506000	5.511839000	0.002202000
C	1.461208000	3.371432000	0.056751000
N	1.726369000	2.278084000	0.786040000
C	2.247599000	1.082290000	2.825339000
H	1.266637000	3.191192000	-0.995918000
H	1.273141000	0.630866000	3.037925000
H	2.782779000	1.256610000	3.769782000
N	2.967628000	0.145833000	1.936834000
N	3.799051000	0.633135000	-0.670685000
N	2.484102000	-1.784588000	-0.015369000
C	2.832986000	-1.268122000	2.328116000
C	4.369905000	0.551387000	1.702954000
C	4.777304000	0.534386000	0.241214000
C	4.112944000	0.714543000	-1.974715000
C	3.047600000	-2.185988000	1.140888000
C	2.572493000	-2.553317000	-1.107960000
H	3.515627000	-1.535024000	3.148182000
H	1.800938000	-1.403130000	2.669500000
H	5.057513000	-0.071309000	2.291943000
H	4.495078000	1.579163000	2.065607000
C	6.123127000	0.497043000	-0.125602000
C	5.431680000	0.700125000	-2.422489000
H	3.264187000	0.787652000	-2.647391000
C	3.734634000	-3.394421000	1.230899000
C	3.234868000	-3.780221000	-1.095596000
H	2.097242000	-2.157639000	-2.000421000
H	6.892806000	0.409528000	0.635746000
C	6.454836000	0.582476000	-1.478256000
H	5.648447000	0.772962000	-3.483084000
H	4.189941000	-3.691817000	2.170532000
C	3.829089000	-4.203644000	0.094327000
H	3.290726000	-4.378833000	-1.998617000
H	7.494933000	0.557746000	-1.789735000
H	4.365887000	-5.146702000	0.138143000
H	-0.969753000	2.115179000	-0.431107000
H	-2.847129000	5.422466000	-2.046284000
C	-2.413866000	4.726345000	-2.771194000
C	-3.263845000	3.457678000	-2.978477000
C	-1.036959000	4.171570000	-2.326708000
H	-2.302130000	5.257926000	-3.723733000
C	-2.266767000	2.463254000	-3.615485000
H	-4.151063000	3.631344000	-3.595111000
H	-3.583961000	3.076038000	-2.001151000
C	-0.961925000	2.829087000	-2.986552000
H	-1.012661000	4.076098000	-1.225500000
H	-0.193757000	4.825174000	-2.593583000
H	-2.217676000	2.627146000	-4.707174000
H	-2.531313000	1.406994000	-3.471293000
H	-0.029632000	2.311582000	-3.185792000

Ia-⁸TS_{Rebhs-is}

Fe	1.607494000	-0.353785000	-0.073330000
O	1.450269000	0.920059000	-1.450603000
Fe	-1.598573000	0.311121000	-0.185783000
O	-1.217928000	0.566302000	-1.969116000
H	-0.242586000	0.715365000	-1.987794000
O	-0.018907000	-0.123725000	0.643565000
N	0.870641000	-2.093441000	-1.201793000
N	2.482322000	0.582253000	1.656896000
N	3.612894000	-0.778700000	-0.503054000
C	0.647573000	-3.198744000	-0.469877000
C	0.219190000	-4.391366000	-1.048087000
H	0.066819000	-5.271172000	-0.430356000
C	-0.009816000	-4.425066000	-2.426269000
H	-0.335263000	-5.343545000	-2.905888000
C	0.187477000	-3.264117000	-3.175452000

H	0.014783000	-3.245538000	-4.246430000
C	0.630958000	-2.115603000	-2.518379000
H	0.790156000	-1.181025000	-3.044358000
C	2.649892000	-0.215037000	2.724845000
C	3.348757000	0.214391000	3.851837000
H	3.481469000	-0.453134000	4.698031000
C	3.868269000	1.511670000	3.867395000
H	4.418454000	1.870174000	4.732251000
C	3.676143000	2.336890000	2.756837000
H	4.065366000	3.349370000	2.732348000
C	2.979809000	1.825776000	1.662418000
H	2.807909000	2.403915000	0.759024000
C	4.180986000	-1.806941000	0.160816000
C	5.554553000	-2.046470000	0.108141000
H	5.974390000	-2.879878000	0.663273000
C	6.365914000	-1.212186000	-0.658286000
H	7.436436000	-1.384281000	-0.714722000
C	5.775638000	-0.146030000	-1.340207000
H	6.363847000	0.539134000	-1.941229000
C	4.403049000	0.039499000	-1.224454000
H	3.912090000	0.879611000	-1.698072000
C	0.841061000	-3.035679000	1.022401000
H	0.971296000	-4.011937000	1.510883000
C	1.962261000	-1.566009000	2.655699000
H	0.912211000	-1.411146000	2.925229000
H	2.405163000	-2.262252000	3.382097000
C	3.269756000	-2.741864000	0.923250000
H	3.068742000	-3.606038000	0.278616000
H	3.786442000	-3.126707000	1.813013000
N	1.974558000	-2.126588000	1.290411000
H	-0.055341000	-2.551429000	1.418209000
H	-4.255910000	-5.098829000	0.486537000
C	-3.728011000	-4.159742000	0.349001000
C	-3.478464000	-3.325108000	1.443279000
C	-3.303923000	-3.762015000	-0.919446000
C	-2.811359000	-2.120936000	1.231413000
H	-3.806922000	-3.596204000	2.442075000
H	-3.486468000	-4.376962000	-1.794372000
C	-2.644180000	-2.539561000	-1.047982000
N	-2.402065000	-1.748791000	0.003697000
C	-2.471775000	-1.157136000	2.351259000
H	-2.294973000	-2.165724000	-2.005259000
H	-1.404360000	-1.255821000	2.579805000
H	-3.046731000	-1.404164000	3.256549000
N	-2.685319000	0.232473000	1.920798000
N	-3.794776000	0.621860000	-0.607155000
N	-1.672892000	2.363355000	0.569875000
C	-1.905841000	1.225429000	2.688646000
C	-4.117171000	0.589297000	1.816472000
C	-4.670118000	0.528419000	0.403576000
C	-4.242345000	0.663513000	-1.873324000
C	-1.823553000	2.516079000	1.898430000
C	-1.592110000	3.438405000	-0.224611000
H	-2.327769000	1.407834000	3.687862000
H	-0.892906000	0.821436000	2.790926000
H	-4.241237000	1.619664000	2.171952000
H	-4.722221000	-0.042576000	2.481472000
C	-6.045624000	0.455588000	0.179621000
C	-5.599995000	0.613012000	-2.181047000
H	-3.467389000	0.732935000	-2.630587000
C	-1.892612000	3.778741000	2.482491000
C	-1.642987000	4.736178000	0.283852000
H	-1.481996000	3.227140000	-1.282870000
H	-6.730627000	0.372664000	1.018568000
C	-6.517134000	0.500187000	-1.133012000
H	-5.926882000	0.654583000	-3.214786000
H	-2.029322000	3.875622000	3.555284000
C	-1.793877000	4.906450000	1.661292000
H	-1.575149000	5.586931000	-0.386047000
H	-7.583145000	0.447803000	-1.333841000
H	-1.848440000	5.902162000	2.091390000
H	1.992946000	0.807951000	-2.245252000
H	1.427160000	3.160623000	-4.963850000
C	1.710096000	3.664485000	-4.034715000
C	3.030752000	3.129289000	-3.439856000

C	0.659343000	3.482582000	-2.904800000
H	1.826007000	4.730964000	-4.259517000
C	2.937243000	3.522571000	-1.947627000
H	3.917419000	3.534755000	-3.936964000
H	3.072664000	2.033481000	-3.539616000
C	1.477626000	3.388228000	-1.653705000
H	0.050336000	2.575388000	-3.041307000
H	-0.055506000	4.320573000	-2.877567000
H	3.266048000	4.571276000	-1.827221000
H	3.577439000	2.925069000	-1.283630000
H	1.055893000	3.420754000	-0.656395000

Ia-⁴TS_{Rebhs-is}

Fe	1.622622000	-0.281924000	0.110907000
O	1.485533000	0.608240000	1.657853000
Fe	-1.613977000	0.346702000	0.213004000
O	-1.223727000	0.521272000	2.045902000
H	-1.761483000	1.069250000	2.634865000
O	-0.034193000	0.077577000	-0.595157000
N	2.589097000	1.026624000	-1.511818000
N	1.042722000	-2.284502000	0.940038000
N	3.598830000	-0.717628000	0.537229000
C	2.666888000	0.393663000	-2.694830000
C	3.362936000	0.928333000	-3.777275000
H	3.418218000	0.384020000	-4.715410000
C	3.982531000	2.172425000	-3.625708000
H	4.534432000	2.614066000	-4.450122000
C	3.885518000	2.833894000	-2.400524000
H	4.351564000	3.801163000	-2.243489000
C	3.181192000	2.216769000	-1.365255000
H	3.079583000	2.679407000	-0.388776000
C	0.900517000	-3.237964000	0.005830000
C	0.648110000	-4.565958000	0.341017000
H	0.554080000	-5.319690000	-0.434971000
C	0.524214000	-4.899097000	1.693897000
H	0.336454000	-5.927600000	1.988416000
C	0.656016000	-3.898528000	2.659237000
H	0.571185000	-4.122523000	3.717662000
C	0.923270000	-2.594776000	2.234902000
H	1.049990000	-1.765306000	2.924467000
C	4.237643000	-1.528290000	-0.326369000
C	5.608256000	-1.765919000	-0.226244000
H	6.099492000	-2.417779000	-0.942521000
C	6.324809000	-1.164474000	0.808269000
H	7.392657000	-1.335637000	0.906172000
C	5.647836000	-0.348117000	1.718079000
H	6.166251000	0.127251000	2.543943000
C	4.282319000	-0.146813000	1.545548000
H	3.684807000	0.470270000	2.205495000
C	1.894670000	-0.904823000	-2.777431000
H	2.210146000	-1.498298000	-3.647153000
C	0.991415000	-2.735596000	-1.418573000
H	0.039973000	-2.258553000	-1.665699000
H	1.179025000	-3.557978000	-2.123204000
C	3.401278000	-2.244755000	-1.364218000
H	3.921978000	-2.249099000	-2.329890000
H	3.311652000	-3.292317000	-1.052175000
N	2.028194000	-1.680677000	-1.522265000
H	0.831727000	-0.662310000	-2.876580000
H	-2.041169000	6.037407000	-1.830228000
C	-1.982683000	5.029245000	-1.431007000
C	-2.024506000	3.927021000	-2.290208000
C	-1.880341000	4.814600000	-0.056050000
C	-1.949930000	2.647599000	-1.745786000
H	-2.120513000	4.055437000	-3.364002000
H	-1.852527000	5.641125000	0.645978000
C	-1.818528000	3.501820000	0.408656000
N	-1.849447000	2.447653000	-0.417217000
C	-1.970565000	1.388460000	-2.585895000
H	-1.730089000	3.274714000	1.463831000
H	-0.939974000	1.037470000	-2.703110000
H	-2.404341000	1.586263000	-3.576616000
N	-2.702118000	0.331140000	-1.853749000
N	-3.902040000	0.349699000	0.673699000
N	-2.222476000	-1.760328000	-0.080002000

C	-2.457084000	-1.022033000	-2.380853000
C	-4.144435000	0.641061000	-1.731439000
C	-4.726643000	0.273754000	-0.383157000
C	-4.391223000	0.087036000	1.895101000
C	-2.649366000	-2.082972000	-1.314729000
C	-2.299411000	-2.658973000	0.908821000
H	-3.088674000	-1.238837000	-3.254858000
H	-1.410969000	-1.053141000	-2.704485000
H	-4.714973000	0.156638000	-2.536244000
H	-4.271105000	1.721945000	-1.862110000
C	-6.074957000	-0.059691000	-0.250399000
C	-5.727522000	-0.234785000	2.121876000
H	-3.672229000	0.116305000	2.707582000
C	-3.174377000	-3.342297000	-1.597874000
C	-2.804157000	-3.942556000	0.705439000
H	-1.938608000	-2.325640000	1.876486000
H	-6.709348000	-0.117163000	-1.129988000
C	-6.586467000	-0.310163000	1.023522000
H	-6.078786000	-0.430096000	3.129641000
H	-3.521360000	-3.573545000	-2.600443000
C	-3.252540000	-4.287179000	-0.570539000
H	-2.849354000	-4.646217000	1.529564000
H	-7.633365000	-0.566924000	1.154922000
H	-3.664601000	-5.273076000	-0.764558000
H	0.535460000	0.752420000	1.898132000
H	0.802547000	3.254175000	0.932646000
C	1.244835000	3.625138000	1.867182000
H	1.554463000	4.670190000	1.683157000
C	2.399936000	2.793313000	2.325111000
H	3.267194000	2.584471000	1.709858000
C	2.369816000	2.560092000	3.804630000
H	3.326318000	2.780703000	4.298632000
H	2.141398000	1.500721000	4.013144000
C	0.279758000	3.564111000	3.075040000
H	-0.405626000	4.417920000	3.125234000
H	-0.310502000	2.642344000	3.002585000
C	1.217951000	3.473020000	4.294264000
H	1.612507000	4.468719000	4.529970000
H	0.719608000	3.088957000	5.189990000

Ia-²TS_{Rebhs-is}

Fe	1.622602000	-0.281906000	0.110903000
O	1.485506000	0.608195000	1.657903000
Fe	-1.613995000	0.346710000	0.213003000
O	-1.223694000	0.521308000	2.045903000
H	-1.761491000	1.069310000	2.634903000
O	-0.034196000	0.077602000	-0.595197000
N	2.589108000	1.026589000	-1.511797000
N	1.042692000	-2.284503000	0.940003000
N	3.598800000	-0.717616000	0.537203000
C	2.666905000	0.393689000	-2.694797000
C	3.362908000	0.928285000	-3.777297000
H	3.418205000	0.383985000	-4.715397000
C	3.982514000	2.172382000	-3.625697000
H	4.534416000	2.614080000	-4.450097000
C	3.885517000	2.833883000	-2.400497000
H	4.351622000	3.801181000	-2.243497000
C	3.181214000	2.216786000	-1.365297000
H	3.079616000	2.679387000	-0.388797000
C	0.900487000	-3.238003000	0.005803000
C	0.648081000	-4.566001000	0.341003000
H	0.554077000	-5.319701000	-0.434997000
C	0.524179000	-4.899101000	1.693903000
H	0.336474000	-5.927600000	1.988403000
C	0.655984000	-3.898501000	2.659203000
H	0.571183000	-4.122501000	3.717703000
C	0.923291000	-2.594803000	2.234903000
H	1.049995000	-1.765303000	2.924503000
C	4.237596000	-1.528319000	-0.326397000
C	5.608295000	-1.765926000	-0.226197000
H	6.099491000	-2.417828000	-0.942497000
C	6.324798000	-1.164529000	0.808303000
H	7.392697000	-1.335634000	0.906203000
C	5.647802000	-0.348126000	1.718103000
H	6.166304000	0.127272000	2.543903000

C	4.282303000	-0.146819000	1.545503000
H	3.684806000	0.470284000	2.205503000
C	1.894699000	-0.904807000	-2.777397000
H	2.210096000	-1.498309000	-3.647197000
C	0.991390000	-2.735603000	-1.418597000
H	0.039992000	-2.258598000	-1.665697000
H	1.178986000	-3.558004000	-2.123197000
C	3.401292000	-2.244815000	-1.364197000
H	3.921992000	-2.249117000	-2.329897000
H	3.311687000	-3.292314000	-1.052197000
N	2.028195000	-1.680708000	-1.522297000
H	0.831700000	-0.662302000	-2.876597000
H	-2.041167000	6.037412000	-1.830197000
C	-1.982672000	5.029212000	-1.430997000
C	-2.024478000	3.927012000	-2.290197000
C	-1.880273000	4.814611000	-0.056097000
C	-1.949884000	2.647611000	-1.745797000
H	-2.120477000	4.055412000	-3.363997000
H	-1.852469000	5.641111000	0.646003000
C	-1.818480000	3.501811000	0.408703000
N	-1.849385000	2.447711000	-0.417197000
C	-1.970590000	1.388512000	-2.585897000
H	-1.730081000	3.274710000	1.463803000
H	-0.939992000	1.037506000	-2.703097000
H	-2.404289000	1.586314000	-3.576597000
N	-2.702095000	0.331115000	-1.853697000
N	-3.901995000	0.349721000	0.673703000
N	-2.222505000	-1.760287000	-0.079997000
C	-2.457102000	-1.021986000	-2.380897000
C	-4.144394000	0.641122000	-1.731397000
C	-4.726595000	0.273825000	-0.383197000
C	-4.391196000	0.087023000	1.895103000
C	-2.649407000	-2.082985000	-1.314697000
C	-2.299410000	-2.658987000	0.908803000
H	-3.088703000	-1.238783000	-3.254897000
H	-1.411002000	-1.053091000	-2.704497000
H	-4.714996000	0.156625000	-2.536197000
H	-4.271088000	1.721923000	-1.862097000
C	-6.074997000	-0.059668000	-0.250397000
C	-5.727498000	-0.234770000	2.121903000
H	-3.672196000	0.116320000	2.707603000
C	-3.174413000	-3.342283000	-1.597897000
C	-2.804216000	-3.942584000	0.705403000
H	-1.938608000	-2.325589000	1.876503000
H	-6.709297000	-0.117165000	-1.129997000
C	-6.586498000	-0.310166000	1.023503000
H	-6.078799000	-0.430068000	3.129603000
H	-3.521414000	-3.573481000	-2.600397000
C	-3.252518000	-4.287182000	-0.570497000
H	-2.849419000	-4.646184000	1.529603000
H	-7.633399000	-0.566861000	1.154903000
H	-3.664622000	-5.273080000	-0.764597000
H	0.535507000	0.752399000	1.898103000
H	0.802519000	3.254198000	0.932603000
C	1.244821000	3.625096000	1.867203000
H	1.554526000	4.670194000	1.683203000
C	2.399917000	2.793290000	2.325103000
H	3.267216000	2.584486000	1.709903000
C	2.369816000	2.560090000	3.804603000
H	3.326317000	2.780686000	4.298603000
H	2.141411000	1.500691000	4.013103000
C	0.279821000	3.564101000	3.075003000
H	-0.405575000	4.417904000	3.125203000
H	-0.310484000	2.642303000	3.002603000
C	1.218020000	3.472996000	4.294303000
H	1.612525000	4.468694000	4.530003000
H	0.719618000	3.088998000	5.190003000

Ia-⁸TS_{Rebis-is}

Fe	-1.622897000	0.246312000	0.116099000
O	-1.467598000	-0.599488000	1.669699000
Fe	1.650503000	-0.286093000	0.122699000
O	1.210102000	-0.514492000	1.924099000
H	1.340601000	-1.457193000	2.125199000
O	0.085903000	-0.078391000	-0.565001000

C	2.025202000	-3.643195000	0.167922000
N	1.946095000	-2.508387000	-0.537301000
C	1.894702000	-1.250005000	-2.615033000
H	2.015810000	-3.538754000	1.249277000
H	0.845213000	-0.945668000	-2.676082000
H	2.309931000	-1.342202000	-3.628426000
N	2.593039000	-0.190760000	-1.840874000
N	3.696123000	-0.330672000	0.655636000
N	2.182090000	1.946641000	-0.084051000
C	2.326248000	1.161859000	-2.375293000
C	4.056468000	-0.464757000	-1.743836000
C	4.592632000	-0.276575000	-0.346490000
C	4.117617000	-0.220981000	1.928320000
C	2.580733000	2.237289000	-1.335049000
C	2.325579000	2.859510000	0.880489000
H	2.915884000	1.353441000	-3.282681000
H	1.267695000	1.180816000	-2.650301000
H	4.610212000	0.162004000	-2.454213000
H	4.234267000	-1.505503000	-2.037204000
C	5.955271000	-0.113194000	-0.103254000
C	5.462826000	-0.071617000	2.251593000
H	3.327081000	-0.241949000	2.671095000
C	3.139746000	3.471074000	-1.663585000
C	2.870071000	4.122503000	0.639498000
H	1.986111000	2.560737000	1.867782000
H	6.652593000	-0.067378000	-0.934301000
C	6.398637000	-0.014600000	1.216044000
H	5.764373000	0.007329000	3.290648000
H	3.459679000	3.673879000	-2.681484000
C	3.285707000	4.430590000	-0.656313000
H	2.969942000	4.837953000	1.449038000
H	7.455670000	0.110393000	1.431003000
H	3.724564000	5.398106000	-0.881679000
H	-0.493618000	-0.636729000	1.875857000
H	-0.137146000	-2.980857000	1.587644000
C	-0.693447000	-3.395196000	2.438531000
H	-0.668719000	-4.494401000	2.327267000
C	-2.098620000	-2.885053000	2.483523000
H	-2.787427000	-2.954189000	1.649226000
C	-2.511661000	-2.515783000	3.874932000
H	-3.493980000	-2.917595000	4.159765000
H	-2.573719000	-1.417416000	3.973008000
C	-0.129068000	-2.989497000	3.823262000
H	0.696818000	-3.627523000	4.157280000
H	0.224839000	-1.951347000	3.791207000
C	-1.358480000	-3.065199000	4.751088000
H	-1.561500000	-4.111135000	5.011140000
H	-1.224472000	-2.505869000	5.682100000

Ia-²TS_{Rebis-is}

Fe	1.585196000	-0.203005000	0.076296000
O	1.466896000	0.682796000	1.621796000
Fe	-1.586604000	0.275897000	0.156596000
O	-1.178004000	0.488996000	2.023796000
H	-1.382503000	1.407596000	2.266896000
O	0.028896000	0.071696000	-0.627004000
N	2.552697000	0.963395000	-1.648004000
N	1.019296000	-2.150704000	1.075296000
N	3.575796000	-0.588605000	0.532096000
C	2.676696000	0.207795000	-2.753804000
C	3.413596000	0.628695000	-3.859004000
H	3.502596000	-0.010505000	-4.732304000
C	4.029297000	1.883195000	-3.816904000
H	4.611797000	2.236894000	-4.662404000
C	3.887797000	2.669495000	-2.672904000
H	4.349497000	3.648795000	-2.600504000
C	3.141697000	2.162995000	-1.607104000
H	3.004397000	2.728695000	-0.690104000
C	0.881295000	-3.183904000	0.230396000
C	0.608095000	-4.472904000	0.681496000
H	0.512494000	-5.293404000	-0.023404000
C	0.466895000	-4.679504000	2.057296000
H	0.263994000	-5.674804000	2.442096000
C	0.598395000	-3.596504000	2.928996000
H	0.497895000	-3.722104000	4.002196000

C	0.879995000	-2.338304000	2.391896000
H	0.998096000	-1.448504000	3.002096000
C	4.232596000	-1.453405000	-0.262804000
C	5.613496000	-1.622106000	-0.176104000
H	6.115895000	-2.324706000	-0.834104000
C	6.326596000	-0.884906000	0.769696000
H	7.402996000	-0.999406000	0.855496000
C	5.634696000	-0.004806000	1.604896000
H	6.150196000	0.580094000	2.359196000
C	4.257296000	0.117295000	1.452296000
H	3.650196000	0.778895000	2.057996000
C	1.912296000	-1.098705000	-2.733004000
H	2.247696000	-1.763305000	-3.541604000
C	0.998295000	-2.818604000	-1.233304000
H	0.044595000	-2.390304000	-1.547304000
H	1.216895000	-3.700704000	-1.851104000
C	3.397695000	-2.304505000	-1.188904000
H	3.914895000	-2.447205000	-2.146204000
H	3.304395000	-3.296805000	-0.731604000
N	2.026196000	-1.763005000	-1.414704000
H	0.850996000	-0.874004000	-2.877904000
H	-2.296502000	5.924197000	-2.258104000
C	-2.186102000	4.960897000	-1.769104000
C	-2.098002000	3.790197000	-2.526404000
C	-2.154702000	4.868897000	-0.376904000
C	-1.958603000	2.569097000	-1.867104000
H	-2.148602000	3.819597000	-3.610804000
H	-2.242302000	5.749497000	0.250796000
C	-2.017503000	3.605797000	0.198196000
N	-1.905703000	2.484097000	-0.524004000
C	-1.872203000	1.256897000	-2.625204000
H	-1.996503000	3.484197000	1.277596000
H	-0.822303000	0.952696000	-2.686404000
H	-2.275103000	1.375897000	-3.641704000
N	-2.580804000	0.193397000	-1.876904000
N	-3.715704000	0.313097000	0.625296000
N	-2.107504000	-1.943703000	-0.095004000
C	-2.302404000	-1.159903000	-2.388104000
C	-4.037504000	0.461997000	-1.783004000
C	-4.590704000	0.256198000	-0.391804000
C	-4.161304000	0.191097000	1.888096000
C	-2.567905000	-2.217403000	-1.330704000
C	-2.269905000	-2.844803000	0.878296000
H	-2.881004000	-1.374703000	-3.298704000
H	-1.240104000	-1.182604000	-2.650304000
H	-4.590704000	-0.153702000	-2.505104000
H	-4.217403000	1.506597000	-2.062304000
C	-5.957404000	0.078198000	-0.176504000
C	-5.511004000	0.028398000	2.187296000
H	-3.386104000	0.211797000	2.647696000
C	-3.209505000	-3.417703000	-1.629104000
C	-2.902305000	-4.071703000	0.667096000
H	-1.870105000	-2.568003000	1.849196000
H	-6.638004000	0.030098000	-1.021404000
C	-6.425804000	-0.031202000	1.132896000
H	-5.832404000	-0.059202000	3.219796000
H	-3.573505000	-3.606303000	-2.634704000
C	-3.382005000	-4.360703000	-0.610204000
H	-3.015205000	-4.775103000	1.485396000
H	-7.485804000	-0.166801000	1.326396000
H	-3.887506000	-5.300203000	-0.813204000
H	0.497996000	0.700196000	1.870596000
H	0.189297000	3.041396000	1.378496000
C	0.754497000	3.532096000	2.178796000
H	0.775298000	4.610496000	1.936896000
C	2.137297000	2.987295000	2.278496000
H	2.820197000	2.925195000	1.440496000
C	2.523897000	2.704395000	3.688896000
H	3.540097000	3.037895000	3.940296000
H	2.492397000	1.612795000	3.860296000
C	0.178397000	3.308096000	3.599996000
H	-0.605202000	4.025296000	3.865996000
H	-0.236603000	2.295996000	3.676896000
C	1.415897000	3.402096000	4.515496000
H	1.684498000	4.452895000	4.676996000

H	1.257497000	2.938596000	5.493696000
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Ia-⁶TS_{RebIs-is}

Fe	-1.525147000	-0.387026000	0.234372000
O	-1.600970000	1.037589000	-1.057669000
Fe	1.649324000	0.283141000	-0.209958000
O	0.931258000	0.327505000	-1.872340000
H	-0.018410000	0.539971000	-1.757069000
O	0.211792000	-0.067426000	0.773635000
N	-2.162368000	0.711414000	1.794225000
N	-0.981554000	-1.898353000	-0.969136000
N	-3.448029000	-1.020465000	-0.149351000
C	-2.028997000	0.090716000	2.988473000
C	-2.492898000	0.673907000	4.164383000
H	-2.386897000	0.146886000	5.107744000
C	-3.100247000	1.931729000	4.105586000
H	-3.472170000	2.403383000	5.010145000
C	-3.238901000	2.560454000	2.867377000
H	-3.718166000	3.529477000	2.776349000
C	-2.761113000	1.908953000	1.731369000
H	-2.859345000	2.326590000	0.734261000
C	-0.714515000	-3.038482000	-0.296066000
C	-0.446439000	-4.230672000	-0.962989000
H	-0.245508000	-5.133837000	-0.395279000
C	-0.444724000	-4.238453000	-2.360501000
H	-0.245372000	-5.157494000	-2.903677000
C	-0.715450000	-3.053203000	-3.045754000
H	-0.731614000	-3.017938000	-4.129808000
C	-0.985555000	-1.901078000	-2.308397000
H	-1.218006000	-0.953477000	-2.778570000
C	-3.901983000	-2.065875000	0.563767000
C	-5.127965000	-2.667725000	0.280881000
H	-5.463906000	-3.516261000	0.869636000
C	-5.906756000	-2.159947000	-0.758742000
H	-6.865521000	-2.610875000	-0.996260000
C	-5.433053000	-1.065887000	-1.487668000
H	-6.006921000	-0.638583000	-2.303132000
C	-4.194142000	-0.528816000	-1.154243000
H	-3.756439000	0.308600000	-1.682018000
C	-1.328217000	-1.254136000	2.955236000
H	-1.570686000	-1.845570000	3.848609000
C	-0.655464000	-2.916323000	1.213152000
H	0.321128000	-2.490848000	1.460017000
H	-0.756075000	-3.900974000	1.689886000
C	-3.049460000	-2.525960000	1.729503000
H	-3.539771000	-2.203787000	2.656311000
H	-3.011396000	-3.622459000	1.760172000
N	-1.677518000	-1.962169000	1.702584000
H	-0.251914000	-1.071077000	2.922095000
H	1.233092000	6.108943000	1.539420000
C	1.324000000	5.089006000	1.177604000
C	1.705699000	4.064740000	2.049269000
C	1.073961000	4.787476000	-0.163425000
C	1.812668000	2.767756000	1.548971000
H	1.917648000	4.267481000	3.094890000
H	0.779148000	5.557030000	-0.869088000
C	1.225113000	3.466509000	-0.585324000
N	1.583032000	2.488716000	0.255200000
C	2.142807000	1.570876000	2.419021000
H	1.059244000	3.159335000	-1.613719000
H	1.197307000	1.111563000	2.726014000
H	2.709785000	1.874287000	3.310618000
N	2.862318000	0.547545000	1.626833000
N	3.545982000	0.534715000	-1.053270000
N	2.502293000	-1.792015000	0.142416000
C	2.885403000	-0.769389000	2.298494000
C	4.227151000	0.999756000	1.240149000
C	4.574887000	0.685526000	-0.198545000
C	3.785033000	0.355233000	-2.362882000
C	3.149805000	-1.894000000	1.316082000
C	2.624800000	-2.759603000	-0.771402000
H	3.618186000	-0.787636000	3.117771000
H	1.888071000	-0.919071000	2.724588000
H	4.980638000	0.578580000	1.918849000
H	4.270117000	2.088815000	1.358243000

C	5.897632000	0.640373000	-0.634619000
C	5.078925000	0.313864000	-2.876086000
H	2.894318000	0.245264000	-2.973350000
C	3.957130000	-2.989268000	1.616456000
C	3.403598000	-3.896630000	-0.548056000
H	2.082013000	-2.600982000	-1.699063000
H	6.708999000	0.758385000	0.077287000
C	6.153266000	0.452026000	-1.994251000
H	5.237303000	0.170975000	-3.939765000
H	4.476961000	-3.042491000	2.568370000
C	4.083138000	-4.008440000	0.666393000
H	3.483930000	-4.664285000	-1.310798000
H	7.175766000	0.415443000	-2.358245000
H	4.709606000	-4.871682000	0.870775000
H	-1.153567000	1.756714000	-0.580827000
H	-3.797312000	4.746539000	-2.021662000
C	-3.241212000	4.136201000	-2.740124000
C	-3.893085000	2.764906000	-3.004577000
C	-1.809318000	3.787446000	-2.255817000
H	-3.180026000	4.699281000	-3.678819000
C	-2.733964000	1.939501000	-3.603532000
H	-4.763727000	2.826206000	-3.664603000
H	-4.213118000	2.321856000	-2.052680000
C	-1.534032000	2.438057000	-2.863839000
H	-1.769937000	3.750221000	-1.153746000
H	-1.064355000	4.538511000	-2.555455000
H	-2.632187000	2.169664000	-4.678732000
H	-2.859637000	0.851026000	-3.530557000
H	-0.530767000	2.085515000	-3.077354000

Ia-⁴TS_{RebIs-is}

Fe	-1.609553000	-0.445351000	-0.029999000
O	-1.759325000	0.974076000	1.188673000
Fe	1.590060000	0.260030000	0.078490000
O	0.947560000	0.573388000	1.740635000
H	0.017536000	0.848635000	1.590581000
O	0.069794000	-0.170614000	-0.726374000
N	-0.913134000	-1.888901000	1.191478000
N	-2.338756000	0.623550000	-1.540447000
N	-3.635261000	-0.891462000	0.353888000
C	-0.640164000	-3.037248000	0.529217000
C	-0.247639000	-4.194580000	1.194390000
H	-0.056645000	-5.102264000	0.630743000
C	-0.100461000	-4.159719000	2.583473000
H	0.193851000	-5.051807000	3.128302000
C	-0.334503000	-2.960314000	3.255693000
H	-0.219906000	-2.882503000	4.331580000
C	-0.739324000	-1.847269000	2.519162000
H	-0.915341000	-0.891952000	2.996240000
C	-2.402129000	-0.063709000	-2.699765000
C	-2.974412000	0.489138000	-3.842017000
H	-3.027075000	-0.089471000	-4.759244000
C	-3.475884000	1.792740000	-3.780348000
H	-3.928747000	2.246315000	-4.656868000
C	-3.394930000	2.496995000	-2.577800000
H	-3.777009000	3.508744000	-2.491356000
C	-2.823769000	1.870036000	-1.471068000
H	-2.743949000	2.338219000	-0.496226000
C	-4.154129000	-1.890787000	-0.382478000
C	-5.520923000	-2.163012000	-0.414287000
H	-5.897372000	-2.974957000	-1.029181000
C	-6.382374000	-1.379756000	0.353121000
H	-7.451091000	-1.571296000	0.349643000
C	-5.844465000	-0.339870000	1.114016000
H	-6.475731000	0.303546000	1.717787000
C	-4.470490000	-0.122707000	1.075443000
H	-4.007179000	0.700190000	1.605146000
C	-0.729484000	-2.947734000	-0.976935000
H	-0.833245000	-3.939593000	-1.436061000
C	-1.743167000	-1.427968000	-2.681492000
H	-0.675990000	-1.276762000	-2.863168000
H	-2.150148000	-2.080616000	-3.464522000
C	-3.161638000	-2.745018000	-1.127485000
H	-2.972840000	-3.644520000	-0.529878000
H	-3.574641000	-3.080790000	-2.086549000

N	-1.858516000	-2.049957000	-1.335800000
H	0.185649000	-2.467977000	-1.327549000
H	4.598632000	-5.015243000	-0.649583000
C	3.982212000	-4.134907000	-0.493163000
C	3.728157000	-3.255071000	-1.550619000
C	3.443615000	-3.859343000	0.764609000
C	2.941412000	-2.131206000	-1.308629000
H	4.138526000	-3.433100000	-2.540107000
H	3.625412000	-4.513894000	1.610829000
C	2.670400000	-2.707077000	0.919029000
N	2.424361000	-1.871549000	-0.094605000
C	2.577566000	-1.127616000	-2.382975000
H	2.229658000	-2.434129000	1.873333000
H	1.530173000	-1.280373000	-2.665174000
H	3.203906000	-1.265537000	-3.275975000
N	2.672663000	0.250530000	-1.862101000
N	3.538586000	0.559453000	0.753177000
N	1.644832000	2.401018000	-0.630479000
C	1.938993000	1.220559000	-2.707445000
C	4.086113000	0.660795000	-1.629215000
C	4.511030000	0.576584000	-0.176875000
C	3.858206000	0.579324000	2.058100000
C	1.785388000	2.528637000	-1.959403000
C	1.485901000	3.488850000	0.130762000
H	2.430573000	1.373388000	-3.678791000
H	0.941756000	0.795388000	-2.864149000
H	4.198035000	1.704314000	-1.945913000
H	4.765765000	0.069137000	-2.256336000
C	5.858656000	0.593036000	0.180700000
C	5.180505000	0.608998000	2.491907000
H	3.007156000	0.573305000	2.731756000
C	1.772319000	3.774385000	-2.584386000
C	1.448850000	4.773327000	-0.413281000
H	1.384924000	3.301958000	1.195260000
H	6.625079000	0.600406000	-0.588584000
C	6.197944000	0.609044000	1.534385000
H	5.404790000	0.627255000	3.553179000
H	1.905252000	3.850084000	-3.659528000
C	1.594114000	4.914787000	-1.795394000
H	1.320337000	5.637340000	0.230538000
H	7.241023000	0.623552000	1.836264000
H	1.582577000	5.899665000	-2.252908000
H	-1.941219000	0.673607000	2.093700000
H	-1.246762000	2.622532000	5.150477000
C	-1.569453000	3.245927000	4.310974000
C	-2.919830000	2.797575000	3.711984000
C	-0.574713000	3.209385000	3.117436000
H	-1.663290000	4.273353000	4.680785000
C	-2.888669000	3.386037000	2.283978000
H	-3.779742000	3.134525000	4.298769000
H	-2.966450000	1.699262000	3.658851000
C	-1.450088000	3.262857000	1.902343000
H	0.053419000	2.306380000	3.120049000
H	0.132691000	4.054530000	3.146256000
H	-3.183612000	4.450737000	2.321166000
H	-3.567839000	2.893297000	1.577017000
H	-1.074187000	3.457294000	0.905410000

Ia-⁴TS_{Rebbs-is}

Fe	-1.651592000	-0.249338000	-0.178169000
O	-1.798684000	1.060372000	1.156753000
Fe	1.574259000	0.191495000	0.142357000
O	0.859683000	0.440716000	1.786332000
H	-0.033001000	0.802323000	1.602615000
O	0.068378000	0.015248000	-0.772109000
N	-1.101001000	-1.847548000	0.920073000
N	-2.264487000	0.997486000	-1.607192000
N	-3.633600000	-0.817954000	0.229335000
C	-0.974961000	-2.960933000	0.162830000
C	-0.792230000	-4.218766000	0.729439000
H	-0.709715000	-5.091915000	0.090023000
C	-0.713101000	-4.329018000	2.120045000
H	-0.583118000	-5.300079000	2.588474000
C	-0.796876000	-3.171111000	2.893831000
H	-0.724936000	-3.206817000	3.975702000

C	-0.991346000	-1.948479000	2.251375000
H	-1.036773000	-1.020473000	2.805761000
C	-2.179402000	0.477717000	-2.851510000
C	-2.596501000	1.192929000	-3.969738000
H	-2.534488000	0.744298000	-4.956537000
C	-3.095151000	2.487642000	-3.794462000
H	-3.428469000	3.066203000	-4.650752000
C	-3.168728000	3.018073000	-2.505978000
H	-3.554735000	4.016486000	-2.329388000
C	-2.747577000	2.234477000	-1.431595000
H	-2.784830000	2.570835000	-0.402090000
C	-4.110420000	-1.824714000	-0.524878000
C	-5.321567000	-2.456747000	-0.247225000
H	-5.663658000	-3.273435000	-0.875869000
C	-6.081890000	-2.011463000	0.833470000
H	-7.028931000	-2.485298000	1.073135000
C	-5.608220000	-0.937441000	1.590052000
H	-6.175078000	-0.541793000	2.426166000
C	-4.380969000	-0.373246000	1.255459000
H	-3.974742000	0.471188000	1.798134000
C	-0.950639000	-2.724537000	-1.330067000
H	-1.140541000	-3.650902000	-1.887700000
C	-1.561944000	-0.903274000	-2.928723000
H	-0.476868000	-0.788377000	-2.928687000
H	-1.876136000	-1.437574000	-3.834657000
C	-3.314373000	-2.159353000	-1.760516000
H	-3.324780000	-3.238089000	-1.958432000
H	-3.809717000	-1.677097000	-2.611731000
N	-1.913065000	-1.655278000	-1.693668000
H	0.045893000	-2.348674000	-1.573551000
H	4.096985000	-5.303619000	-0.780230000
C	3.558967000	-4.376976000	-0.603342000
C	3.487651000	-3.401418000	-1.603310000
C	2.940351000	-4.137934000	0.624658000
C	2.797445000	-2.221194000	-1.336096000
H	3.963813000	-3.550511000	-2.567788000
H	2.980020000	-4.867457000	1.426967000
C	2.273907000	-2.925094000	0.808424000
N	2.203175000	-1.997028000	-0.150607000
C	2.626962000	-1.114508000	-2.356192000
H	1.778501000	-2.676338000	1.742346000
H	1.605233000	-1.153081000	-2.748418000
H	3.322807000	-1.249143000	-3.196815000
N	2.791453000	0.209843000	-1.725742000
N	3.499895000	0.240310000	0.957650000
N	1.893502000	2.358892000	-0.397089000
C	2.202701000	1.298546000	-2.538292000
C	4.213031000	0.476620000	-1.368529000
C	4.529302000	0.223850000	0.091346000
C	3.731189000	0.122139000	2.275606000
C	2.117520000	2.561111000	-1.705759000
C	1.789129000	3.405141000	0.429613000
H	2.767124000	1.472654000	-3.465550000
H	1.183835000	0.980144000	-2.783676000
H	4.426071000	1.532374000	-1.572625000
H	4.886566000	-0.108080000	-2.008811000
C	5.843930000	0.062374000	0.526760000
C	5.017238000	-0.027621000	2.787319000
H	2.841264000	0.155851000	2.896113000
C	2.248000000	3.841035000	-2.240995000
C	1.894797000	4.720600000	-0.024020000
H	1.611722000	3.161206000	1.472312000
H	6.656761000	0.045541000	-0.193141000
C	6.091226000	-0.065150000	1.894570000
H	5.170142000	-0.116508000	3.857677000
H	2.446325000	3.974421000	-3.300333000
C	2.127079000	4.938793000	-1.383775000
H	1.806865000	5.548248000	0.672151000
H	7.107331000	-0.189432000	2.257085000
H	2.226314000	5.948467000	-1.771236000
H	-1.951971000	0.713629000	2.051265000
H	0.188736000	2.259542000	3.099720000
C	-1.303782000	3.296985000	1.894363000
H	-0.814626000	3.426340000	0.937037000
C	-0.573802000	3.044604000	3.172834000

H	-0.050029000	3.966516000	3.491458000
C	-1.715080000	2.741589000	4.169007000
H	-1.430476000	2.901468000	5.213180000
H	-2.021237000	1.689122000	4.065892000
C	-2.731268000	3.669325000	2.152489000
H	-3.006451000	4.634793000	1.702579000
H	-3.402325000	2.917517000	1.704293000
C	-2.850975000	3.672459000	3.699898000
H	-2.668603000	4.684769000	4.079495000
H	-3.839270000	3.360726000	4.052071000

Ia-²TS_{Rebls-is}

Fe	-1.542833000	-0.444099000	-0.074867000
O	-1.671248000	1.036699000	1.139204000
Fe	1.626284000	0.296450000	0.109247000
O	0.962859000	0.582575000	1.765013000
H	0.029461000	0.848901000	1.604057000
O	0.128395000	-0.133162000	-0.735572000
N	-0.848757000	-1.871064000	1.177870000
N	-2.277531000	0.557000000	-1.639335000
N	-3.551949000	-0.984897000	0.307623000
C	-0.561225000	-3.026918000	0.533701000
C	-0.176538000	-4.172535000	1.224651000
H	0.029942000	-5.086870000	0.677390000
C	-0.057990000	-4.118999000	2.615742000
H	0.229180000	-5.002710000	3.177841000
C	-0.311935000	-2.912483000	3.268175000
H	-0.220960000	-2.820818000	4.345230000
C	-0.704417000	-1.810860000	2.508712000
H	-0.893767000	-0.848555000	2.966351000
C	-2.295502000	-0.151063000	-2.788244000
C	-2.865915000	0.366040000	-3.948174000
H	-2.881436000	-0.227731000	-4.857082000
C	-3.415743000	1.651138000	-3.915965000
H	-3.868577000	2.074557000	-4.807483000
C	-3.384160000	2.375287000	-2.723086000
H	-3.805590000	3.372951000	-2.658482000
C	-2.809544000	1.785889000	-1.597634000
H	-2.762568000	2.271476000	-0.628765000
C	-4.041336000	-2.002228000	-0.424695000
C	-5.396633000	-2.332764000	-0.424288000
H	-5.750903000	-3.157829000	-1.035119000
C	-6.275216000	-1.592366000	0.364595000
H	-7.334089000	-1.831727000	0.383592000
C	-5.767669000	-0.531191000	1.117413000
H	-6.412388000	0.083022000	1.737078000
C	-4.406077000	-0.256390000	1.050187000
H	-3.974481000	0.584046000	1.577631000
C	-0.612150000	-2.973072000	-0.979280000
H	-0.666610000	-3.983179000	-1.407578000
C	-1.598640000	-1.498134000	-2.742181000
H	-0.529771000	-1.317544000	-2.885355000
H	-1.958879000	-2.155040000	-3.545469000
C	-3.046721000	-2.816390000	-1.219939000
H	-2.862646000	-3.751556000	-0.677363000
H	-3.477405000	-3.096574000	-2.189766000
N	-1.748070000	-2.123642000	-1.408755000
H	0.303328000	-2.480661000	-1.314266000
H	4.783461000	-4.868355000	-0.651991000
C	4.140930000	-4.007001000	-0.495006000
C	3.903302000	-3.105728000	-1.538063000
C	3.551183000	-3.778713000	0.749387000
C	3.080310000	-2.007946000	-1.296711000
H	4.351872000	-3.248753000	-2.516567000
H	3.718495000	-4.451754000	1.583966000
C	2.746280000	-2.648970000	0.906123000
N	2.516058000	-1.793285000	-0.094859000
C	2.718124000	-0.995026000	-2.363490000
H	2.266779000	-2.409791000	1.850787000
H	1.691416000	-1.189930000	-2.692393000
H	3.384030000	-1.088977000	-3.233225000
N	2.732035000	0.376988000	-1.816694000
N	3.557286000	0.661149000	0.814714000
N	1.546993000	2.436896000	-0.562981000
C	1.966075000	1.324065000	-2.659283000

C	4.117336000	0.857434000	-1.554148000
C	4.537585000	0.728227000	-0.104805000
C	3.864050000	0.650616000	2.122484000
C	1.696942000	2.599514000	-1.886562000
C	1.249683000	3.485549000	0.211464000
H	2.477643000	1.534117000	-3.609345000
H	1.002810000	0.844133000	-2.862272000
H	4.164392000	1.921246000	-1.814860000
H	4.834373000	0.342000000	-2.206633000
C	5.881091000	0.763699000	0.265330000
C	5.181721000	0.697256000	2.569639000
H	3.007104000	0.606246000	2.787252000
C	1.570036000	3.848667000	-2.492023000
C	1.090151000	4.768249000	-0.314081000
H	1.136649000	3.265674000	1.268510000
H	6.653867000	0.811429000	-0.496047000
C	6.207445000	0.747052000	1.622501000
H	5.395995000	0.690216000	3.633100000
H	1.715582000	3.957049000	-3.562747000
C	1.257318000	4.949747000	-1.689315000
H	0.852810000	5.601858000	0.338868000
H	7.247154000	0.775413000	1.934849000
H	1.155393000	5.936593000	-2.131178000
H	-1.961173000	0.725321000	2.013839000
H	-1.620267000	2.372892000	5.105094000
C	-1.972884000	3.035708000	4.308803000
C	-3.276061000	2.537468000	3.645344000
C	-0.952276000	3.173939000	3.143021000
H	-2.152807000	4.019266000	4.757102000
C	-3.256463000	3.221922000	2.260197000
H	-4.169156000	2.776373000	4.230804000
H	-3.247991000	1.443274000	3.524750000
C	-1.803827000	3.226699000	1.908191000
H	-0.240831000	2.335707000	3.104339000
H	-0.334362000	4.079902000	3.250894000
H	-3.631145000	4.256725000	2.361345000
H	-3.885484000	2.735432000	1.503035000
H	-1.424559000	3.556148000	0.948038000

Ia-⁴TS_{Rebls-ls}

Fe	-1.433394000	-0.310486000	0.292307000
O	-1.416618000	1.144596000	-1.045685000
Fe	1.788316000	0.216850000	-0.080124000
O	1.109713000	0.239025000	-1.752668000
H	0.200008000	0.592399000	-1.641630000
O	0.272421000	-0.147350000	0.875023000
N	-2.062182000	0.721895000	1.893969000
N	-0.994447000	-1.793497000	-1.003057000
N	-3.417030000	-0.776244000	-0.133289000
C	-2.013139000	0.020934000	3.049620000
C	-2.480815000	0.561056000	4.244681000
H	-2.443519000	-0.028706000	5.155588000
C	-3.004601000	1.857308000	4.246849000
H	-3.378514000	2.295737000	5.167190000
C	-3.058005000	2.568883000	3.047611000
H	-3.471942000	3.570750000	3.002986000
C	-2.580402000	1.957653000	1.889233000
H	-2.616023000	2.443340000	0.918809000
C	-0.833516000	-2.986480000	-0.390868000
C	-0.677348000	-4.162772000	-1.120096000
H	-0.560588000	-5.109013000	-0.600929000
C	-0.678337000	-4.098969000	-2.515839000
H	-0.566423000	-5.003375000	-3.106677000
C	-0.842051000	-2.860084000	-3.137577000
H	-0.859389000	-2.768623000	-4.218476000
C	-1.004999000	-1.728258000	-2.340197000
H	-1.154652000	-0.740460000	-2.757879000
C	-3.967915000	-1.816626000	0.513180000
C	-5.258021000	-2.262302000	0.221672000
H	-5.670955000	-3.112314000	0.757100000
C	-5.999026000	-1.598460000	-0.755117000
H	-7.005309000	-1.926438000	-0.997834000
C	-5.425884000	-0.505856000	-1.411694000
H	-5.967091000	0.044156000	-2.174392000
C	-4.130630000	-0.131322000	-1.072853000

H	-3.614581000	0.696607000	-1.538156000
C	-1.398072000	-1.363795000	2.955888000
H	-1.701823000	-1.983340000	3.811257000
C	-0.774443000	-2.952634000	1.124640000
H	0.217167000	-2.585856000	1.400483000
H	-0.925412000	-3.958605000	1.541020000
C	-3.149367000	-2.464141000	1.613276000
H	-3.634010000	-2.246407000	2.573314000
H	-3.169166000	-3.555660000	1.497831000
N	-1.751133000	-1.979411000	1.660377000
H	-0.312133000	-1.247781000	2.961718000
H	1.079545000	5.794956000	1.576293000
C	1.194106000	4.771752000	1.231202000
C	1.564681000	3.763648000	2.126186000
C	0.995861000	4.448981000	-0.112434000
C	1.703845000	2.461019000	1.654741000
H	1.748831000	3.983213000	3.173338000
H	0.718760000	5.203024000	-0.840855000
C	1.174362000	3.126195000	-0.514663000
N	1.503419000	2.159723000	0.353041000
C	2.065097000	1.287597000	2.541628000
H	1.056564000	2.798611000	-1.541054000
H	1.136065000	0.786606000	2.822034000
H	2.608459000	1.613872000	3.437979000
N	2.852665000	0.314455000	1.736357000
N	3.691526000	0.573666000	-0.827769000
N	2.351783000	-1.676549000	-0.078233000
C	2.799156000	-1.085330000	2.233007000
C	4.248126000	0.792459000	1.515624000
C	4.683372000	0.651895000	0.075333000
C	3.985395000	0.536908000	-2.138329000
C	2.909337000	-2.073054000	1.086628000
C	2.332190000	-2.496213000	-1.136201000
H	3.568799000	-1.274235000	2.992522000
H	1.816760000	-1.217084000	2.693886000
H	4.942862000	0.277311000	2.190523000
H	4.283877000	1.857068000	1.775610000
C	6.023892000	0.682751000	-0.303530000
C	5.299410000	0.580705000	-2.597473000
H	3.123348000	0.464795000	-2.793329000
C	3.478347000	-3.336091000	1.219537000
C	2.873695000	-3.779323000	-1.072457000
H	1.866711000	-2.079756000	-2.023206000
H	6.802916000	0.739071000	0.450868000
C	6.336352000	0.647948000	-1.663627000
H	5.502297000	0.553975000	-3.662884000
H	3.931749000	-3.632899000	2.160279000
C	3.458166000	-4.203307000	0.121854000
H	2.842627000	-4.423761000	-1.944389000
H	7.372326000	-0.672299000	-1.988045000
H	3.900970000	-5.191768000	0.199804000
H	-1.029284000	1.884708000	-0.551475000
H	-3.448630000	4.893362000	-2.588637000
C	-2.888484000	4.144407000	-3.157129000
C	-3.638700000	2.807298000	-3.305518000
C	-1.551849000	3.747837000	-2.478225000
H	-2.682685000	4.561676000	-4.149955000
C	-2.513182000	1.817007000	-3.675320000
H	-4.436702000	2.845047000	-4.053189000
H	-4.088180000	2.532357000	-2.342304000
C	-1.324280000	2.321702000	-2.914054000
H	-1.648828000	3.820814000	-1.382151000
H	-0.719520000	4.408824000	-2.757107000
H	-2.308415000	1.878868000	-4.757841000
H	-2.744700000	0.764644000	-3.464287000
H	-0.330388000	1.938544000	-3.118781000

Ia-²TS_{Reb}ls-ls

Fe	-1.593584000	0.317918000	-0.100962000
O	-1.478973000	-0.681862000	1.406282000
Fe	1.717030000	-0.161913000	0.013558000
O	1.081859000	-0.187750000	1.831934000
H	1.480354000	-0.939595000	2.294726000
O	0.164025000	0.190528000	-0.748241000
N	-2.138289000	-1.038318000	-1.440252000

N	-1.120862000	2.026456000	0.833816000
N	-3.588172000	0.634835000	0.298703000
C	-2.243335000	-0.563010000	-2.699924000
C	-2.669932000	-1.373959000	-3.748339000
H	-2.763207000	-0.963234000	-4.749097000
C	-2.971529000	-2.713585000	-3.486575000
H	-3.311101000	-3.364435000	-4.286691000
C	-2.834063000	-3.199355000	-2.184984000
H	-3.055860000	-4.233580000	-1.943548000
C	-2.417017000	-2.323898000	-1.183761000
H	-2.289517000	-2.619979000	-0.149986000
C	-0.997957000	3.093752000	0.014649000
C	-0.795593000	4.376714000	0.511637000
H	-0.718632000	5.216618000	-0.171665000
C	-0.700992000	4.556373000	1.894791000
H	-0.554621000	5.549291000	2.309764000
C	-0.808582000	3.445260000	2.730911000
H	-0.743040000	3.542414000	3.809576000
C	-1.023826000	2.190811000	2.159958000
H	-1.122419000	1.283446000	2.742399000
C	-4.259392000	1.399896000	-0.578675000
C	-5.642643000	1.566034000	-0.511736000
H	-6.151816000	2.184542000	-1.245080000
C	-6.347126000	0.937928000	0.514649000
H	-7.424471000	1.050311000	0.590345000
C	-5.641123000	0.173446000	1.446785000
H	-6.147088000	-0.318102000	2.271114000
C	-4.263244000	0.045365000	1.301799000
H	-3.647838000	-0.524937000	1.983337000
C	-1.775360000	0.864260000	-2.896542000
H	-2.236781000	1.315887000	-3.784979000
C	-1.051450000	2.769480000	-1.461047000
H	-0.071339000	2.385439000	-1.746444000
H	-1.290378000	3.656916000	-2.062259000
C	-3.431157000	2.152096000	-1.595248000
H	-3.905056000	2.110047000	-2.583625000
H	-3.416821000	3.208789000	-1.301824000
N	-2.023014000	1.667976000	-1.675893000
H	-0.692194000	0.836117000	-3.040110000
H	1.565558000	-5.772770000	-1.724654000
C	1.571519000	-4.751812000	-1.355055000
C	1.693196000	-3.678484000	-2.243275000
C	1.480522000	-4.488854000	0.011167000
C	1.705273000	-2.382377000	-1.738970000
H	1.790391000	-3.842595000	-3.311989000
H	1.395491000	-5.288971000	0.738633000
C	1.504113000	-3.162371000	0.440213000
N	1.605119000	-2.134170000	-0.410226000
C	1.837855000	-1.155799000	-2.615140000
H	1.430920000	-2.905026000	1.488367000
H	0.842411000	-0.730317000	-2.761502000
H	2.292553000	-1.404044000	-3.583522000
N	2.625478000	-0.141816000	-1.865947000
N	3.706571000	-0.379464000	0.638114000
N	2.172114000	1.764229000	0.008930000
C	2.459890000	1.251080000	-2.344818000
C	4.057445000	-0.549517000	-1.758751000
C	4.608546000	-0.392322000	-0.360547000
C	4.138909000	-0.263683000	1.905263000
C	2.582797000	2.227562000	-1.191073000
C	2.190129000	2.558822000	1.086299000
H	3.170369000	1.495373000	-3.145517000
H	1.448003000	1.325690000	-2.752137000
H	4.669943000	0.006731000	-2.479098000
H	4.130668000	-1.607835000	-2.034688000
C	5.979516000	-0.312698000	-0.121007000
C	5.490553000	-0.196643000	2.230580000
H	3.360874000	-0.190145000	2.656656000
C	3.030456000	3.536546000	-1.342979000
C	2.618129000	3.882954000	1.006969000
H	1.843708000	2.085848000	1.998571000
H	6.677713000	-0.319390000	-0.952666000
C	6.429393000	-0.223890000	1.196810000
H	5.795220000	-0.110570000	3.268220000
H	3.367480000	3.887109000	-2.313753000

C	3.047859000	4.377574000	-0.225286000
H	2.619641000	4.505127000	1.895300000
H	7.492118000	-0.163889000	1.411282000
H	3.401076000	5.400286000	-0.317770000
H	-0.505227000	-0.624891000	1.652602000
H	-0.774804000	-3.710924000	1.383781000
C	-1.240166000	-3.670103000	2.374997000
H	-1.630156000	-4.684538000	2.580752000
C	-2.342495000	-2.668864000	2.468612000
H	-3.184071000	-2.652185000	1.786002000
C	-2.382656000	-2.034489000	3.824117000
H	-3.367697000	-2.113472000	4.305475000
H	-2.160388000	-0.958998000	3.726883000
C	-0.294026000	-3.243065000	3.518180000
H	0.377705000	-4.041046000	3.851918000
H	0.306672000	-3.184154000	3.184154000
C	-1.265693000	-2.763704000	4.614793000
H	-1.686462000	-3.631487000	5.136516000
H	-0.785840000	-2.123778000	5.361520000

Ia-²TS_{Rebls-ls}

Fe	1.517677000	0.190744000	-0.281234000
O	1.515911000	-1.096783000	1.180700000
Fe	-1.740120000	-0.141675000	0.054844000
O	-1.051137000	-0.171664000	1.725862000
H	-0.198852000	-0.646977000	1.602768000
O	-0.189514000	0.016883000	-0.898467000
N	1.093765000	1.858266000	0.776272000
N	2.081003000	-1.121805000	-1.662836000
N	3.548394000	0.620667000	0.154638000
C	1.043870000	2.954685000	-0.014041000
C	0.956196000	4.239649000	0.513351000
H	0.928536000	5.095829000	-0.153341000
C	0.906873000	4.400417000	1.900263000
H	0.852513000	5.392881000	2.337735000
C	0.930788000	3.265120000	2.710301000
H	0.886522000	3.340591000	3.791738000
C	1.022526000	2.012361000	2.104865000
H	1.009362000	1.102812000	2.690441000
C	2.062647000	-0.629248000	-2.920307000
C	2.448361000	-1.403822000	-4.010491000
H	2.441845000	-0.978373000	-5.009492000
C	2.844928000	-2.726754000	-3.791620000
H	3.152552000	-3.350846000	-4.625286000
C	2.852261000	-3.227195000	-2.488682000
H	3.160686000	-4.246096000	-2.279113000
C	2.467287000	-2.385506000	-1.445245000
H	2.457752000	-2.693820000	-0.405581000
C	4.099486000	1.583580000	-0.607175000
C	5.346841000	2.139433000	-0.323694000
H	5.746830000	2.923203000	-0.960208000
C	6.066340000	1.663994000	0.771643000
H	7.039254000	2.079914000	1.015180000
C	5.514870000	0.635239000	1.537791000
H	6.043820000	0.216154000	2.387292000
C	4.257619000	0.147401000	1.195116000
H	3.799906000	-0.660275000	1.749848000
C	1.012712000	2.678660000	-1.500872000
H	1.252840000	3.581083000	-2.079326000
C	1.552032000	0.792385000	-3.048145000
H	0.461750000	0.756537000	-3.079685000
H	1.928011000	1.273319000	-3.960971000
C	3.347798000	1.967203000	-1.858848000
H	3.432354000	3.044395000	-2.049584000
H	3.832921000	1.460342000	-2.701842000
N	1.920033000	1.553527000	-1.826832000
H	0.001913000	2.342618000	-1.742088000
H	-3.460806000	5.392719000	-0.446186000
C	-3.085998000	4.380418000	-0.328066000
C	-3.139097000	3.481839000	-1.398731000
C	-2.562314000	3.954562000	0.893505000
C	-2.659443000	2.188271000	-1.214484000
H	-3.554714000	3.776075000	-2.357564000
H	-2.514097000	4.619944000	1.748696000
C	-2.106350000	2.642351000	1.006203000

N	-2.147138000	1.793863000	-0.027873000
C	-2.618914000	1.150297000	-2.319790000
H	-1.694973000	2.224510000	1.917695000
H	-1.622159000	1.170194000	-2.768575000
H	-3.356757000	1.377532000	-3.100348000
N	-2.810003000	-0.213908000	-1.765114000
N	-3.669652000	-0.293527000	0.807843000
N	-1.659602000	-2.118577000	-0.296394000
C	-2.119502000	-1.293700000	-2.522397000
C	-4.245839000	-0.542121000	-1.529297000
C	-4.664118000	-0.312021000	-0.094967000
C	-3.957949000	-0.191402000	2.115920000
C	-1.889535000	-2.458379000	-1.583007000
C	-1.455036000	-3.070150000	0.620506000
H	-2.686206000	-1.598118000	-3.411957000
H	-1.142291000	-0.900693000	-2.809705000
H	-4.387848000	-1.605938000	-1.753351000
H	-4.887344000	0.016663000	-2.222020000
C	-6.001883000	-0.209917000	0.281892000
C	-5.270102000	-0.102210000	2.573640000
H	-3.091976000	-0.179836000	2.769701000
C	-1.904793000	-3.788957000	-1.990079000
C	-1.441526000	-4.424108000	0.286870000
H	-1.302612000	-2.708361000	1.629453000
H	-6.783561000	-0.220590000	-0.471820000
C	-6.309197000	-0.104130000	1.639493000
H	-5.469572000	-0.025642000	3.637291000
H	-2.109440000	-4.036798000	-3.027066000
C	-1.666455000	-4.788350000	-1.041301000
H	-1.270843000	-5.170245000	1.055901000
H	-7.343043000	-0.025198000	1.962011000
H	-1.676555000	-5.834091000	-1.333738000
H	1.819375000	-0.664068000	1.993559000
H	1.286437000	-1.914903000	5.348102000
C	1.587552000	-2.660584000	4.606048000
C	2.930220000	-2.326276000	3.923367000
C	0.571924000	-2.789756000	3.436882000
H	1.676859000	-3.623208000	5.122147000
C	2.867795000	-3.139290000	2.611749000
H	3.797991000	-2.573291000	4.542215000
H	2.981660000	-1.250006000	3.698383000
C	1.424640000	-3.056809000	2.227740000
H	-0.026560000	-1.874726000	3.310246000
H	-0.155140000	-3.598220000	3.611024000
H	3.140310000	-4.188914000	2.822487000
H	3.545571000	-2.791379000	1.822046000
H	1.036530000	-3.522598000	1.330892000

Ib-²TS_{2Hhs-hs}

Fe	1.653795000	-0.455665000	-0.145892000
O	1.069331000	-1.755544000	1.412545000
Fe	-1.523511000	0.233741000	-0.058953000
O	-1.082991000	-0.362509000	1.734370000
H	-0.188362000	-0.794151000	1.547303000
O	-0.018901000	-0.049433000	-0.948061000
N	1.669437000	1.504857000	1.016232000
N	2.409323000	-1.761369000	-1.809785000
N	3.755398000	-0.460088000	0.654484000
C	2.132011000	2.525662000	0.270942000
C	2.486267000	3.747982000	0.839885000
H	2.864288000	4.549921000	0.213022000
C	2.351249000	3.914011000	2.221292000
H	2.631368000	4.852496000	2.691080000
C	1.859363000	2.855606000	2.986879000
H	1.741875000	2.943744000	4.062240000
C	1.532701000	1.664308000	2.336126000
H	1.134107000	0.807515000	2.870903000
C	2.729596000	-1.054521000	-2.913286000
C	3.272216000	-1.662904000	-4.044225000
H	3.532359000	-1.062384000	-4.910781000
C	3.479872000	-3.044712000	-4.036840000
H	3.903243000	-3.540733000	-4.905206000
C	3.149139000	-3.772475000	-2.893149000
H	3.304313000	-4.845065000	-2.840847000
C	2.620077000	-3.083701000	-1.801524000

H	2.359744000	-3.598498000	-0.880372000
C	4.630045000	0.382266000	0.082946000
C	5.864533000	0.670627000	0.667394000
H	6.545910000	1.364471000	0.183623000
C	6.203786000	0.049061000	1.869130000
H	7.159762000	0.253986000	2.341981000
C	5.295890000	-0.838117000	2.453298000
H	5.523686000	-1.344074000	3.385848000
C	4.078196000	-1.056028000	1.813954000
H	3.312218000	-1.712727000	2.214301000
C	2.195170000	2.278900000	-1.226212000
H	2.720120000	3.108284000	-1.725339000
C	2.452621000	0.438541000	-2.859167000
H	1.374437000	0.591086000	-2.977228000
H	2.979141000	0.952255000	-3.677843000
C	4.262211000	0.949898000	-1.276007000
H	4.700446000	1.951272000	-1.394772000
H	4.734298000	0.311863000	-2.033418000
N	2.809249000	0.976880000	-1.533469000
H	1.165564000	2.237636000	-1.595839000
H	-1.039108000	6.257299000	-0.535647000
C	-1.123681000	5.181468000	-0.413757000
C	-1.397464000	4.367324000	-1.516677000
C	-0.978664000	4.595452000	0.844766000
C	-1.506582000	2.991250000	-1.325662000
H	-1.535243000	4.790899000	-2.506891000
H	-0.774620000	5.192819000	1.726613000
C	-1.110075000	3.211988000	0.953068000
N	-1.359249000	2.434866000	-0.107822000
C	-1.781424000	2.020752000	-2.457239000
H	-1.006493000	2.696353000	1.901612000
H	-0.834752000	1.561491000	-2.761495000
H	-2.216918000	2.545351000	-3.320020000
N	-2.646649000	0.927480000	-1.972150000
N	-3.652428000	0.682461000	0.629890000
N	-2.611930000	-1.543798000	-0.770802000
C	-2.603779000	-0.278150000	-2.824161000
C	-4.025569000	1.386026000	-1.685027000
C	-4.551553000	0.966738000	-0.323735000
C	-4.079504000	0.382565000	1.866845000
C	-3.055880000	-1.490898000	-2.038831000
C	-2.934926000	-2.582346000	0.008636000
H	-3.205729000	-0.155861000	-3.736233000
H	-1.555496000	-0.431803000	-3.103145000
H	-4.714003000	1.045482000	-2.470154000
H	-4.037449000	2.482620000	-1.716982000
C	-5.924358000	0.951438000	-0.070908000
C	-5.429393000	0.361686000	2.208556000
H	-3.297839000	0.147858000	2.581987000
C	-3.845760000	-2.504909000	-2.576567000
C	-3.709351000	-3.644028000	-0.456134000
H	-2.563083000	-2.531190000	1.026312000
H	-6.627154000	1.177684000	-0.867582000
C	-6.370028000	0.647091000	1.215538000
H	-5.733762000	0.121069000	3.221849000
H	-4.199363000	-2.434498000	-3.600604000
C	-4.171282000	-3.601831000	-1.773572000
H	-3.951209000	-4.473218000	0.200499000
H	-7.432802000	0.630563000	1.438165000
H	-4.785446000	-4.405515000	-2.168690000
H	0.701322000	-2.543004000	0.981271000
H	-1.104077000	-1.170759000	2.799105000
C	-0.824005000	-1.979247000	3.767043000
H	-0.954866000	-1.275513000	4.595484000
C	0.493980000	-2.412662000	3.505329000
H	1.380665000	-1.862082000	3.795752000
C	0.530025000	-3.873104000	3.182430000
H	0.753891000	-4.388320000	4.132886000
H	1.304641000	-4.159497000	2.466004000
C	-1.751880000	-3.205002000	3.639850000
H	-1.939455000	-3.649755000	4.625798000
H	-2.726759000	-2.960132000	3.201496000
C	-0.925358000	-4.173509000	2.763569000
H	-1.198976000	-5.222784000	2.902796000
H	-1.053988000	-3.926564000	1.701472000

Ib-¹⁰TS_{2Hhs-hs}			
C	-2.267957000	4.006245000	-1.368613000
C	-1.597164000	4.684200000	-2.589906000
C	-1.832699000	3.716415000	-3.702597000
C	-2.737015000	2.640212000	-3.288291000
C	-3.405179000	3.179460000	-2.002063000
H	-3.409841000	2.272537000	-4.074191000
H	-1.387430000	3.805437000	-4.689228000
H	-2.091302000	5.644492000	-2.824135000
H	-0.535446000	4.925965000	-2.439552000
H	-4.258207000	3.822302000	-2.252674000
H	-3.755788000	2.368137000	-1.356457000
H	-2.611485000	4.729030000	-0.620995000
H	-1.556341000	3.316153000	-0.898562000
H	-2.126639000	1.755246000	-2.937477000
O	-1.496699000	0.717670000	-1.516063000
Fe	-1.564853000	-0.265482000	0.017773000
N	-2.474226000	0.830467000	1.749822000
C	-2.370707000	0.200081000	2.933478000
C	-2.885516000	0.746378000	4.107654000
C	-3.511925000	1.994330000	4.049369000
C	-3.608361000	2.648400000	2.819798000
C	-3.077340000	2.025036000	1.690242000
C	-1.627293000	-1.119154000	2.901745000
N	-1.907465000	-1.833281000	1.637535000
C	-3.310923000	-2.317797000	1.579260000
C	-4.021713000	-1.981125000	0.284934000
N	-3.528356000	-0.971060000	-0.452858000
C	-4.169616000	-0.597045000	-1.574095000
C	-5.346059000	-1.208948000	-1.996377000
C	-5.861310000	-2.262742000	-1.237807000
C	-5.185383000	-2.657018000	-0.083366000
O	0.127467000	0.035906000	0.661273000
Fe	1.653387000	0.340113000	-0.296020000
N	2.872003000	0.599070000	1.664874000
C	4.276020000	0.972842000	1.381320000
C	4.770476000	0.453597000	0.048614000
N	3.861104000	0.376683000	-0.937053000
C	4.255715000	-0.026105000	-2.154472000
C	5.579191000	-0.345275000	-2.450627000
C	6.526085000	-0.263346000	-1.427660000
C	6.113145000	0.136014000	-0.155444000
O	1.100282000	0.408800000	-2.116140000
N	2.364321000	-1.723807000	0.182648000
C	2.920636000	-1.869911000	1.399244000
C	3.538655000	-3.058817000	1.783103000
C	3.567282000	-4.126170000	0.881096000
C	2.977725000	-3.969269000	-0.374222000
C	2.392061000	-2.742533000	-0.685506000
C	2.755578000	-0.701126000	2.350875000
N	1.687127000	2.512254000	0.134289000
C	1.934989000	2.847893000	1.414399000
C	1.955226000	4.175716000	1.835486000
C	1.693933000	5.182141000	0.902057000
C	1.419542000	4.826503000	-0.419538000
C	1.423858000	3.474337000	-0.759590000
C	2.144231000	1.683519000	2.358824000
N	-0.940812000	-2.211027000	-0.933323000
C	-0.864436000	-3.257825000	-0.098904000
C	-0.659013000	-4.555903000	-0.562930000
C	-0.512115000	-4.756332000	-1.938878000
C	-0.574001000	-3.657714000	-2.799408000
C	-0.800398000	-2.393653000	-2.250697000
C	-0.921125000	-2.902677000	1.371019000
H	-0.555785000	0.727687000	-1.847531000
H	3.988551000	-3.144439000	2.767608000
H	4.046172000	-5.061660000	1.154789000
H	2.976915000	-4.772728000	-1.103031000
H	1.923506000	-2.558091000	-1.647224000
H	2.175685000	4.413677000	2.871611000
H	1.710835000	6.225822000	1.201336000
H	1.213295000	5.578645000	-1.173171000
H	1.203335000	3.132392000	-1.766128000
H	6.818678000	0.203824000	0.667304000
H	7.566350000	-0.512768000	-1.614352000

H	5.854540000	-0.658564000	-3.452227000
H	3.467927000	-0.112667000	-2.896471000
H	3.467092000	-0.783016000	3.185732000
H	1.157985000	1.284453000	2.619428000
H	2.657912000	2.008443000	3.275134000
H	4.939872000	0.641430000	2.192351000
H	4.332074000	2.067318000	1.350145000
H	1.741125000	-0.753761000	2.762019000
H	-0.357688000	-5.756817000	-2.332654000
H	-0.613697000	-5.386913000	0.134607000
H	-0.465445000	-3.776528000	-3.872602000
H	-0.865126000	-1.492645000	-2.852347000
H	0.061825000	-2.501786000	1.641413000
H	-1.120329000	-3.792311000	1.985872000
H	-1.876293000	-1.730240000	3.781299000
H	-0.553565000	-0.906498000	2.906599000
H	-3.870907000	-1.847291000	2.396623000
H	-3.350527000	-3.400596000	1.757081000
H	-3.692759000	0.201361000	-2.130342000
H	-3.128716000	2.482713000	0.707515000
H	-5.553667000	-3.474662000	0.529258000
H	-5.837489000	-0.872813000	-2.903275000
H	-2.801320000	0.203403000	5.044360000
H	-4.092923000	3.615207000	2.731772000
H	-6.770634000	-2.772235000	-1.542239000
H	-3.925366000	2.442526000	4.947974000
H	1.592280000	0.969332000	-2.733753000

Ib-¹²TS_{2Hhs-hs}

C	-2.683347000	3.964430000	-1.685451000
C	-1.910112000	4.272267000	-2.993143000
C	-2.047356000	3.004641000	-3.782738000
C	-2.981165000	2.135568000	-3.196374000
C	-3.744389000	2.928701000	-2.123549000
H	-3.488328000	1.385412000	-3.809888000
H	-1.501914000	2.806083000	-4.700766000
H	-2.398192000	5.095253000	-3.544408000
H	-0.870961000	4.589577000	-2.832481000
H	-4.621629000	3.428940000	-2.557361000
H	-4.100715000	2.300646000	-1.297028000
H	-3.112637000	4.858955000	-1.223891000
H	-1.994384000	3.494749000	-0.971211000
H	-2.165937000	1.380582000	-2.344428000
O	-1.491728000	0.808466000	-1.490125000
Fe	-1.487483000	-0.238363000	0.130869000
N	-2.486746000	0.810199000	1.744077000
C	-2.373845000	0.228635000	2.959370000
C	-2.942108000	0.803537000	4.093644000
C	-3.627544000	2.014760000	3.970121000
C	-3.729667000	2.613645000	2.710795000
C	-3.145756000	1.973796000	1.620898000
C	-1.564894000	-1.049099000	3.002730000
N	-1.790712000	-1.822434000	1.763006000
C	-3.151596000	-2.404679000	1.713597000
C	-3.858471000	-2.198201000	0.390305000
N	-3.489324000	-1.138639000	-0.351960000
C	-4.155235000	-0.876368000	-1.491023000
C	-5.222699000	-1.652779000	-1.931077000
C	-5.602667000	-2.758961000	-1.167217000
C	-4.905163000	-3.036764000	0.008667000
O	0.180005000	0.113611000	0.818374000
Fe	1.688586000	0.385476000	-0.236264000
N	2.975852000	0.827334000	1.596634000
C	4.328176000	1.276010000	1.186359000
C	4.775827000	0.624815000	-0.097723000
N	3.814993000	0.444523000	-1.028894000
C	4.157139000	-0.095089000	-2.213384000
C	5.464295000	-0.444432000	-2.532747000
C	6.462851000	-0.246964000	-1.572231000
C	6.106647000	0.287566000	-0.332841000
O	1.046938000	0.439236000	-2.022041000
N	2.443199000	-1.575667000	0.264390000
C	3.165501000	-1.633550000	1.416681000
C	3.910553000	-2.755172000	1.755538000
C	3.903684000	-3.866849000	0.903413000

C	3.140227000	-3.806799000	-0.271866000
C	2.437639000	-2.644524000	-0.560271000
C	2.998471000	-0.454141000	2.340482000
N	1.550191000	2.551876000	0.081468000
C	1.844414000	2.978924000	1.327467000
C	1.719332000	4.318506000	1.689671000
C	1.246110000	5.232122000	0.745800000
C	0.911666000	4.775640000	-0.533260000
C	1.084277000	3.426207000	-0.825084000
C	2.241381000	1.898018000	2.304996000
N	-0.870994000	-2.090482000	-0.823291000
C	-0.707270000	-3.148698000	0.003293000
C	-0.486078000	-4.431333000	-0.487624000
C	-0.418022000	-4.628238000	-1.871069000
C	-0.558944000	-3.519221000	-2.718386000
C	-0.791561000	-2.269269000	-2.156669000
C	-0.722931000	-2.807889000	1.472458000
H	-0.546108000	0.805550000	-1.832302000
H	4.481446000	-2.762028000	2.679403000
H	4.478821000	-4.753624000	1.149079000
H	3.097793000	-4.645026000	-0.959372000
H	1.845326000	-2.543733000	-1.464053000
H	1.985105000	4.634532000	2.693793000
H	1.140954000	6.281783000	1.002730000
H	0.532467000	5.451684000	-1.291695000
H	0.833679000	3.009929000	-1.795027000
H	6.848878000	0.445654000	0.443778000
H	7.494167000	-0.513647000	-1.781251000
H	5.691731000	-0.867260000	-3.505610000
H	3.341069000	-0.267490000	-2.908079000
H	3.774409000	-0.449342000	3.118438000
H	1.322847000	1.444855000	2.694073000
H	2.821067000	2.312315000	3.141683000
H	5.055665000	1.097137000	1.989683000
H	4.277317000	2.359966000	1.023696000
H	2.018209000	-0.541669000	2.828035000
H	-0.256766000	-5.620929000	-2.279293000
H	-0.372503000	-5.260243000	0.204407000
H	-0.508182000	-3.625874000	-3.797032000
H	-0.920328000	-1.374697000	-2.754625000
H	0.228741000	-2.315745000	1.706295000
H	-0.829041000	-3.710807000	2.089720000
H	-1.804572000	-1.632731000	3.902633000
H	-0.501327000	-0.786287000	3.018511000
H	-3.756453000	-1.916871000	2.488454000
H	-3.121859000	-3.473735000	1.961602000
H	-3.801861000	-0.025112000	-2.058795000
H	-3.195420000	2.389320000	0.619657000
H	-5.169709000	-3.888043000	0.628902000
H	-5.735414000	-1.399329000	-2.852977000
H	-2.850702000	0.306764000	5.054784000
H	-4.257768000	3.550996000	2.572046000
H	-6.424267000	-3.395111000	-1.482240000
H	-4.080826000	2.478927000	4.840752000
H	1.578284000	0.924739000	-2.671113000

Ib-¹⁰TS_{2Hhs-is}

C	-2.266409000	4.006291000	-1.369695000
C	-1.595058000	4.683529000	-2.591086000
C	-1.831084000	3.715635000	-3.703576000
C	-2.736032000	2.640040000	-3.289090000
C	-3.404025000	3.179982000	-2.003063000
H	-3.408977000	2.272539000	-4.074969000
H	-1.385692000	3.804180000	-4.690194000
H	-2.088546000	5.644085000	-2.825595000
H	-0.533195000	4.924643000	-2.440696000
H	-4.256671000	3.823230000	-2.253922000
H	-3.755140000	2.369015000	-1.357284000
H	-2.609624000	4.729482000	-0.622326000
H	-1.555259000	3.315922000	-0.899350000
H	-2.126153000	1.754830000	-2.938000000
O	-1.496589000	0.717548000	-1.516261000
Fe	-1.564920000	-0.265413000	0.017678000
N	-2.474143000	0.831047000	1.749474000
C	-2.370998000	0.200786000	2.933229000

C	-2.886002000	0.747301000	4.107217000
C	-3.512211000	1.995341000	4.048630000
C	-3.608254000	2.649281000	2.818959000
C	-3.077060000	2.025700000	1.689603000
C	-1.627759000	-1.118553000	2.901808000
N	-1.907911000	-1.832876000	1.637702000
C	-3.311412000	-2.317261000	1.579402000
C	-4.022178000	-1.980491000	0.285085000
N	-3.528598000	-0.970623000	-0.452822000
C	-4.169828000	-0.596536000	-1.574053000
C	-5.346448000	-1.208175000	-1.996222000
C	-5.861927000	-2.261774000	-1.237536000
C	-5.186042000	-2.656117000	-0.083096000
O	0.127416000	0.035738000	0.661185000
Fe	1.653459000	0.339977000	-0.295941000
N	2.871967000	0.598438000	1.665098000
C	4.276034000	0.972156000	1.381711000
C	4.770528000	0.453213000	0.048901000
N	3.861201000	0.376550000	-0.936826000
C	4.255863000	-0.025957000	-2.154322000
C	5.579348000	-0.345078000	-2.450492000
C	6.526196000	-0.263406000	-1.427461000
C	6.113202000	0.135658000	-0.155170000
O	1.100434000	0.408930000	-2.116080000
N	2.364190000	-1.724069000	0.182359000
C	2.920396000	-1.870493000	1.398963000
C	3.538263000	-3.059547000	1.782610000
C	3.566851000	-4.126704000	0.880370000
C	2.977408000	-3.969468000	-0.374960000
C	2.391895000	-2.742604000	-0.686020000
C	2.755396000	-0.701890000	2.350828000
N	1.687317000	2.512029000	0.134830000
C	1.935113000	2.847383000	1.415028000
C	1.955335000	4.175113000	1.836409000
C	1.694061000	5.181745000	0.903197000
C	1.419713000	4.826402000	-0.418485000
C	1.424078000	3.474313000	-0.758842000
C	2.144248000	1.682806000	2.359226000
N	-0.941232000	-2.211187000	-0.933036000
C	-0.864931000	-3.257836000	-0.098420000
C	-0.659579000	-4.556009000	-0.562211000
C	-0.512687000	-4.756698000	-1.938121000
C	-0.574510000	-3.658237000	-2.798856000
C	-0.800824000	-2.394063000	-2.250376000
C	-0.921657000	-2.902417000	1.371438000
H	-0.555624000	0.727598000	-1.847610000
H	3.988080000	-3.145431000	2.767129000
H	4.045626000	-5.062303000	1.153895000
H	2.976580000	-4.772767000	-1.103947000
H	1.923443000	-2.557888000	-1.647733000
H	2.175751000	4.412845000	2.872596000
H	1.710935000	6.225358000	1.202714000
H	1.213439000	5.578708000	-1.171947000
H	1.203605000	3.132592000	-1.765467000
H	6.818698000	0.203261000	0.667627000
H	7.566466000	-0.512799000	-1.614164000
H	5.854738000	-0.658134000	-3.452153000
H	3.468110000	-0.112331000	-2.896378000
H	3.466865000	-0.784015000	3.185700000
H	1.157965000	1.283765000	2.619724000
H	2.657920000	2.007517000	3.275618000
H	4.939810000	0.640472000	2.192693000
H	4.332195000	2.066635000	1.350827000
H	1.740921000	-0.754522000	2.761921000
H	-0.358318000	-5.757266000	-2.331712000
H	-0.614321000	-5.386898000	0.135476000
H	-0.465965000	-3.777256000	-3.872028000
H	-0.865506000	-1.493157000	-2.852188000
H	0.061312000	-2.501567000	1.641822000
H	-1.120983000	-3.791923000	1.986437000
H	-1.876917000	-1.729448000	3.781449000
H	-0.554003000	-0.906037000	2.906722000
H	-3.871363000	-1.846753000	2.396787000
H	-3.351106000	-3.400065000	1.757172000
H	-3.692808000	0.201711000	-2.130387000

H	-3.128128000	2.483265000	0.706805000
H	-5.554505000	-3.473611000	0.529622000
H	-5.837841000	-0.871990000	-2.903122000
H	-2.802105000	0.204431000	5.044011000
H	-4.092647000	3.616152000	2.730706000
H	-6.771396000	-2.771062000	-1.541876000
H	-3.925799000	2.443708000	4.947083000
H	1.592407000	0.969576000	-2.733609000

Ib-⁸TS_{2H_{hs}-is}

C	-3.040496000	4.273988000	-0.645330000
C	-1.985312000	5.165718000	-1.340852000
C	-1.446463000	4.287733000	-2.416039000
C	-2.236982000	3.090676000	-2.585015000
C	-3.531578000	3.349543000	-1.779408000
H	-2.348601000	2.744677000	-3.621223000
H	-0.591272000	4.548511000	-3.033191000
H	-2.468929000	6.039187000	-1.816889000
H	-1.216914000	5.568726000	-0.669459000
H	-4.269613000	3.871313000	-2.401403000
H	-3.988458000	2.419993000	-1.423342000
H	-3.841881000	4.851466000	-0.175194000
H	-2.538134000	3.681479000	0.129550000
H	-1.720415000	2.185302000	-2.067651000
O	-1.360023000	0.613068000	-1.627616000
Fe	-1.479669000	-0.462473000	-0.140993000
N	-2.825860000	0.364991000	1.553502000
C	-2.787176000	-0.417989000	2.646253000
C	-3.600087000	-0.187633000	3.754855000
C	-4.477910000	0.899274000	3.730351000
C	-4.521176000	1.706046000	2.592668000
C	-3.680191000	1.393961000	1.523834000
C	-1.789742000	-1.552505000	2.590513000
N	-1.780074000	-2.162447000	1.241846000
C	-3.057278000	-2.869533000	0.939294000
C	-3.905564000	-2.170238000	-0.101753000
N	-3.345397000	-1.159568000	-0.788272000
C	-4.035487000	-0.560162000	-1.775150000
C	-5.332694000	-0.937946000	-2.104097000
C	-5.930886000	-1.974384000	-1.382077000
C	-5.205361000	-2.601394000	-0.369750000
O	-0.008665000	-0.014884000	0.619323000
Fe	1.677352000	0.367585000	-0.325654000
N	2.619876000	0.791633000	1.773865000
C	4.022907000	1.242400000	1.647262000
C	4.693858000	0.774785000	0.370835000
N	3.904107000	0.606593000	-0.702349000
C	4.460828000	0.245807000	-1.869157000
C	5.832709000	0.062224000	-2.025342000
C	6.656108000	0.239292000	-0.911128000
C	6.075852000	0.593609000	0.307572000
O	1.239328000	0.261925000	-2.185573000
N	2.481725000	-1.609249000	0.340410000
C	2.917463000	-1.655360000	1.613979000
C	3.654263000	-2.733859000	2.098606000
C	3.940504000	-3.796650000	1.235889000
C	3.480663000	-3.744128000	-0.080594000
C	2.757296000	-2.623131000	-0.488787000
C	2.497799000	-0.490754000	2.488697000
N	1.495639000	2.547939000	0.013199000
C	1.604251000	2.958655000	1.292001000
C	1.601459000	4.309385000	1.632949000
C	1.485450000	5.262897000	0.616715000
C	1.372766000	4.831127000	-0.705296000
C	1.373173000	3.459459000	-0.959614000
C	1.739481000	1.849610000	2.314964000
N	-0.611912000	-2.269393000	-1.225315000
C	-0.395301000	-3.320772000	-0.419871000
C	0.046033000	-4.548486000	-0.908454000
C	0.289742000	-4.670881000	-2.279793000
C	0.087281000	-3.565330000	-3.108442000
C	-0.374103000	-2.377080000	-2.536685000
C	-0.606230000	-3.043306000	1.050951000
H	-0.415615000	0.582013000	-1.954097000
H	3.999523000	-2.738134000	3.128067000

H	4.518161000	-4.646700000	1.586847000
H	3.682538000	-4.547133000	-0.781715000
H	2.378228000	-2.520297000	-1.501528000
H	1.703558000	4.607192000	2.672079000
H	1.498758000	6.322508000	0.854207000
H	1.293587000	5.538618000	-1.523854000
H	1.286188000	3.060882000	-1.965838000
H	6.682567000	0.730974000	1.197816000
H	7.729892000	0.096336000	-0.987303000
H	6.239908000	-0.221828000	-2.990080000
H	3.764249000	0.080096000	-2.685436000
H	3.069170000	-0.490368000	3.429015000
H	0.754426000	1.395380000	2.462101000
H	2.105593000	2.247159000	3.272911000
H	4.613811000	0.931818000	2.520789000
H	4.027937000	2.338865000	1.638311000
H	1.436101000	-0.617506000	2.727346000
H	0.628276000	-5.616234000	-2.693991000
H	0.197991000	-5.383917000	-0.231707000
H	0.267383000	-3.622189000	-4.176975000
H	-0.549088000	-1.479367000	-3.118172000
H	0.263267000	-2.488692000	1.416153000
H	-0.706344000	-3.976592000	1.622938000
H	-2.004367000	-2.301874000	3.365523000
H	-0.786359000	-1.145300000	2.750348000
H	-3.639231000	-3.006402000	1.859324000
H	-2.823794000	-3.873897000	0.565642000
H	-3.496350000	0.226207000	-2.291576000
H	-3.689577000	1.975811000	0.610192000
H	-5.634694000	-3.417477000	0.203856000
H	-5.859160000	-0.432066000	-2.906469000
H	-3.548303000	-0.848586000	4.614920000
H	-5.197116000	2.552245000	2.525864000
H	-6.944224000	-2.293022000	-1.607496000
H	-5.123535000	1.103261000	4.579351000
H	1.690046000	0.852279000	-2.806347000

Ib-⁴TS_{2H_{hs}-is}

Fe	1.702498000	-0.314305000	-0.262339000
O	1.352034000	0.547841000	-1.957575000
Fe	-1.572267000	0.219808000	-0.201502000
O	-1.390835000	0.419859000	-2.026616000
H	-0.422894000	0.447238000	-2.206627000
O	0.076117000	0.012489000	0.509439000
N	1.148649000	-2.409210000	-1.078870000
N	2.764547000	1.036128000	1.292234000
N	3.690579000	-0.649703000	-0.756856000
C	0.987837000	-3.297004000	-0.083268000
C	0.650818000	-4.628242000	-0.321301000
H	0.545535000	-5.320976000	0.508157000
C	0.453835000	-5.044109000	-1.640234000
H	0.198250000	-6.077038000	-1.857762000
C	0.595925000	-4.115094000	-2.672337000
H	0.450322000	-4.395747000	-3.710368000
C	0.946871000	-2.805875000	-2.340066000
H	1.066384000	-2.043926000	-3.105450000
C	2.903739000	0.394790000	2.464848000
C	3.663277000	0.917560000	3.510812000
H	3.764576000	0.366126000	4.440922000
C	4.284416000	2.156959000	3.335281000
H	4.882429000	2.589113000	4.132084000
C	4.129651000	2.825831000	2.119843000
H	4.597100000	3.789143000	1.943273000
C	3.364636000	2.218983000	1.122890000
H	3.221255000	2.686062000	0.151776000
C	4.354606000	-1.466148000	0.086936000
C	5.740099000	-1.619290000	0.020103000
H	6.243711000	-2.280113000	0.719197000
C	6.457545000	-0.917673000	-0.947227000
H	7.535695000	-1.025226000	-1.017724000
C	5.767024000	-0.067408000	-1.815148000
H	6.284985000	0.505548000	-2.576947000
C	4.388495000	0.041835000	-1.676550000
H	3.804496000	0.712076000	-2.297634000
C	1.143840000	-2.735365000	1.311987000

H	1.350179000	-3.533564000	2.039565000
C	2.131354000	-0.900844000	2.591028000
H	1.076537000	-0.648748000	2.741041000
H	2.490030000	-1.489698000	3.447458000
C	3.540317000	-2.257755000	1.087454000
H	3.418978000	-3.272272000	0.689864000
H	4.097272000	-2.353836000	2.028630000
N	2.187240000	-1.687344000	1.338927000
H	0.207902000	-2.237750000	1.570760000
H	-3.533327000	-5.453851000	0.645360000
C	-3.134472000	-4.456770000	0.482958000
C	-2.984581000	-3.575223000	1.557506000
C	-2.782047000	-4.032508000	-0.799033000
C	-2.484294000	-2.297387000	1.314421000
H	-3.265459000	-3.866195000	2.565292000
H	-2.894097000	-4.683145000	-1.659700000
C	-2.290948000	-2.737331000	-0.959508000
N	-2.141417000	-1.901547000	0.075125000
C	-2.265603000	-1.280076000	2.419181000
H	-2.010938000	-2.333608000	-1.927391000
H	-1.203696000	-1.271190000	2.687414000
H	-2.834590000	-1.569265000	3.316141000
N	-2.606809000	0.073048000	1.963535000
N	-3.855386000	0.271779000	-0.525439000
N	-1.895080000	2.269953000	0.537202000
C	-1.887647000	1.148424000	2.674601000
C	-4.066294000	0.300827000	1.904901000
C	-4.665333000	0.091279000	0.526870000
C	-4.358567000	0.187026000	-1.767711000
C	-1.997978000	2.426721000	1.870021000
C	-2.008632000	3.330761000	-0.270004000
H	-2.258177000	1.301615000	3.699166000
H	-0.832989000	0.853127000	2.708029000
H	-4.264006000	1.340423000	2.193190000
H	-4.587557000	-0.328447000	2.640098000
C	-6.022143000	-0.197132000	0.374466000
C	-5.705718000	-0.078040000	-2.007934000
H	-3.634862000	0.328920000	-2.564274000
C	-2.211707000	3.678283000	2.443107000
C	-2.218548000	4.618252000	0.224988000
H	-1.927603000	3.118449000	-1.330696000
H	-6.649355000	-0.346825000	1.248615000
C	-6.550836000	-0.280267000	-0.914465000
H	-6.077617000	-0.132574000	-3.025828000
H	-2.305545000	3.773936000	3.520524000
C	-2.317543000	4.793171000	1.606204000
H	-2.308427000	5.456168000	-0.458177000
H	-7.604051000	-0.500789000	-1.061706000
H	-2.490590000	5.779192000	2.027129000
H	1.815247000	0.077945000	-2.670940000
H	1.521892000	1.978051000	-2.418700000
C	1.554512000	3.028786000	-3.018453000
H	2.276650000	2.786667000	-3.810746000
C	1.960612000	4.013187000	-2.075791000
H	2.976783000	4.120544000	-1.702941000
C	0.821350000	4.861473000	-1.623914000
H	1.125960000	5.889907000	-1.392558000
H	0.394734000	4.447009000	-0.692713000
C	0.095422000	3.352787000	-3.429097000
H	-0.030547000	3.366193000	-4.515790000
H	-0.576518000	2.583593000	-3.029502000
C	-0.180670000	4.745185000	-2.800842000
H	0.040115000	5.531300000	-3.531020000
H	-1.220686000	4.874641000	-2.486779000

Ib-²TS_{2H_{hs}-is}

Fe	-1.624403000	0.112673000	0.056237000
O	-1.351412000	0.098674000	1.938341000
Fe	1.535939000	0.334721000	-0.026676000
O	1.116154000	-1.098834000	1.106847000
H	0.311928000	-0.838988000	1.607691000
O	-0.107523000	0.803772000	-0.640871000
N	-1.227509000	-1.938330000	-0.657186000
N	-2.818746000	1.944474000	-0.196482000
N	-3.714393000	-0.677199000	0.362209000

C	-1.212595000	-2.093575000	-1.993358000
C	-0.904991000	-3.318236000	-2.583193000
H	-0.916552000	-3.417227000	-3.664220000
C	-0.596068000	-4.403601000	-1.759321000
H	-0.360901000	-5.371332000	-2.192843000
C	-0.611221000	-4.231044000	-0.373790000
H	-0.387184000	-5.050460000	0.300946000
C	-0.936057000	-2.975690000	0.137095000
H	-0.966891000	-2.786887000	1.204517000
C	-3.207219000	2.228213000	-1.453666000
C	-4.089389000	3.271284000	-1.724775000
H	-4.395346000	3.472984000	-2.746762000
C	-4.570848000	4.040389000	-0.661174000
H	-5.261061000	4.858138000	-0.845956000
C	-4.164862000	3.735490000	0.639490000
H	-4.526078000	4.302333000	1.491103000
C	-3.288545000	2.667636000	0.828466000
H	-2.953257000	2.355170000	1.813081000
C	-4.512562000	-0.788514000	-0.709428000
C	-5.880638000	-1.035852000	-0.583261000
H	-6.503933000	-1.112087000	-1.469580000
C	-6.424180000	-1.183940000	0.692917000
H	-7.485354000	-1.378617000	0.817071000
C	-5.586073000	-1.071331000	1.805369000
H	-5.971077000	-1.175364000	2.814429000
C	-4.235478000	-0.806913000	1.594477000
H	-3.527532000	-0.673876000	2.406634000
C	-1.521883000	-0.849376000	-2.797412000
H	-1.832456000	-1.113859000	-3.818768000
C	-2.591086000	1.359471000	-2.529918000
H	-1.553852000	1.682283000	-2.671727000
H	-3.132475000	1.475955000	-3.480119000
C	-3.870251000	-0.700874000	-2.083401000
H	-3.754766000	-1.724537000	-2.460305000
H	-4.552757000	-0.191448000	-2.777228000
N	-2.541829000	-0.047745000	-2.092597000
H	-0.611175000	-0.243227000	-2.842123000
H	3.682585000	-1.554319000	-5.400287000
C	3.223489000	-1.279382000	-4.455250000
C	3.040638000	0.067749000	-4.126740000
C	2.816803000	-2.261875000	-3.551251000
C	2.452642000	0.384756000	-2.903719000
H	3.349552000	0.856692000	-4.805961000
H	2.947535000	-3.316793000	-3.769530000
C	2.246590000	-1.856924000	-2.342792000
N	2.068380000	-0.568593000	-2.033331000
C	2.145851000	1.813260000	-2.491134000
H	1.919382000	-2.571570000	-1.592782000
H	1.068403000	1.972872000	-2.601263000
H	2.678813000	2.526087000	-3.136133000
N	2.456807000	2.045626000	-1.061651000
N	3.634448000	-0.031951000	0.317075000
N	1.629227000	1.928692000	1.556630000
C	1.741835000	3.216020000	-0.496549000
C	3.920524000	2.109738000	-0.806949000
C	4.493931000	0.811482000	-0.279827000
C	4.095036000	-1.154786000	0.892524000
C	1.758568000	3.157238000	1.020455000
C	1.603395000	1.784000000	2.887889000
H	2.164193000	4.165454000	-0.854813000
H	0.702370000	3.132498000	-0.829651000
H	4.102562000	2.882125000	-0.049961000
H	4.455812000	2.424590000	-1.712310000
C	5.861320000	0.544005000	-0.338383000
C	5.447561000	-1.485140000	0.890745000
C	3.335107000	-1.777842000	1.351607000
C	1.870922000	4.295156000	1.818294000
C	1.690887000	2.872235000	3.756738000
H	1.516446000	0.761897000	3.248277000
H	6.531673000	1.240355000	-0.833431000
C	6.344951000	-0.621923000	0.256698000
H	5.786539000	-2.398032000	1.369044000
H	1.990962000	5.272742000	1.361003000
C	1.828373000	4.149368000	3.208102000
H	1.663688000	2.719612000	4.830643000

H	7.405853000	-0.851935000	0.226865000
H	1.913166000	5.019789000	3.851938000
H	-0.772583000	0.825972000	2.220145000
H	1.204397000	-2.616488000	2.087274000
C	1.318458000	-3.195681000	3.057891000
H	2.107206000	-3.936567000	2.865714000
C	0.030442000	-3.763869000	3.458062000
H	-0.373216000	-4.701685000	3.085026000
C	-0.654357000	-2.917171000	4.479566000
H	-0.660509000	-3.449244000	5.448068000
H	-1.709255000	-2.713281000	4.244264000
C	1.627890000	-2.135407000	4.140981000
H	2.133771000	-2.601689000	4.995070000
H	2.269176000	-1.335912000	3.754067000
C	0.223977000	-1.642253000	4.551908000
H	0.205363000	-1.175455000	5.541610000
H	-0.155338000	-0.919609000	3.819604000

Ib-⁶TS_{2HIs-is}

Fe	1.733331000	-0.118022000	-0.133098000
O	1.680806000	1.037682000	-1.763624000
Fe	-1.546966000	0.031656000	-0.237686000
O	-0.991589000	0.205194000	-1.952565000
H	-0.132783000	0.678228000	-1.910007000
O	0.024561000	0.178697000	0.569960000
N	1.210944000	-1.915260000	-0.891704000
N	2.465063000	1.323964000	1.087550000
N	3.739901000	-0.697396000	-0.605685000
C	1.310878000	-2.915505000	0.014549000
C	1.255891000	-4.253267000	-0.365516000
H	1.354946000	-5.029804000	0.386474000
C	1.066576000	-4.571610000	-1.712856000
H	1.036328000	-5.608419000	-2.034504000
C	0.904651000	-3.535264000	-2.632502000
H	0.732542000	-3.733408000	-3.685234000
C	0.980902000	-2.218746000	-2.176978000
H	0.823229000	-1.377269000	-2.839527000
C	2.532832000	0.965790000	2.390346000
C	3.093558000	1.804633000	3.349599000
H	3.143117000	1.482695000	4.385342000
C	3.600828000	3.045691000	2.954773000
H	4.049541000	3.713148000	3.684281000
C	3.541911000	3.398883000	1.606760000
H	3.944507000	4.342097000	1.252986000
C	2.965398000	2.504770000	0.704924000
H	2.894900000	2.715498000	-0.355919000
C	4.352032000	-1.539184000	0.246975000
C	5.568890000	-2.150367000	-0.056598000
H	6.021686000	-2.832860000	0.656664000
C	6.190679000	-1.859785000	-1.269565000
H	7.138147000	-2.322502000	-1.528717000
C	5.575838000	-0.953734000	-2.136594000
H	6.028299000	-0.680531000	-3.084007000
C	4.353857000	-0.401471000	-1.766027000
H	3.839032000	0.313843000	-2.394767000
C	1.389012000	-2.488363000	1.467417000
H	1.675851000	-3.336992000	2.105062000
C	1.969404000	-0.401687000	2.728433000
H	0.881772000	-0.319018000	2.761411000
H	2.343278000	-0.746678000	3.702819000
C	3.718153000	-1.717109000	1.609050000
H	3.856340000	-2.747350000	1.964750000
H	4.260376000	-1.069113000	2.308891000
N	2.293274000	-1.339332000	1.634423000
H	0.389223000	-2.151742000	1.747756000
H	-3.111180000	-5.574630000	1.812638000
C	-2.745868000	-4.628214000	1.424937000
C	-2.695763000	-3.499561000	2.249448000
C	-2.335117000	-4.514472000	0.096461000
C	-2.231929000	-2.300419000	1.712656000
H	-3.021078000	-3.545215000	3.284507000
H	-2.368683000	-5.363228000	-0.578808000
C	-1.882493000	-3.273745000	-0.356213000
N	-1.825633000	-2.198409000	0.434433000
C	-2.143149000	-1.017923000	2.511177000

H	-1.550493000	-3.127128000	-1.379268000
H	-1.095224000	-0.804707000	2.739456000
H	-2.698114000	-1.106618000	3.456340000
N	-2.635008000	0.111094000	1.700292000
N	-3.487977000	-0.399871000	-0.891532000
N	-2.447693000	2.140506000	-0.012608000
C	-2.243849000	1.424576000	2.268374000
C	-4.102118000	-0.001240000	1.450413000
C	-4.450612000	-0.456801000	0.045780000
C	-3.770874000	-0.718688000	-2.165323000
C	-2.610570000	2.502315000	1.270559000
C	-2.847481000	2.962376000	-0.987351000
H	-2.719689000	1.609807000	3.242061000
H	-1.155123000	1.387463000	2.388106000
H	-4.563705000	0.980098000	1.608534000
H	-4.559716000	-0.678984000	2.182352000
C	-5.747061000	-0.863599000	-0.269467000
C	-5.043327000	-1.123896000	-2.558120000
H	-2.933752000	-0.627442000	-2.850508000
C	-3.141355000	3.740315000	1.626974000
C	-3.399460000	4.216496000	-0.722213000
H	-2.711000000	2.592671000	-1.998192000
H	-6.506556000	-0.906926000	0.505629000
C	-6.047247000	-1.202523000	-1.589321000
H	-5.239866000	-1.372450000	-3.595709000
H	-3.267437000	4.002282000	2.673219000
C	-3.532830000	4.615878000	0.609044000
H	-3.717988000	4.857494000	-1.537715000
H	-7.050436000	-1.520544000	-1.857345000
H	-3.957496000	5.584810000	0.854739000
H	1.788688000	0.514308000	-2.577657000
H	1.756761000	2.479990000	-2.338285000
C	1.453694000	3.560622000	-2.765516000
H	1.649406000	3.497785000	-3.841858000
C	2.200821000	4.520332000	-2.016920000
H	3.204617000	4.855529000	-2.266479000
C	1.426090000	5.021968000	-0.844347000
H	1.114145000	6.060045000	-1.062186000
H	2.001998000	5.071286000	0.088467000
C	-0.004550000	3.671352000	-2.268003000
H	-0.541518000	4.448806000	-2.827626000
H	-0.537177000	2.724583000	-2.371900000
C	0.194215000	4.085437000	-0.794531000
H	-0.681190000	4.570948000	-0.357199000
H	0.422950000	3.190417000	-0.203180000

Ib-⁴TS_{2Hls-is}

Fe	1.755143000	-0.289924000	-0.003844000
O	1.837465000	0.909593000	-1.516187000
Fe	-1.539414000	0.088281000	-0.211728000
O	-0.918584000	0.307950000	-1.904211000
H	-0.001524000	0.626665000	-1.792817000
O	0.013594000	0.029956000	0.622324000
N	1.178742000	-1.975630000	-0.946390000
N	2.397313000	1.075768000	1.289413000
N	3.722579000	-0.864073000	-0.428824000
C	1.116739000	-3.027258000	-0.097861000
C	0.957537000	-4.332651000	-0.552527000
H	0.927672000	-5.152140000	0.158578000
C	0.829541000	-4.560430000	-1.925121000
H	0.717259000	-5.570582000	-2.307481000
C	0.838019000	-3.467610000	-2.792004000
H	0.721300000	-3.593813000	-3.863226000
C	1.014484000	-2.190983000	-2.258342000
H	1.000698000	-1.310964000	-2.888997000
C	2.332028000	0.675525000	2.578105000
C	2.755154000	1.497550000	3.618617000
H	2.708687000	1.143939000	4.644180000
C	3.239909000	2.773826000	3.316194000
H	3.575172000	3.434241000	4.110240000
C	3.300680000	3.178174000	1.981804000
H	3.678077000	4.157006000	1.705048000
C	2.876866000	2.290286000	0.994210000
H	2.908024000	2.522174000	-0.063075000
C	4.233884000	-1.795062000	0.397690000

C	5.439853000	-2.444835000	0.138304000
H	5.807918000	-3.198870000	0.827642000
C	6.161118000	-2.098439000	-1.003535000
H	7.103029000	-2.588465000	-1.230567000
C	5.654024000	-1.100841000	-1.838784000
H	6.189043000	-0.781554000	-2.726962000
C	4.434296000	-0.514017000	-1.515556000
H	4.002309000	0.274719000	-2.118771000
C	1.127044000	-2.665380000	1.369382000
H	1.346872000	-3.538277000	1.998510000
C	1.735530000	-0.700721000	2.789707000
H	0.649988000	-0.595667000	2.799695000
H	2.075153000	-1.148699000	3.732840000
C	3.483911000	-2.018833000	1.686528000
H	3.525876000	-3.071972000	1.990831000
H	3.994943000	-1.443701000	2.467895000
N	2.071292000	-1.551087000	1.616613000
H	0.130361000	-2.287691000	1.602190000
H	-3.658424000	-5.546802000	0.983743000
C	-3.196719000	-4.590544000	0.755960000
C	-3.118908000	-3.593961000	1.734256000
C	-2.686176000	-4.332645000	-0.516906000
C	-2.529365000	-2.376242000	1.401103000
H	-3.516839000	-3.753987000	2.731927000
H	-2.735997000	-5.076405000	-1.305474000
C	-2.112825000	-3.083968000	-0.763109000
N	-2.031954000	-2.136499000	0.175377000
C	-2.378196000	-1.235298000	2.384849000
H	-1.701439000	-2.821621000	-1.732959000
H	-1.337152000	-1.186284000	2.718258000
H	-3.012824000	-1.397701000	3.268418000
N	-2.678017000	0.050247000	1.731673000
N	-3.508212000	-0.031245000	-0.923443000
N	-2.126017000	2.248566000	0.312030000
C	-2.130683000	1.204379000	2.479483000
C	-4.132162000	0.185868000	1.437696000
C	-4.492632000	-0.093030000	-0.008942000
C	-3.793382000	-0.192569000	-2.226243000
C	-2.278816000	2.449416000	1.632318000
C	-2.313469000	3.266630000	-0.532465000
H	-2.617016000	1.334220000	3.457332000
H	-1.064495000	0.994647000	2.619659000
H	-4.440524000	1.212945000	1.664185000
H	-4.718440000	-0.466138000	2.098560000
C	-5.814534000	-0.339951000	-0.379476000
C	-5.090290000	-0.428197000	-2.674240000
H	-2.935184000	-0.123766000	-2.887614000
C	-2.595492000	3.700166000	2.158390000
C	-2.637386000	4.551528000	-0.093925000
H	-2.204185000	3.028498000	-1.585435000
H	-6.590264000	-0.392704000	0.378769000
C	-6.117966000	-0.508611000	-1.731030000
H	-5.286635000	-0.550682000	-3.734194000
H	-2.723602000	3.826298000	3.229322000
C	-2.768102000	4.772264000	1.277876000
H	-2.790902000	5.351658000	-0.810727000
H	-7.140696000	-0.700037000	-2.042097000
H	-3.022979000	5.757273000	1.657585000
H	1.951403000	0.427996000	-2.352448000
H	1.245129000	2.284989000	-2.089145000
C	0.633669000	3.248450000	-2.395598000
H	-0.338297000	2.798776000	-2.628157000
C	1.323520000	3.896844000	-3.469886000
H	1.268244000	3.589378000	-4.511335000
C	2.134930000	5.052676000	-3.001094000
H	1.640817000	5.979700000	-3.347427000
H	3.148429000	5.084040000	-3.423242000
C	0.749306000	4.201808000	-1.184302000
H	-0.087684000	4.909813000	-1.180827000
H	0.738249000	3.663063000	-0.232088000
C	2.075759000	4.944162000	-1.456743000
H	2.131615000	5.918754000	-0.963613000
H	2.925800000	4.343257000	-1.111108000

Ib-⁴TS_{2Hls-is}

C	3.231414000	-4.575118000	-0.575672000
C	3.043680000	-3.710747000	-1.659049000
C	2.822034000	-4.169770000	0.695482000
C	2.450492000	-2.471315000	-1.429324000
H	3.358843000	-3.988769000	-2.660327000
H	2.957797000	-4.808962000	1.561773000
C	2.238205000	-2.909757000	0.835753000
N	2.054460000	-2.088607000	-0.202652000
C	2.171746000	-1.471581000	-2.531953000
H	1.902528000	-2.535733000	1.798268000
H	1.101982000	-1.497888000	-2.767013000
H	2.732054000	-1.729425000	-3.442389000
N	2.470504000	-0.098683000	-2.081585000
N	3.551380000	0.192142000	0.465383000
N	1.829484000	2.212168000	-0.894482000
C	1.808133000	0.920715000	-2.925432000
C	3.934599000	0.139739000	-1.951950000
C	4.446511000	0.045113000	-0.527943000
C	3.964340000	0.205171000	1.743326000
C	1.863543000	2.266956000	-2.234528000
C	1.850617000	3.341674000	-0.180676000
H	2.248493000	0.972103000	-3.931671000
H	0.757603000	0.619874000	-2.999955000
H	4.150380000	1.152492000	-2.311823000
H	4.494828000	-0.547886000	-2.599362000
C	5.806840000	-0.112950000	-0.263050000
C	5.306320000	0.066036000	2.086125000
H	3.169474000	0.330376000	2.472198000
C	1.925135000	3.479564000	-2.919647000
C	1.901689000	4.598440000	-0.783678000
H	1.826146000	3.206076000	0.895244000
H	6.509271000	-0.235995000	-1.082063000
C	6.242639000	-0.101991000	1.062655000
H	5.607563000	0.082997000	3.128270000
H	1.968693000	3.494723000	-4.004617000
C	1.938120000	4.664641000	-2.178888000
H	1.926662000	5.499454000	-0.178800000
H	7.297195000	-0.222340000	1.292378000
H	1.989808000	5.624597000	-2.684106000
H	-1.879657000	0.856920000	2.298971000
H	-1.339512000	2.640574000	2.096227000
C	-1.230217000	3.535856000	2.907549000
H	-2.055516000	4.213065000	2.660781000
C	0.097546000	4.016331000	2.738998000
H	0.388771000	4.762265000	2.004471000
C	1.060726000	3.333586000	3.650910000
H	1.467500000	4.077796000	4.357855000
H	1.921487000	2.902366000	3.120627000
C	-1.245621000	2.798623000	4.265307000
H	-1.465328000	3.506394000	5.073730000
H	-2.000964000	2.004673000	4.306091000
C	0.200356000	2.263870000	4.371930000
H	0.516422000	2.097108000	5.405442000
H	0.301497000	1.323711000	3.819458000

Ib-⁴TS_{2Hls-ls}

Fe	1.607795000	0.294592000	0.047813000
O	1.298964000	-1.038214000	1.611426000
Fe	-1.626211000	-0.070454000	-0.255682000
O	-1.330385000	-0.073883000	1.562883000
H	-0.437716000	-0.461640000	1.662578000
O	-0.009760000	0.456642000	-0.796195000
N	1.103871000	1.974342000	1.098382000
N	2.227811000	-0.970143000	-1.356645000
N	3.685615000	0.331335000	0.617566000
C	1.118251000	3.087015000	0.327129000
C	0.772487000	4.336279000	0.837854000
H	0.817409000	5.209785000	0.194616000
C	0.370651000	4.442304000	2.170739000
H	0.103856000	5.407725000	2.590448000
C	0.324971000	3.287664000	2.951050000
H	0.014189000	3.316485000	3.990070000
C	0.700100000	2.076591000	2.372399000
H	0.658672000	1.156267000	2.940007000
C	2.637214000	-0.373828000	-2.498384000

C	3.210893000	-1.110963000	-3.532087000
H	3.544062000	-0.607233000	-4.434549000
C	3.354101000	-2.493616000	-3.385285000
H	3.804312000	-3.084499000	-4.177350000
C	2.920833000	-3.097818000	-2.204283000
H	3.016756000	-4.167203000	-2.048782000
C	2.367960000	-2.295010000	-1.208406000
H	2.021182000	-2.690787000	-0.260171000
C	4.476355000	1.159968000	-0.092752000
C	5.867893000	1.088090000	-0.039003000
H	6.465177000	1.773327000	-0.633126000
C	6.468907000	0.132759000	0.779839000
H	7.550538000	0.059535000	0.840213000
C	5.650802000	-0.734517000	1.505762000
H	6.069449000	-1.504685000	2.145089000
C	4.270098000	-0.607557000	1.385083000
H	3.590432000	-1.285090000	1.888244000
C	1.445012000	2.907787000	-1.144911000
H	1.791481000	3.856967000	-1.578569000
C	2.367461000	1.119280000	-2.629090000
H	1.346445000	1.231963000	-3.007628000
H	3.053751000	1.562481000	-3.365209000
C	3.782239000	2.219805000	-0.917839000
H	3.691853000	3.121113000	-0.299148000
H	4.398296000	2.490729000	-1.786927000
N	2.425067000	1.818986000	-1.333012000
H	0.520112000	2.595181000	-1.635053000
H	-3.755842000	5.286009000	-0.980980000
C	-3.332585000	4.300693000	-0.809902000
C	-3.100549000	3.439625000	-1.887615000
C	-3.018860000	3.877719000	0.483011000
C	-2.562063000	2.181239000	-1.634810000
H	-3.332829000	3.739308000	-2.905006000
H	-3.183627000	4.521065000	1.340790000
C	-2.496121000	2.597493000	0.661371000
N	-2.281379000	1.781414000	-0.377547000
C	-2.161560000	1.209932000	-2.729129000
H	-2.222973000	2.179795000	1.624489000
H	-1.107052000	1.391990000	-2.956015000
H	-2.750623000	1.371562000	-3.641325000
N	-2.257599000	-0.194816000	-2.255167000
N	-3.597822000	-0.606741000	0.067725000
N	-1.114892000	-1.978256000	-0.600075000
C	-1.257567000	-1.118107000	-2.857235000
C	-3.640535000	-0.747804000	-2.351011000
C	-4.369677000	-0.722234000	-1.025963000
C	-4.158755000	-0.649406000	1.287851000
C	-1.032471000	-2.281137000	-1.913545000
C	-0.885448000	-2.919456000	0.320532000
H	-1.562009000	-1.461661000	-3.854648000
H	-0.317807000	-0.564180000	-2.920632000
H	-3.566434000	-1.792159000	-2.677228000
H	-4.213128000	-0.216720000	-3.121294000
C	-5.751834000	-0.879699000	-0.937410000
C	-5.530065000	-0.817589000	1.459676000
H	-3.454160000	-0.529322000	2.104914000
C	-0.719517000	-3.568189000	-2.341503000
C	-0.547815000	-4.225613000	-0.029603000
H	-0.982250000	-2.583092000	1.344835000
H	-6.350431000	-0.964251000	-1.839524000
C	-6.340799000	-0.929589000	0.326981000
H	-5.952765000	-0.849068000	2.458437000
H	-0.675399000	-3.791427000	-3.402909000
C	-0.467979000	-4.555282000	-1.383907000
H	-0.367068000	-4.967194000	0.741796000
H	-7.415410000	-1.050470000	0.425584000
H	-0.226265000	-5.568029000	-1.692713000
H	1.679986000	-0.495202000	2.322211000
H	0.929277000	-2.098486000	2.567539000
C	0.806449000	-2.705671000	3.642409000
H	1.637174000	-3.419166000	3.603761000
C	-0.512942000	-3.221530000	3.662385000
H	-0.811529000	-4.168940000	3.220107000
C	-1.469764000	-2.301299000	4.344157000
H	-1.834621000	-2.793575000	5.262561000

H	-2.359614000	-2.081756000	3.737855000
C	0.836074000	-1.572936000	4.693063000
H	1.088996000	-1.986101000	5.677046000
H	1.577306000	-0.796373000	4.465747000
C	-0.617507000	-1.047148000	4.668184000
H	-0.910795000	-0.574355000	5.609704000
H	-0.752832000	-0.324891000	3.856404000

Ib-²TS_{2Hls-ls}

Fe	1.541785000	-0.403587000	0.196761000
O	1.410150000	0.904855000	-1.275879000
Fe	-1.720420000	0.099223000	-0.113775000
O	-1.129569000	0.099766000	-1.827388000
H	-0.259843000	0.545692000	-1.752643000
O	-0.249473000	-0.400672000	0.765646000
N	1.122735000	-2.049216000	-0.912145000
N	1.929157000	0.914115000	1.643752000
N	3.532151000	-0.755659000	-0.222355000
C	1.035717000	-3.160153000	-0.146472000
C	0.838562000	-4.424371000	-0.696018000
H	0.789738000	-5.292852000	-0.046463000
C	0.698427000	-4.547627000	-2.079715000
H	0.552034000	-5.522928000	-2.534255000
C	0.748028000	-3.395228000	-2.863725000
H	0.630970000	-3.437391000	-3.941472000
C	0.962910000	-2.168967000	-2.236999000
H	0.976250000	-1.251409000	-2.810552000
C	1.861827000	0.378120000	2.884396000
C	2.085292000	1.141233000	4.027472000
H	2.041940000	0.673627000	5.006582000
C	2.365762000	2.503262000	3.891043000
H	2.547926000	3.117672000	4.767589000
C	2.415523000	3.053563000	2.610221000
H	2.628981000	4.106161000	2.457013000
C	2.197090000	2.221443000	1.513667000
H	2.222416000	2.593507000	0.498189000
C	4.097571000	-1.709772000	0.543191000
C	5.362393000	-2.232118000	0.275236000
H	5.771669000	-3.009979000	0.913024000
C	6.086119000	-1.734555000	-0.807375000
H	7.073183000	-2.123745000	-1.037351000
C	5.516381000	-0.722521000	-1.582950000
H	6.044114000	-0.293532000	-2.428285000
C	4.241963000	-0.269923000	-1.258101000
H	3.764411000	0.512342000	-1.832900000
C	1.033341000	-2.930124000	1.346494000
H	1.321819000	-3.836960000	1.894827000
C	1.453364000	-1.078328000	2.948346000
H	0.363147000	-1.118436000	2.967304000
H	1.845600000	-1.565109000	3.851511000
C	3.332063000	-2.120902000	1.776923000
H	3.460996000	-3.191695000	1.978233000
H	3.771263000	-1.585371000	2.627353000
N	1.885859000	-1.771491000	1.709245000
H	0.008957000	-2.650674000	1.604695000
H	-3.927124000	-5.274959000	0.197162000
C	-3.482699000	-4.288181000	0.107540000
C	-3.468927000	-3.421862000	1.205077000
C	-2.929463000	-3.865663000	-1.102503000
C	-2.896033000	-2.161229000	1.057932000
H	-3.897406000	-3.717539000	2.157920000
H	-2.926701000	-4.509686000	-1.975420000
C	-2.387929000	-2.583446000	-1.180180000
N	-2.373486000	-1.765063000	-0.121106000
C	-2.738506000	-1.188164000	2.212490000
H	-1.945934000	-2.166313000	-2.078470000
H	-1.760300000	-1.371035000	2.663973000
H	-3.509500000	-1.356296000	2.975828000
N	-2.737224000	0.220441000	1.739887000
N	-3.649142000	0.580934000	-0.784915000
N	-1.290972000	2.008348000	0.334838000
C	-1.875425000	1.140520000	2.528308000
C	-4.111492000	0.774042000	1.576755000
C	-4.605987000	0.672040000	0.153268000
C	-3.991407000	0.578498000	-2.083819000

C	-1.462421000	2.299869000	1.643650000
C	-0.920346000	2.970401000	-0.517976000
H	-2.378292000	1.496173000	3.437631000
H	-0.974382000	0.587119000	2.794365000
H	-4.078965000	1.836614000	1.845554000
H	-4.807784000	0.291291000	2.273877000
C	-5.957973000	0.750221000	-0.174730000
C	-5.319134000	0.671661000	-2.494496000
H	-3.154008000	0.488586000	-2.768232000
C	-1.260159000	3.586334000	2.135535000
C	-0.696159000	4.281282000	-0.097543000
H	-0.818503000	2.655832000	-1.550056000
H	-6.707167000	0.814322000	0.608738000
C	-6.319851000	0.751217000	-1.523062000
H	-5.560816000	0.670818000	-3.552199000
H	-1.421715000	3.794274000	3.188650000
C	-0.867458000	4.594040000	1.251528000
H	-0.419852000	5.041508000	-0.818434000
H	-7.365585000	0.811594000	-1.809330000
H	-0.718927000	5.609150000	1.607866000
H	1.726044000	0.445243000	-2.070491000
H	2.163681000	2.131000000	-1.522531000
C	2.830064000	3.029284000	-2.065429000
H	3.786186000	3.031442000	-1.530800000
C	2.002947000	4.177460000	-1.972861000
H	1.997386000	4.868006000	-1.134860000
C	1.122547000	4.321167000	-3.169998000
H	1.477390000	5.186331000	-3.758624000
H	0.070437000	4.531565000	-2.934237000
C	2.776054000	2.580520000	-3.543929000
H	3.529265000	3.117584000	-4.133609000
H	2.954441000	1.506414000	-3.675666000
C	1.347531000	3.001453000	-3.950864000
H	1.222339000	3.122715000	-5.029822000
H	0.631688000	2.247353000	-3.600232000

Ib-²TS_{2Hls-ls}

Fe	1.589788000	-0.361440000	0.122912000
O	1.370300000	1.317835000	-0.783596000
Fe	-1.711195000	0.092805000	0.124701000
O	-1.155418000	0.531749000	-1.624991000
H	-0.212296000	0.749303000	-1.521172000
O	-0.154652000	-0.396005000	0.825968000
N	1.089552000	-1.547777000	-1.410732000
N	2.224382000	0.389119000	1.862650000
N	3.568304000	-0.525063000	-0.367259000
C	0.899547000	-2.833535000	-1.040941000
C	0.648020000	-3.836725000	-1.971753000
H	0.515185000	-4.861646000	-1.639787000
C	0.567468000	-3.496430000	-3.324670000
H	0.379418000	-4.260324000	-4.073357000
C	0.741686000	-2.163439000	-3.697393000
H	0.686473000	-1.856378000	-4.736409000
C	1.004340000	-1.218256000	-2.706258000
H	1.154587000	-0.170839000	-2.934146000
C	2.303890000	-0.535657000	2.844489000
C	2.831359000	-0.227487000	4.095923000
H	2.896055000	-0.995083000	4.861099000
C	3.276680000	1.074452000	4.341114000
H	3.693733000	1.338094000	5.308354000
C	3.192900000	2.023050000	3.320175000
H	3.539521000	3.040757000	3.466132000
C	2.666838000	1.633205000	2.089768000
H	2.597849000	2.306688000	1.241637000
C	4.199039000	-1.612557000	0.109548000
C	5.575251000	-1.791067000	-0.032399000
H	6.051477000	-2.680244000	0.370161000
C	6.317507000	-0.815847000	-0.696609000
H	7.389791000	-0.931471000	-0.821834000
C	5.658270000	0.312673000	-1.191465000
H	6.199321000	1.097455000	-1.709677000
C	4.285047000	0.421792000	-0.999529000
H	3.715259000	1.279774000	-1.334843000
C	0.932167000	-3.080276000	0.451268000
H	1.117119000	-4.138334000	0.681041000

C	1.736790000	-1.896996000	2.498102000
H	0.655697000	-1.850835000	2.645443000
H	2.156654000	-2.679881000	3.143872000
C	3.335570000	-2.665039000	0.768889000
H	3.270741000	-3.526732000	0.093976000
H	3.813326000	-3.024096000	1.688692000
N	1.952031000	-2.188567000	1.059900000
H	-0.032906000	-2.312002000	0.858622000
H	-3.719405000	-5.293728000	-0.727311000
C	-3.293056000	-4.302892000	-0.601278000
C	-3.223257000	-3.726509000	0.673077000
C	-2.821100000	-3.588926000	-1.703577000
C	-2.684019000	-2.450696000	0.801732000
H	-3.588850000	-4.255046000	1.548140000
H	-2.862290000	-4.006634000	-2.703865000
C	-2.297543000	-2.312002000	-1.501570000
N	-2.234570000	-1.774081000	-0.279065000
C	-2.492071000	-1.744689000	2.133558000
H	-1.909864000	-1.670477000	-2.287339000
H	-1.457865000	-1.899879000	2.452628000
H	-3.163277000	-2.159010000	2.898118000
N	-2.668382000	-0.283554000	1.965516000
N	-3.650527000	0.547767000	-0.432423000
N	-1.551812000	1.913595000	0.900107000
C	-1.888086000	0.576526000	2.892274000
C	-4.103975000	0.115533000	1.914055000
C	-4.595215000	0.373514000	0.505304000
C	-4.002046000	0.852722000	-1.693064000
C	-1.702945000	1.936455000	2.243157000
C	-1.373566000	3.048911000	0.211894000
H	-2.360075000	0.667186000	3.879909000
H	-0.900386000	0.117118000	2.984079000
H	-4.224972000	1.040565000	2.490592000
H	-4.728654000	-0.640979000	2.405417000
C	-5.952540000	0.487959000	0.208535000
C	-5.336205000	0.996612000	-2.064775000
H	-3.160850000	0.964933000	-2.370656000
C	-1.661769000	3.137664000	2.946070000
C	-1.305235000	4.285296000	0.852217000
H	-1.291178000	2.910376000	-0.861806000
H	-6.696663000	0.335404000	0.984714000
C	-6.327362000	0.805543000	-1.098044000
H	-5.591192000	1.245062000	-3.089665000
H	-1.798905000	3.141832000	4.023001000
C	-1.450796000	4.327557000	2.241143000
H	-1.158370000	5.190263000	0.271976000
H	-7.377715000	0.901074000	-1.356933000
H	-1.418849000	5.275588000	2.769848000
H	0.885556000	1.939842000	-0.219336000
H	2.240483000	5.715973000	-2.207021000
C	2.709988000	3.777091000	-3.083909000
H	3.795417000	3.799569000	-3.144044000
C	1.871643000	5.000514000	-2.954564000
H	1.902204000	5.536423000	-3.921566000
C	0.451286000	4.442106000	-2.688333000
H	-0.338987000	5.104533000	-3.053058000
H	0.318103000	4.312474000	-1.606274000
C	1.914565000	2.591404000	-3.125240000
H	2.311600000	1.753072000	-3.713206000
H	1.860433000	2.125985000	-2.022496000
C	0.460171000	3.059990000	-3.376578000
H	0.282447000	3.169356000	-4.454189000
H	-0.278404000	2.363392000	-2.967371000

Ia-²P_{Rebbs-hs}

Fe	1.631501000	0.157931000	-0.048020000
O	1.332395000	0.737280000	-2.106122000
Fe	-1.653544000	0.181133000	-0.317149000
O	-1.147038000	-0.061642000	-2.156304000
H	-1.749759000	0.191768000	-2.869843000
O	-0.127248000	0.456502000	0.534005000
N	1.271871000	-1.997062000	-0.757491000
N	2.498099000	1.629457000	1.488825000
N	3.718185000	-0.543923000	-0.567252000
C	1.414991000	-2.895173000	0.232959000

C	1.476764000	-4.265527000	-0.016074000
H	1.603768000	-4.962349000	0.807029000
C	1.373779000	-4.716123000	-1.334593000
H	1.425002000	-5.777949000	-1.557884000
C	1.216959000	-3.780501000	-2.358690000
H	1.141262000	-4.087396000	-3.396872000
C	1.182294000	-2.426010000	-2.021907000
H	1.079265000	-1.649782000	-2.771907000
C	2.454276000	1.123729000	2.739500000
C	2.898320000	1.842468000	3.848572000
H	2.863090000	1.389514000	4.834903000
C	3.390484000	3.136836000	3.667343000
H	3.743648000	3.715876000	4.515437000
C	3.431629000	3.662142000	2.376466000
H	3.812898000	4.659199000	2.182075000
C	2.979748000	2.869207000	1.321411000
H	3.004698000	3.235852000	0.303655000
C	4.290834000	-1.370868000	0.326514000
C	5.419713000	-2.129367000	0.016071000
H	5.849618000	-2.790256000	0.762889000
C	5.980457000	-2.020695000	-1.256610000
H	6.861718000	-2.597805000	-1.520466000
C	5.383162000	-1.165573000	-2.184358000
H	5.779027000	-1.054845000	-3.188423000
C	4.248394000	-0.456807000	-1.798243000
H	3.727770000	0.194391000	-2.489069000
C	1.428073000	-2.335710000	1.641962000
H	1.751544000	-3.108714000	2.356086000
C	1.869500000	-0.267061000	2.890591000
H	0.778132000	-0.182853000	2.862337000
H	2.167921000	-0.701768000	3.856816000
C	3.700674000	-1.400171000	1.722172000
H	3.923727000	-2.362756000	2.204817000
H	4.208561000	-0.626716000	2.310387000
N	2.250805000	-1.119350000	1.751051000
H	0.399594000	-2.049318000	1.885962000
H	-2.796207000	-5.305125000	2.023359000
C	-2.542252000	-4.342900000	1.588583000
C	-2.673460000	-3.172618000	2.342477000
C	-2.091228000	-4.254853000	0.270895000
C	-2.345302000	-1.953534000	1.753294000
H	-3.029009000	-3.202659000	3.367919000
H	-1.977571000	-5.138153000	-0.348189000
C	-1.791456000	-2.995493000	-0.247453000
N	-1.911247000	-1.879316000	0.481123000
C	-2.387933000	-0.641571000	2.509683000
H	-1.439915000	-2.858451000	-1.264798000
H	-1.365019000	-0.394714000	2.812922000
H	-3.003949000	-0.738109000	3.415619000
N	-2.854631000	0.459283000	1.648581000
N	-3.864365000	-0.373270000	-0.829283000
N	-2.353664000	2.284220000	-0.268424000
C	-2.387999000	1.789568000	2.099133000
C	-4.318402000	0.428735000	1.428629000
C	-4.728629000	-0.354201000	0.198640000
C	-4.215073000	-1.012550000	-1.955584000
C	-2.563185000	2.779582000	0.967804000
C	-2.509086000	3.083889000	-1.331195000
H	-2.916472000	2.131287000	3.000609000
H	-1.319295000	1.692991000	2.316258000
H	-4.663853000	1.460246000	1.293531000
H	-4.835663000	0.037022000	2.315611000
C	-5.979039000	-0.969664000	0.127546000
C	-5.449290000	-1.636857000	-2.120168000
H	-3.462407000	-1.039772000	-2.737217000
C	-2.927880000	4.107866000	1.172815000
C	-2.868361000	4.425118000	-1.212755000
H	-2.332751000	2.627543000	-2.298359000
H	-6.648216000	-0.939434000	0.982396000
C	-6.349618000	-1.614414000	-1.053023000
H	-5.690420000	-2.133508000	-3.054154000
H	-3.102720000	4.472548000	2.180332000
C	-3.074962000	4.946865000	0.064813000
H	-2.986280000	5.037532000	-2.100337000
H	-7.319082000	-2.096706000	-1.135096000

H	-3.361003000	5.985870000	0.198059000
H	-0.457752000	2.214648000	-3.227911000
H	0.376907000	0.448595000	-2.262441000
C	0.489617000	2.761527000	-3.205183000
H	0.603812000	3.287819000	-4.161391000
C	1.679519000	1.806920000	-3.012678000
H	1.995694000	1.347998000	-3.957263000
C	2.795820000	2.674330000	-2.377564000
H	3.667562000	2.762341000	-3.033973000
H	3.128470000	2.181168000	-1.457088000
C	0.638090000	3.757852000	-2.045781000
H	0.019403000	4.653894000	-2.158249000
H	0.369673000	3.267407000	-1.100548000
C	2.146363000	4.054346000	-2.091910000
H	2.354008000	4.736560000	-2.924811000
H	2.525631000	4.537554000	-1.185476000

Ia-¹⁰P_{Rebhs-hs}

Fe	-1.610002000	0.431294000	0.012104000
O	-1.185701000	0.236795000	2.026004000
Fe	1.736999000	-0.107099000	0.226404000
O	1.333999000	0.251600000	2.090604000
H	1.778700000	-0.252499000	2.786604000
O	0.207998000	0.298698000	-0.638896000
N	-2.033398000	-1.671707000	-0.667496000
N	-1.778806000	2.647794000	-0.312596000
N	-3.861201000	0.247989000	0.298504000
C	-2.355897000	-1.785708000	-1.968096000
C	-2.821595000	-2.984009000	-2.507896000
H	-3.086195000	-3.040509000	-3.559596000
C	-2.947793000	-4.096109000	-1.671496000
H	-3.314491000	-5.039410000	-2.065296000
C	-2.608593000	-3.971608000	-0.323196000
H	-2.698091000	-4.808408000	0.361304000
C	-2.162995000	-2.732907000	0.136704000
H	-1.899296000	-2.569807000	1.177404000
C	-1.768107000	2.999394000	-1.614196000
C	-1.806110000	4.330894000	-2.022796000
H	-1.815410000	4.572493000	-3.081396000
C	-1.837512000	5.335293000	-1.052596000
H	-1.867814000	6.380793000	-1.344496000
C	-1.846011000	4.970793000	0.294004000
H	-1.881513000	5.716193000	1.081504000
C	-1.822708000	3.614093000	0.616304000
H	-1.839708000	3.284693000	1.648704000
C	-4.576402000	0.312888000	-0.840396000
C	-5.896101000	-0.132915000	-0.914496000
H	-6.436701000	-0.067816000	-1.853996000
C	-6.501400000	-0.655416000	0.229004000
H	-7.529199000	-1.004318000	0.197504000
C	-5.757699000	-0.729715000	1.407604000
H	-6.181599000	-1.136415000	2.319804000
C	-4.440300000	-0.276612000	1.390504000
H	-3.816300000	-0.343211000	2.274604000
C	-2.123100000	-0.552907000	-2.820296000
H	-2.679300000	-0.630008000	-3.766296000
C	-1.690105000	1.856794000	-2.604596000
H	-0.644604000	1.537196000	-2.669496000
H	-2.034805000	2.180693000	-3.597596000
C	-3.906003000	0.954589000	-2.038596000
H	-4.401402000	0.634688000	-2.966196000
H	-4.048605000	2.037989000	-1.956496000
N	-2.450902000	0.692392000	-2.102296000
H	-1.054800000	-0.508605000	-3.059196000
H	0.538811000	-6.079702000	0.132804000
C	0.740809000	-5.014001000	0.187004000
C	1.057708000	-4.297101000	-0.969696000
C	0.702808000	-4.345501000	1.411804000
C	1.326905000	-2.934100000	-0.862696000
H	1.106609000	-4.786201000	-1.937696000
H	0.470209000	-4.867502000	2.334204000
C	0.986005000	-2.980101000	1.429904000
N	1.295204000	-2.296400000	0.321704000
C	1.658303000	-2.061699000	-2.055196000
H	0.965204000	-2.401801000	2.348804000

H	0.754902000	-1.507401000	-2.328396000
H	1.982004000	-2.674299000	-2.909396000
N	2.669601000	-1.055597000	-1.670196000
N	3.930100000	-0.592795000	0.787304000
N	2.888796000	1.552103000	-0.688596000
C	2.744699000	0.081003000	-2.608996000
C	3.988702000	-1.668495000	-1.399896000
C	4.701001000	-1.065893000	-0.205596000
C	4.521499000	-0.097994000	1.885504000
C	3.317596000	1.315504000	-1.942396000
C	3.298694000	2.652204000	-0.044896000
H	3.320999000	-0.174596000	-3.510296000
H	1.715498000	0.312501000	-2.904096000
H	4.632002000	-1.616993000	-2.289696000
H	3.830605000	-2.732295000	-1.186096000
C	6.094001000	-1.067890000	-0.125796000
C	5.903799000	-0.076891000	2.056404000
H	3.853198000	0.314505000	2.635604000
C	4.186795000	2.186906000	-2.594996000
C	4.156192000	3.582406000	-0.632096000
H	2.927293000	2.773103000	0.969104000
H	6.684702000	-1.452689000	-0.951996000
C	6.705800000	-0.572589000	1.026404000
H	6.335998000	0.326810000	2.966004000
H	4.524795000	1.964106000	-3.602496000
C	4.610192000	3.340907000	-1.929696000
H	4.465090000	4.464106000	-0.080496000
H	7.788100000	-0.566087000	1.114504000
H	5.288691000	4.035708000	-2.415796000
H	-2.463299000	-0.853308000	4.027004000
H	-0.154401000	0.202097000	2.135504000
C	-1.998301000	0.097093000	4.314104000
H	-2.660702000	0.605992000	5.026904000
C	-1.757503000	1.013594000	3.110704000
H	-2.672404000	1.460692000	2.711504000
C	-0.750405000	2.060096000	3.633504000
H	-1.295507000	2.941895000	3.989404000
H	-0.076806000	2.375297000	2.831604000
C	-0.589701000	-0.053104000	4.914304000
H	-0.598900000	-0.435704000	5.939004000
H	-0.011999000	-0.756703000	4.299804000
C	0.011696000	1.370097000	4.804504000
H	-0.149605000	1.920197000	5.737004000
H	1.088796000	1.344599000	4.616904000

Ia-⁸P_{Rebhs-is}

Fe	1.647935000	-0.377324000	-0.073195000
O	1.216668000	-0.908540000	1.954194000
Fe	-1.650326000	0.377460000	0.370660000
O	-0.938620000	0.387782000	2.184832000
H	-1.483578000	0.232603000	2.967239000
O	0.088055000	-0.151697000	-0.613241000
N	1.963419000	1.646712000	0.472560000
N	1.826835000	-2.157546000	-1.273323000
N	3.723577000	-0.491209000	0.448538000
C	2.407033000	2.416578000	-0.538624000
C	2.873080000	3.710406000	-0.317159000
H	3.232763000	4.306366000	-1.150404000
C	2.878358000	4.213094000	0.986701000
H	3.249467000	5.214194000	1.185692000
C	2.407850000	3.409712000	2.025554000
H	2.396448000	3.762023000	3.051786000
C	1.957010000	2.125159000	1.723920000
H	1.576289000	1.449514000	2.480980000
C	1.955470000	-1.878970000	-2.588705000
C	2.019898000	-2.886050000	-3.549571000
H	2.143710000	-2.624725000	-4.596271000
C	1.925195000	-4.219669000	-3.145963000
H	1.974883000	-5.020676000	-3.877414000
C	1.773343000	-4.501873000	-1.788487000
H	1.696367000	-5.521853000	-1.426945000
C	1.731659000	-3.438555000	-0.887947000
H	1.610380000	-3.608782000	0.174272000
C	4.614843000	-0.113064000	-0.489454000
C	5.974115000	0.020058000	-0.205788000

H	6.657854000	0.334023000	-0.988753000	O	1.323794000	-1.044560000	1.907445000
C	6.431700000	-0.254387000	1.081679000	Fe	-1.533580000	0.238120000	0.186021000
H	7.486328000	-0.162034000	1.323060000	O	-1.038825000	-0.019313000	2.025256000
C	5.505466000	-0.634426000	2.054711000	H	-1.637023000	-0.391691000	2.686096000
H	5.809203000	-0.842849000	3.075045000	O	-0.037908000	-0.040857000	-0.722315000
C	4.164085000	-0.727811000	1.699871000	N	1.833283000	1.592746000	0.578719000
H	3.400580000	-0.969055000	2.425956000	N	1.866362000	-1.926554000	-1.304326000
C	2.316763000	1.820513000	-1.933915000	N	3.837254000	-0.314390000	0.308083000
H	2.949860000	2.389955000	-2.629807000	C	2.143376000	2.509683000	-0.366505000
C	1.979232000	-0.411826000	-2.983463000	C	2.431289000	3.831082000	-0.033468000
H	0.945272000	-0.060327000	-3.042906000	H	2.689834000	4.537988000	-0.815862000
H	2.450322000	-0.293538000	-3.970267000	C	2.394402000	4.221253000	1.307148000
C	4.101526000	0.116323000	-1.893241000	H	2.628626000	5.243706000	1.588403000
H	4.666727000	0.928821000	-2.370823000	C	2.066171000	3.272105000	2.274707000
H	4.305072000	-0.790301000	-2.476241000	H	2.032861000	3.526674000	3.329004000
N	2.650447000	0.385369000	-1.943988000	C	1.795829000	1.966652000	1.867886000
H	1.278000000	1.918004000	-2.262331000	H	1.552209000	1.180314000	2.571619000
H	-0.482461000	6.168228000	-1.111212000	C	1.984469000	-1.623972000	-2.621094000
C	-0.677759000	5.138744000	-0.825485000	C	2.111089000	-2.614340000	-3.591925000
C	-1.022903000	4.191530000	-1.793680000	H	2.223237000	-2.331513000	-4.634238000
C	-0.605326000	4.745679000	0.511776000	C	2.097188000	-3.957129000	-3.207933000
C	-1.277228000	2.882127000	-1.388219000	H	2.198106000	-4.743651000	-3.949660000
H	-1.105601000	4.464073000	-2.841840000	C	1.962595000	-4.264172000	-1.854653000
H	-0.347477000	5.452151000	1.293593000	H	1.950466000	-5.291167000	-1.505178000
C	-0.884984000	3.416681000	0.831340000	C	1.853928000	-3.218565000	-0.939284000
N	-1.210223000	2.510782000	-0.098496000	H	1.749847000	-3.409011000	0.120526000
C	-1.608686000	1.775240000	-2.367920000	C	4.651337000	0.223721000	-0.617906000
H	-0.845036000	3.037537000	1.847742000	C	6.005365000	0.452681000	-0.370882000
H	-0.687388000	1.233828000	-2.599253000	H	6.626210000	0.896412000	-1.143788000
H	-2.011883000	2.191491000	-3.303455000	C	6.538728000	0.104590000	0.868875000
N	-2.524021000	0.797456000	-1.754521000	H	7.590413000	0.269728000	1.082608000
N	-3.806272000	0.846333000	0.764716000	C	5.691213000	-0.447901000	1.831513000
N	-2.701631000	-1.582618000	-0.283384000	H	6.056423000	-0.723687000	2.815197000
C	-2.482329000	-0.507970000	-2.438933000	C	4.348888000	-0.628710000	1.513140000
C	-3.895200000	1.340503000	-1.628303000	H	3.642047000	-1.013055000	2.236976000
C	-4.584788000	0.997548000	-0.321001000	C	2.109268000	2.044529000	-1.813048000
C	-4.390599000	0.646197000	1.955945000	H	2.670989000	2.748029000	-2.445496000
C	-3.087537000	-1.587993000	-1.574229000	C	1.928564000	-0.152658000	-2.994812000
C	-3.197229000	-2.523149000	0.532501000	H	0.876675000	0.144198000	-3.009740000
H	-2.984913000	-0.469136000	-3.417436000	H	2.357787000	0.001070000	-3.995900000
H	-1.424458000	-0.750474000	-2.587659000	C	4.057763000	0.527622000	-1.981150000
H	-4.517973000	1.024356000	-2.477285000	H	4.529834000	1.427525000	-2.400388000
H	-3.827146000	2.434148000	-1.676163000	H	4.317421000	-0.302175000	-2.650332000
C	-5.976620000	0.932846000	-0.246604000	N	2.592540000	0.662438000	-1.963594000
C	-5.771629000	0.587227000	2.123737000	H	1.063368000	2.061306000	-2.131864000
H	-3.715722000	0.526915000	2.798961000	H	-1.162137000	6.211225000	-0.749381000
C	-3.968812000	-2.538178000	-2.086531000	C	-1.224991000	5.145158000	-0.551919000
C	-4.075026000	-3.518368000	0.102466000	C	-1.496520000	4.251226000	-1.592312000
H	-2.878274000	-2.474865000	1.566634000	C	-1.053107000	4.651318000	0.741936000
H	-6.573061000	1.049281000	-1.146656000	C	-1.580113000	2.890857000	-1.303309000
C	-6.580710000	0.726299000	0.993957000	H	-1.652478000	4.602619000	-2.607901000
H	-6.196999000	0.430155000	3.109385000	H	-0.849243000	5.313740000	1.576271000
H	-4.258635000	-2.498054000	-3.132145000	C	-1.161466000	3.276415000	0.949552000
C	-4.468545000	-3.526274000	-1.235356000	N	-1.414177000	2.425326000	-0.051239000
H	-4.443440000	-4.258311000	0.805399000	C	-1.841319000	1.837431000	-2.361507000
H	-7.662192000	0.675196000	1.077126000	H	-1.041575000	2.822877000	1.928119000
H	-5.157700000	-4.278352000	-1.607827000	H	-0.887070000	1.387690000	-2.650338000
H	2.126392000	-1.570013000	4.334818000	H	-2.302204000	2.288856000	-3.252222000
H	0.317413000	-0.429308000	2.150681000	N	-2.663814000	0.752064000	-1.796116000
C	1.349455000	-2.259892000	3.986500000	N	-3.753611000	0.706200000	0.799198000
H	1.619847000	-3.272963000	4.311558000	N	-2.592172000	-1.633857000	-0.408611000
C	1.205086000	-2.255129000	2.460903000	C	-2.559204000	-0.511812000	-2.548813000
H	2.041512000	-2.762044000	1.969854000	C	-4.064577000	1.174491000	-1.578687000
C	-0.153434000	-2.930477000	2.214375000	C	-4.623511000	0.807904000	-0.218112000
H	-0.014608000	-4.015930000	2.145460000	C	-4.234010000	0.519274000	2.037933000
H	-0.583190000	-2.583902000	1.269399000	C	-3.009392000	-1.670854000	-1.688766000
C	-0.061683000	-1.897778000	4.481467000	C	-2.920552000	-2.635986000	0.416612000
H	-0.243294000	-2.219684000	5.510592000	H	-3.131274000	-0.478635000	-3.487685000
H	-0.186320000	-0.809346000	4.448485000	H	-1.498135000	-0.657122000	-2.778683000
C	-1.020130000	-2.578337000	3.463375000	H	-4.714595000	0.780337000	-2.371780000
H	-1.467760000	-3.482260000	3.887872000	H	-4.106414000	2.268083000	-1.656616000
H	-1.837260000	-1.898634000	3.203233000	C	-6.001745000	0.686319000	-0.032947000
				C	-5.593458000	0.406084000	2.318435000
				H	-3.494330000	0.473982000	2.830992000
				C	-3.774076000	-2.725543000	-2.181776000

Ia-⁴P_{Rebhs-is}
Fe 1.742729000 -0.294948000 -0.119751000

C	-3.672466000	-3.733851000	0.000759000
H	-2.563989000	-2.547582000	1.436418000
H	-6.672540000	0.763492000	-0.883654000
C	-6.495691000	0.478699000	1.254921000
H	-5.931363000	0.262229000	3.339360000
H	-4.102562000	-2.718963000	-3.216549000
C	-4.107943000	-3.777261000	-1.324290000
H	-3.914597000	-4.525144000	0.702367000
H	-7.563731000	0.382393000	1.425822000
H	-4.704664000	-4.610250000	-1.683783000
H	2.259572000	-1.469546000	4.316479000
H	0.384634000	-0.682465000	2.048319000
C	1.560502000	-2.255970000	4.011227000
H	1.924620000	-3.214101000	4.404889000
C	1.433869000	-2.355504000	2.486268000
H	2.316291000	-2.811449000	2.026711000
C	0.144243000	-3.175695000	2.269678000
H	0.390694000	-4.238882000	2.170020000
H	-0.346918000	-2.860791000	1.343787000
C	0.112046000	-2.012163000	4.466209000
H	-0.044656000	-2.222411000	5.527991000
H	-0.150138000	-0.961944000	4.290296000
C	-0.723410000	-2.939170000	3.545419000
H	-0.922111000	-3.891898000	4.046159000
H	-1.699832000	-2.496832000	3.313003000

Ia-⁶P_{Rebis-is}

Fe	1.649534000	-0.413230000	0.073539000
O	1.217442000	-0.096390000	2.054044000
Fe	-1.622234000	0.366879000	0.197766000
O	-1.303037000	-0.020771000	2.062631000
H	-1.445185000	0.793182000	2.575232000
O	-0.116273000	0.019311000	-0.474416000
N	2.301073000	1.296616000	-0.988673000
N	0.989183000	-2.492924000	0.230644000
N	3.639342000	-0.750770000	0.271924000
C	2.557732000	1.114830000	-2.295594000
C	3.118203000	2.127382000	-3.075404000
H	3.330305000	1.947841000	-4.125410000
C	3.399677000	3.360873000	-2.485460000
H	3.841144000	4.161045000	-3.072108000
C	3.110564000	3.546569000	-1.131602000
H	3.311366000	4.489472000	-0.634217000
C	2.567149000	2.480970000	-0.418445000
H	2.330009000	2.559987000	0.638793000
C	0.708094000	-3.088592000	-0.941332000
C	0.160943000	-4.368618000	-1.007799000
H	-0.034923000	-4.825760000	-1.973192000
C	-0.121577000	-5.042772000	0.181836000
H	-0.542971000	-6.043470000	0.159083000
C	0.161508000	-4.416854000	1.396890000
H	-0.032306000	-4.908273000	2.344763000
C	0.721065000	-3.139661000	1.372663000
H	0.962504000	-2.603937000	2.283261000
C	4.261802000	-1.366848000	-0.758973000
C	5.650939000	-1.451710000	-0.836574000
H	6.110100000	-1.950734000	-1.684525000
C	6.429819000	-0.892673000	0.176391000
H	7.513108000	-0.952496000	0.136188000
C	5.787328000	-0.241861000	1.230399000
H	6.347130000	0.225455000	2.033611000
C	4.397144000	-0.185849000	1.231533000
H	3.857136000	0.338664000	2.007811000
C	2.118737000	-0.203856000	-2.916513000
H	2.749838000	-0.432257000	-3.788263000
C	0.974355000	-2.266941000	-2.187067000
H	0.081665000	-1.664068000	-2.371547000
H	1.148412000	-2.924212000	-3.052502000
C	3.383416000	-2.009788000	-1.809695000
H	3.919799000	-2.067400000	-2.767857000
H	3.183748000	-3.039736000	-1.492056000
N	2.084462000	-1.324121000	-1.964159000
H	1.098580000	-0.057697000	-3.290999000
H	0.153806000	6.141179000	-0.890293000
C	-0.211538000	5.154353000	-0.621540000

C	-0.588557000	4.246938000	-1.613486000
C	-0.327982000	4.779262000	0.718237000
C	-1.058463000	2.989501000	-1.233684000
H	-0.522945000	4.507780000	-2.665693000
H	-0.058043000	5.456798000	1.521751000
C	-0.824594000	3.508162000	1.006835000
N	-1.179576000	2.633505000	0.057875000
C	-1.401420000	1.935398000	-2.271879000
H	-0.944536000	3.174969000	2.034094000
H	-0.494871000	1.353172000	-2.460668000
H	-1.729546000	2.410765000	-3.207633000
N	-2.413570000	0.982716000	-1.761799000
N	-3.660989000	0.735484000	0.664976000
N	-2.540089000	-1.551189000	-0.530415000
C	-2.505973000	-0.243379000	-2.585666000
C	-3.731728000	1.644315000	-1.581570000
C	-4.445739000	1.165357000	-0.342262000
C	-4.229127000	0.338023000	1.817302000
C	-2.970936000	-1.459349000	-1.798990000
C	-2.840623000	-2.631220000	0.196908000
H	-3.153106000	-0.085307000	-3.459830000
H	-1.496978000	-0.450381000	-2.956256000
H	-4.360991000	1.508645000	-2.471313000
H	-3.558433000	2.720819000	-1.471700000
C	-5.832738000	1.220086000	-0.222020000
C	-5.605466000	0.380070000	2.020467000
H	-3.537237000	-0.037794000	2.563368000
C	-3.736740000	-2.464778000	-2.388077000
C	-3.589519000	-3.690267000	-0.318352000
H	-2.462788000	-2.629159000	1.215230000
H	-6.435296000	1.565078000	-1.056664000
C	-6.422640000	0.828447000	0.980707000
H	-6.023076000	0.056544000	2.967980000
H	-4.082702000	-2.361113000	-3.412421000
C	-4.049005000	-3.599669000	-1.633386000
H	-3.814903000	-4.553513000	0.299314000
H	-7.501319000	0.864687000	1.100059000
H	-4.647905000	-4.395845000	-2.065723000
H	2.683443000	1.762280000	3.177059000
H	0.187217000	-0.090209000	2.101300000
C	2.155833000	1.144008000	3.914084000
H	2.796598000	1.034752000	4.798926000
C	1.795373000	-0.243545000	3.366367000
H	2.652327000	-0.916760000	3.267717000
C	0.748547000	-0.767780000	4.373604000
H	1.256816000	-1.347481000	5.151107000
H	0.024964000	-1.423494000	3.880422000
C	0.781225000	1.705606000	4.315844000
H	0.843524000	2.580035000	4.970256000
H	0.250972000	2.002542000	3.401272000
C	0.071640000	0.498852000	4.979288000
H	0.219866000	0.525835000	6.063304000
H	-1.008416000	0.504345000	4.800466000

Ia-²P_{Rebis-is}

Fe	1.649502000	-0.413207000	0.073506000
O	1.217403000	-0.096406000	2.054006000
Fe	-1.622196000	0.366900000	0.197806000
O	-1.302997000	-0.020801000	2.062606000
H	-1.445195000	0.793200000	2.575206000
O	-0.116297000	0.019297000	-0.474394000
N	2.301106000	1.296592000	-0.988694000
N	0.989198000	-2.492905000	0.230606000
N	3.639301000	-0.750811000	0.271906000
C	2.557705000	1.114791000	-2.295594000
C	3.118208000	2.127390000	-3.075394000
H	3.330307000	1.947790000	-4.125394000
C	3.399710000	3.360889000	-2.485494000
H	3.841112000	4.160989000	-3.072094000
C	3.110611000	3.546590000	-1.131594000
H	3.311413000	4.489490000	-0.634194000
C	2.567108000	2.480991000	-0.418394000
H	2.330009000	2.559992000	0.638806000
C	0.708096000	-3.088605000	-0.941294000
C	0.160894000	-4.368604000	-1.007794000

H	-0.034907000	-4.825803000	-1.973194000
C	-0.121608000	-5.042803000	0.181806000
H	-0.543010000	-6.043502000	0.159106000
C	0.161494000	-4.416904000	1.396906000
H	-0.032307000	-4.908303000	2.344806000
C	0.721096000	-3.139705000	1.372706000
H	0.962497000	-2.603905000	2.283306000
C	4.261800000	-1.366812000	-0.758994000
C	5.650900000	-1.451715000	-0.836594000
H	6.110099000	-1.950716000	-1.684494000
C	6.429801000	-0.892717000	0.176406000
H	7.513101000	-0.952519000	0.136206000
C	5.787303000	-0.241916000	1.230406000
H	6.347104000	0.225483000	2.033606000
C	4.397103000	-0.185813000	1.231506000
H	3.857104000	0.338688000	2.007806000
C	2.118703000	-0.203908000	-2.916494000
H	2.749802000	-0.432309000	-3.788294000
C	0.974398000	-2.266905000	-2.187094000
H	0.081700000	-1.664103000	-2.371494000
H	1.148397000	-2.924206000	-3.052494000
C	3.383399000	-2.009811000	-1.809694000
H	3.919799000	-2.067412000	-2.767894000
H	3.183697000	-3.039710000	-1.492094000
N	2.084500000	-1.324108000	-1.964194000
H	1.098603000	-0.057706000	-3.290994000
H	0.153816000	6.141196000	-0.890294000
C	-0.211486000	5.154397000	-0.621494000
C	-0.588588000	4.246898000	-1.613494000
C	-0.327987000	4.779297000	0.718206000
C	-1.058491000	2.989499000	-1.233694000
H	-0.522887000	4.507798000	-2.665694000
H	-0.057985000	5.456797000	1.521806000
C	-0.824589000	3.508198000	1.006806000
N	-1.179591000	2.633499000	0.057906000
C	-1.401393000	1.935400000	-2.271894000
H	-0.944490000	3.174999000	2.034106000
H	-0.494894000	1.353198000	-2.460694000
H	-1.729492000	2.410800000	-3.207594000
N	-2.413595000	0.982702000	-1.761794000
N	-3.660995000	0.735505000	0.665006000
N	-2.540100000	-1.551198000	-0.530394000
C	-2.505997000	-0.243398000	-2.585694000
C	-3.731693000	1.644305000	-1.581594000
C	-4.445694000	1.165406000	-0.342294000
C	-4.229096000	0.338006000	1.817306000
C	-2.970900000	-1.459297000	-1.798994000
C	-2.840603000	-2.631197000	0.196906000
H	-3.153097000	-0.085297000	-3.459794000
H	-1.496998000	-0.450400000	-2.956294000
H	-4.360994000	1.508606000	-2.471294000
H	-3.558391000	2.720804000	-1.471694000
C	-5.832694000	1.220109000	-0.221994000
C	-5.605496000	0.380109000	2.020506000
H	-3.537197000	-0.037796000	2.563406000
C	-3.736702000	-2.464795000	-2.388094000
C	-3.589505000	-3.690296000	-0.318394000
H	-2.462803000	-2.629198000	1.215206000
H	-6.435294000	1.565110000	-1.056694000
C	-6.422595000	0.828410000	0.980706000
H	-6.023097000	0.056510000	2.968006000
H	-4.082702000	-2.361095000	-3.412394000
C	-4.049005000	-3.599695000	-1.633394000
H	-3.814907000	-4.553495000	0.299306000
H	-7.501295000	0.864713000	1.100106000
H	-4.647906000	-4.395793000	-2.065694000
H	2.683407000	1.762291000	3.177106000
H	0.187203000	-0.090204000	2.101306000
C	2.155806000	1.143992000	3.914106000
H	2.796605000	1.034791000	4.798906000
C	1.795403000	-0.243507000	3.366406000
H	2.652301000	-0.916809000	3.267706000
C	0.748501000	-0.767805000	4.373606000
H	1.256800000	-1.347506000	5.151106000
H	0.025000000	-1.423503000	3.880406000

C	0.781207000	1.705595000	4.315806000
H	0.843509000	2.579995000	4.970306000
H	0.251007000	2.002496000	3.401306000
C	0.071604000	0.498897000	4.979306000
H	0.219904000	0.525796000	6.063306000
H	-1.008396000	0.504299000	4.800506000

Ia-⁴P_{Rebls-is}

Fe	1.659496000	-0.550472000	0.025606000
O	1.360146000	0.595631000	1.696293000
Fe	-1.596457000	0.303219000	0.151416000
O	-1.115340000	0.034402000	2.011559000
H	-1.380353000	0.830291000	2.503386000
O	-0.128294000	-0.089199000	-0.564031000
N	2.244828000	0.933514000	-1.146834000
N	0.937631000	-2.242022000	0.826072000
N	3.670336000	-0.972158000	0.206396000
C	2.304625000	0.584069000	-2.448599000
C	2.742107000	1.477154000	-3.424267000
H	2.798201000	1.164291000	-4.462660000
C	3.100389000	2.772511000	-3.041541000
H	3.450041000	3.485019000	-3.782652000
C	3.000437000	3.134775000	-1.697011000
H	3.256115000	4.134226000	-1.361699000
C	2.571955000	2.179817000	-0.777383000
H	2.463430000	2.388284000	0.280646000
C	0.520037000	-3.120329000	-0.116060000
C	-0.031454000	-4.353240000	0.215934000
H	-0.335025000	-5.038355000	-0.569504000
C	-0.185635000	-4.684812000	1.564516000
H	-0.606844000	-5.643888000	1.850890000
C	0.218275000	-3.766457000	2.533044000
H	0.116931000	-3.979442000	3.591906000
C	0.777793000	-2.557891000	2.119820000
H	1.108670000	-1.815705000	2.833160000
C	4.133294000	-1.772044000	-0.780608000
C	5.490812000	-1.969846000	-1.018702000
H	5.805631000	-2.618200000	-1.830726000
C	6.423773000	-1.329345000	-0.203093000
H	7.488287000	-1.468814000	-0.364189000
C	5.954013000	-0.498699000	0.813323000
H	6.634300000	0.032999000	1.470164000
C	4.579404000	-0.342564000	0.973460000
H	4.189908000	0.318394000	1.730581000
C	1.753525000	-0.786401000	-2.794928000
H	2.257887000	-1.206647000	-3.674725000
C	0.648521000	-2.644103000	-1.545454000
H	-0.245947000	-2.065090000	-1.780113000
H	0.743716000	-3.485670000	-2.244828000
C	3.081424000	-2.492470000	-1.578164000
H	3.438891000	-2.735010000	-2.586796000
H	2.865733000	-3.440822000	-1.072756000
N	1.810896000	-1.717024000	-1.636584000
H	0.696013000	-0.655464000	-3.044025000
H	0.217285000	5.962786000	-1.299386000
C	-0.158488000	4.998978000	-0.968541000
C	-0.618078000	4.063848000	-1.897972000
C	-0.203394000	4.681260000	0.390317000
C	-1.097876000	2.837369000	-1.437768000
H	-0.605317000	4.278420000	-2.962522000
H	0.136969000	5.380030000	1.147522000
C	-0.716945000	3.438910000	0.761420000
N	-1.155193000	2.540815000	-0.127773000
C	-1.517074000	1.745555000	-2.407015000
H	-0.777820000	3.147181000	1.805406000
H	-0.627653000	1.151383000	-2.634961000
H	-1.903907000	2.184927000	-3.337974000
N	-2.497781000	0.823069000	-1.791929000
N	-3.604565000	0.715013000	0.720071000
N	-2.597354000	-1.642875000	-0.422191000
C	-2.631811000	-0.448302000	-2.535685000
C	-3.804011000	1.494874000	-1.572172000
C	-4.441766000	1.104835000	-0.260420000
C	-4.109272000	0.387499000	1.922913000
C	-3.125356000	-1.586048000	-1.657136000

C	-2.927865000	-2.647382000	0.394807000
H	-3.281794000	-0.331047000	-3.414384000
H	-1.628647000	-0.709676000	-2.890537000
H	-4.488801000	1.297094000	-2.407916000
H	-3.629612000	2.576644000	-1.550667000
C	-5.817892000	1.195701000	-0.058670000
C	-5.468966000	0.468609000	2.207447000
H	-3.383913000	0.032157000	2.646851000
C	-4.017742000	-2.551399000	-2.119598000
C	-3.806348000	-3.662030000	0.009545000
H	-2.468766000	-2.619767000	1.379010000
H	-6.464642000	1.507723000	-0.873026000
C	-6.339898000	0.881626000	1.196690000
H	-5.833302000	0.202437000	3.193969000
H	-4.435225000	-2.477671000	-3.119453000
C	-4.362508000	-3.607713000	-1.269671000
H	-4.054021000	-4.463609000	0.697886000
H	-7.408253000	0.948354000	1.379047000
H	-5.059859000	-4.371207000	-1.601699000
H	3.389809000	2.178878000	2.227874000
H	0.368030000	0.373378000	1.848849000
C	2.823414000	1.902850000	3.124016000
H	3.535564000	1.794877000	3.951828000
C	2.052768000	0.585933000	2.964646000
H	2.691171000	-0.304069000	3.006499000
C	1.068565000	0.643704000	4.143135000
H	1.620689000	0.375727000	5.051245000
H	0.236134000	-0.056276000	4.029775000
C	1.730391000	2.936565000	3.478475000
H	2.126116000	3.750389000	4.092620000
H	1.335703000	3.380294000	2.558481000
C	0.619845000	2.126075000	4.210999000
H	0.487802000	2.452613000	5.246361000
H	-0.349956000	2.262537000	3.715219000

Ia-²P_{Rebls-is}

Fe	-1.433202000	0.369722000	-0.005482000
O	-0.941514000	0.113389000	2.086805000
Fe	1.886267000	-0.242264000	0.050755000
O	1.621810000	0.337971000	1.835423000
H	1.932325000	-0.348605000	2.446821000
O	0.314458000	0.207171000	-0.626365000
N	-2.053332000	-1.739554000	-0.739633000
N	-1.609813000	2.628236000	-0.187289000
N	-3.653386000	0.229479000	0.471215000
C	-2.502630000	-1.734371000	-2.008096000
C	-3.146106000	-2.838359000	-2.566922000
H	-3.504550000	-2.799045000	-3.591335000
C	-3.332842000	-3.979792000	-1.781992000
H	-3.839287000	-4.849436000	-2.190482000
C	-2.874545000	-3.976175000	-0.464154000
H	-3.011431000	-4.836232000	0.183429000
C	-2.243922000	-2.826555000	0.013957000
H	-1.876774000	-2.760381000	1.033651000
C	-1.672419000	3.016486000	-1.477245000
C	-1.705575000	4.360114000	-1.847347000
H	-1.775094000	4.631578000	-2.896541000
C	-1.659028000	5.337899000	-0.851115000
H	-1.685740000	6.391515000	-1.113073000
C	-1.598491000	4.936162000	0.483299000
H	-1.576448000	5.659828000	1.291509000
C	-1.582139000	3.570086000	0.766190000
H	-1.548474000	3.212677000	1.788523000
C	-4.472644000	0.390622000	-0.583476000
C	-5.815798000	0.015676000	-0.540992000
H	-6.444665000	0.155845000	-1.415175000
C	-6.328986000	-0.536061000	0.633276000
H	-7.372423000	-0.831190000	0.692005000
C	-5.474794000	-0.713256000	1.723165000
H	-5.826285000	-1.149363000	2.652441000
C	-4.143266000	-0.325945000	1.590992000
H	-3.431849000	-0.473704000	2.395607000
C	-2.241830000	-0.471314000	-2.812425000
H	-2.855281000	-0.476003000	-3.726936000
C	-1.690930000	1.909260000	-2.514110000

H	-0.661476000	1.559821000	-2.655547000
H	-2.075151000	2.291917000	-3.472144000
C	-3.890193000	1.052353000	-1.817911000
H	-4.479496000	0.776131000	-2.704482000
H	-3.994019000	2.136213000	-1.692822000
N	-2.458236000	0.749520000	-2.020477000
H	-1.190357000	-0.467257000	-3.122313000
H	0.301649000	-5.892722000	0.282753000
C	0.556950000	-4.837425000	0.293002000
C	0.825425000	-4.164020000	-0.901413000
C	0.625198000	-4.133632000	1.495363000
C	1.161865000	-2.814883000	-0.853735000
H	0.775333000	-4.675223000	-1.857603000
H	0.418604000	-4.614253000	2.445811000
C	0.977768000	-2.785255000	1.461181000
N	1.256774000	-2.145325000	0.318254000
C	1.402649000	-1.980901000	-2.091977000
H	1.027867000	-2.193122000	2.367768000
H	0.486878000	-1.422298000	-2.290707000
H	1.666964000	-2.604593000	-2.955642000
N	2.458668000	-0.972679000	-1.794356000
N	3.894848000	-0.691360000	0.489685000
N	2.613763000	1.464965000	-0.612026000
C	2.431337000	0.222039000	-2.683163000
C	3.800899000	-1.627897000	-1.736459000
C	4.606219000	-1.172362000	-0.547023000
C	4.550421000	-0.289085000	1.592940000
C	2.883422000	1.458548000	-1.933072000
C	2.887497000	2.544077000	0.131734000
H	3.027676000	0.060570000	-3.589910000
H	1.387044000	0.375632000	-2.967264000
H	4.348670000	-1.459398000	-2.671219000
H	3.643876000	-2.709356000	-1.649094000
C	5.994013000	-1.290115000	-0.506837000
C	5.932786000	-0.389911000	1.720135000
H	3.937295000	0.155072000	2.368441000
C	3.465587000	2.558069000	-2.556839000
C	3.452952000	3.689427000	-0.427211000
H	2.639214000	2.446823000	1.183513000
H	6.530797000	-1.677879000	-1.367330000
C	6.669754000	-0.902000000	0.650398000
H	6.416868000	-0.058640000	2.632678000
H	3.688660000	2.527529000	-3.618956000
C	3.751888000	3.692317000	-1.790920000
H	3.662980000	4.551350000	0.197170000
H	7.750606000	-0.985382000	0.710309000
H	4.207311000	4.562566000	-2.253901000
H	-2.044851000	-0.949199000	4.195270000
H	0.069208000	0.200627000	2.018749000
C	-1.532892000	-0.009431000	4.432974000
H	-2.103586000	0.509457000	5.214481000
C	-1.396572000	0.903410000	3.209063000
H	-2.341498000	1.364666000	2.904923000
C	-0.342452000	1.940085000	3.651311000
H	-0.853805000	2.795185000	4.108683000
H	0.232154000	2.303988000	2.795210000
C	-0.070994000	-0.194148000	4.877427000
H	0.024589000	-0.577178000	5.897547000
H	0.415480000	-0.915400000	4.205227000
C	0.555162000	1.212927000	4.696172000
H	0.549302000	1.755123000	5.646906000
H	1.591989000	1.156664000	4.352553000

Ia-²P_{Rebls-ls}

Fe	-1.658836000	0.269957000	-0.031501000
O	-1.107759000	-0.892586000	1.586836000
Fe	1.700458000	-0.116500000	-0.015909000
O	1.183531000	0.110992000	1.837488000
H	0.878941000	1.023806000	1.950516000
O	0.121067000	0.228358000	-0.715303000
N	-2.062134000	-1.323398000	-1.140788000
N	-1.240115000	2.123687000	0.676479000
N	-3.737056000	0.423027000	0.290842000
C	-2.245946000	-1.027111000	-2.445914000
C	-2.609216000	-1.998955000	-3.375329000

H	-2.764627000	-1.724558000	-4.414462000
C	-2.766296000	-3.319496000	-2.946947000
H	-3.055263000	-4.094156000	-3.650821000
C	-2.548443000	-3.622920000	-1.601856000
H	-2.653513000	-4.636017000	-1.228210000
C	-2.201859000	-2.592878000	-0.729699000
H	-2.011117000	-2.760663000	0.322962000
C	-1.047182000	3.022679000	-0.317768000
C	-0.720246000	4.351760000	-0.061028000
H	-0.593703000	5.043564000	-0.888182000
C	-0.561454000	4.772015000	1.261036000
H	-0.310742000	5.804416000	1.485599000
C	-0.748665000	3.842934000	2.284916000
H	-0.646581000	4.120697000	3.328816000
C	-1.094470000	2.535353000	1.946546000
H	-1.259245000	1.781830000	2.703326000
C	-4.373919000	1.030162000	-0.735726000
C	-5.757275000	1.003441000	-0.895296000
H	-6.209323000	1.499141000	-1.749111000
C	-6.539104000	0.351405000	0.057714000
H	-7.619699000	0.316159000	-0.040995000
C	-5.895525000	-0.242934000	1.141735000
H	-6.451788000	-0.749704000	1.923228000
C	-4.505348000	-0.186810000	1.212219000
H	-3.987747000	-0.639922000	2.040224000
C	-1.921052000	0.395599000	-2.851096000
H	-2.496928000	0.696881000	-3.736137000
C	-1.160952000	2.480847000	-1.724332000
H	-0.185936000	2.080446000	-2.000222000
H	-1.460303000	3.264858000	-2.433184000
C	-3.510778000	1.852806000	-1.651229000
H	-3.951277000	1.933083000	-2.652943000
H	-3.471802000	2.867220000	-1.236530000
N	-2.116371000	1.342131000	-1.723505000
H	-0.859667000	0.425809000	-3.109832000
H	1.081090000	-5.896364000	-0.489804000
C	1.175999000	-4.822513000	-0.359286000
C	1.296185000	-3.984836000	-1.472763000
C	1.212033000	-4.263789000	0.919187000
C	1.423048000	-2.614800000	-1.269838000
H	1.303735000	-4.386981000	-2.480969000
H	1.147235000	-4.882733000	1.807866000
C	1.348364000	-2.881819000	1.042291000
N	1.428622000	-2.083520000	-0.026850000
C	1.567293000	-1.605606000	-2.386739000
H	1.401223000	-2.376533000	1.998255000
H	0.589662000	-1.153121000	-2.567207000
H	1.944276000	-2.072650000	-3.306118000
N	2.459095000	-0.511839000	-1.907519000
N	3.658346000	-0.462687000	0.541427000
N	2.315001000	1.750288000	-0.417387000
C	2.302572000	0.767616000	-2.637733000
C	3.884490000	-0.958638000	-1.828267000
C	4.506478000	-0.721412000	-0.467746000
C	4.132287000	-0.310950000	1.789621000
C	2.613923000	1.934405000	-1.723423000
C	2.535118000	2.741761000	0.456406000
H	2.921605000	0.800706000	-3.544037000
H	1.252941000	0.834999000	-2.931815000
H	4.478139000	-0.471582000	-2.611219000
H	3.918335000	-2.034919000	-2.034675000
C	5.881261000	-0.828080000	-0.262224000
C	5.490041000	-0.415909000	2.078662000
H	3.372204000	-0.096678000	2.534121000
C	3.132317000	3.139958000	-2.188364000
C	3.039133000	3.980439000	0.065110000
H	2.308318000	2.515275000	1.492318000
H	6.544462000	-1.032617000	-1.097572000
C	6.379870000	-0.674213000	1.032382000
H	5.840327000	-0.292085000	3.098000000
H	3.375810000	3.254995000	-3.240150000
C	3.342365000	4.183086000	-1.281743000
H	3.202473000	4.757140000	0.804537000
H	7.446305000	-0.754247000	1.220624000
H	3.750632000	5.130269000	-1.621106000

H	-0.378063000	-3.146946000	2.873217000
H	-0.149786000	-0.553087000	1.806346000
C	-0.917232000	-2.441805000	3.508168000
H	-1.587250000	-3.030304000	4.146768000
C	-1.795073000	-1.470590000	2.707383000
H	-2.662006000	-1.991756000	2.290941000
C	-2.155906000	-0.435066000	3.783166000
H	-2.899661000	-0.878415000	4.457497000
H	-2.599449000	0.474589000	3.365984000
C	-0.020606000	-1.535397000	4.382987000
H	0.204014000	-2.004603000	5.345115000
H	0.927029000	-1.320767000	3.879897000
C	-0.826023000	-0.208678000	4.546050000
H	-1.004707000	0.048922000	5.593681000
H	-0.254402000	0.612457000	4.099677000

Ib-²P_{2Hs-hs}

Fe	1.495742000	-0.319521000	0.054755000
O	1.461084000	0.905548000	-1.728652000
Fe	-1.645481000	0.390120000	-0.239331000
O	-1.062177000	0.375562000	-2.077424000
H	-1.611887000	0.809906000	-2.745476000
O	-0.180160000	0.192730000	0.733177000
N	0.674333000	-2.193970000	-0.944330000
N	2.739729000	0.677370000	1.616231000
N	3.384628000	-1.275853000	-0.663349000
C	0.632331000	-3.235908000	-0.093188000
C	0.394607000	-4.537048000	-0.533762000
H	0.375147000	-5.356861000	0.178029000
C	0.186095000	-4.759698000	-1.897790000
H	0.007761000	-5.764841000	-2.269052000
C	0.219815000	-3.673770000	-2.774367000
H	0.067696000	-3.804434000	-3.840909000
C	0.474758000	-2.404265000	-2.250818000
H	0.502767000	-1.519975000	-2.878195000
C	2.692932000	0.033609000	2.800564000
C	3.423862000	0.470955000	3.903975000
H	3.375631000	-0.078360000	4.839414000
C	4.219826000	1.612979000	3.779240000
H	4.800100000	1.971912000	4.624103000
C	4.270833000	2.271694000	2.549984000
H	4.887508000	3.152800000	2.405323000
C	3.515133000	1.762180000	1.494289000
H	3.528386000	2.225178000	0.513667000
C	3.830581000	-2.330082000	0.039406000
C	4.856885000	-3.148848000	-0.434643000
H	5.189662000	-3.998553000	0.154471000
C	5.444028000	-2.853664000	-1.664826000
H	6.246614000	-3.474072000	-2.052567000
C	4.979575000	-1.753884000	-2.390564000
H	5.405285000	-1.492305000	-3.353643000
C	3.940648000	-0.997334000	-1.855130000
H	3.510333000	-0.150201000	-2.379211000
C	0.790561000	-2.899017000	1.378404000
H	0.912313000	-3.820395000	1.968620000
C	1.794098000	-1.189751000	2.859111000
H	0.754066000	-0.853069000	2.933030000
H	2.035634000	-1.798400000	3.743571000
C	3.229113000	-2.569573000	1.414273000
H	3.190573000	-3.648873000	1.618627000
H	3.915990000	-2.138653000	2.153045000
N	1.898513000	-1.955458000	1.601776000
H	-0.128186000	-2.394751000	1.698521000
H	-4.242861000	-4.793133000	1.619653000
C	-3.731918000	-3.902027000	1.267193000
C	-3.637451000	-2.773013000	2.086118000
C	-3.167245000	-3.863145000	-0.008217000
C	-2.979664000	-1.643861000	1.602809000
H	-4.068344000	-2.765001000	3.082642000
H	-3.217395000	-4.716603000	-0.675833000
C	-2.534713000	-2.690731000	-0.420624000
N	-2.441972000	-1.613117000	0.368141000
C	-2.761386000	-0.406653000	2.448610000
H	-2.080405000	-2.602778000	-1.402229000
H	-1.728441000	-0.431014000	2.812543000

H	-3.439105000	-0.407230000	3.314918000
N	-2.899825000	0.826663000	1.651871000
N	-3.863017000	0.406062000	-0.942566000
N	-1.764181000	2.589233000	-0.051260000
C	-2.187897000	1.979708000	2.246399000
C	-4.308650000	1.151859000	1.334284000
C	-4.783544000	0.560043000	0.023201000
C	-4.250316000	-0.068888000	-2.136197000
C	-2.001057000	3.049376000	1.191868000
C	-1.555656000	3.456307000	-1.049540000
H	-2.711200000	2.381818000	3.125604000
H	-1.198183000	1.619357000	2.545524000
H	-4.393917000	2.241982000	1.253433000
H	-4.973007000	0.841988000	2.153038000
C	-6.129202000	0.251941000	-0.180109000
C	-5.574308000	-0.385059000	-2.431398000
H	-3.458235000	-0.219062000	-2.863728000
C	-2.048994000	4.413864000	1.469412000
C	-1.580202000	4.836385000	-0.856375000
H	-1.357003000	3.013104000	-2.019330000
H	-6.844145000	0.383243000	0.626716000
C	-6.533118000	-0.220761000	-1.429361000
H	-5.841395000	-0.757979000	-3.414626000
H	-2.257196000	4.756071000	2.478474000
C	-1.832425000	5.321528000	0.428632000
H	-1.405653000	5.507308000	-1.690694000
H	-7.575156000	-0.463994000	-1.614247000
H	-1.868578000	6.390234000	0.617838000
H	0.498674000	0.765725000	-2.012359000
H	1.546377000	1.865118000	-1.561795000
C	1.917173000	4.396363000	-1.198978000
H	1.167196000	4.782269000	-0.514302000
C	1.662700000	3.874128000	-2.407923000
H	0.675820000	3.783431000	-2.854748000
C	2.935608000	3.506524000	-3.143690000
H	3.151084000	4.253500000	-3.921758000
H	2.875808000	2.530838000	-3.639780000
C	3.407376000	4.504788000	-0.951264000
H	3.733576000	5.540187000	-1.131366000
H	3.705612000	4.263967000	0.076379000
C	3.997446000	3.542157000	-2.013663000
H	4.987692000	3.846783000	-2.363664000
H	4.089306000	2.534549000	-1.583177000

Ib-¹⁰P_{2Hhs-hs}

C	-0.785219000	-2.312634000	-2.287724000
N	-0.929014000	-2.102876000	-0.973130000
C	-0.874098000	-3.148390000	-0.129174000
C	-0.683796000	-4.453456000	-0.581598000
C	-0.527035000	-4.674660000	-1.952319000
C	-0.569506000	-3.584135000	-2.822946000
Fe	-1.571516000	-0.161542000	0.048746000
O	0.212115000	0.242823000	0.753329000
Fe	1.690282000	0.351246000	-0.236624000
N	1.923555000	2.535145000	-0.009012000
C	2.196705000	2.953145000	1.241706000
C	2.296730000	4.307069000	1.555314000
C	2.090841000	5.250329000	0.545232000
C	1.795492000	4.809460000	-0.746432000
C	1.721273000	3.437111000	-0.977956000
C	2.348490000	1.853175000	2.270555000
N	2.995057000	0.678649000	1.644185000
C	2.807192000	-0.563580000	2.417671000
C	2.910060000	-1.795292000	1.540827000
N	2.339373000	-1.700268000	0.324632000
C	2.317322000	-2.766405000	-0.484481000
C	2.865665000	-3.993116000	-0.111129000
C	3.467961000	-4.099233000	1.143163000
C	3.490868000	-2.981956000	1.983233000
C	-0.946260000	-2.809508000	1.345198000
N	-1.966941000	-1.785730000	1.626069000
C	-3.348800000	-2.300638000	1.532541000
C	-4.028427000	-2.005842000	0.206173000
N	-3.560374000	-0.981959000	-0.527009000
C	-4.178917000	-0.665130000	-1.677621000

C	-5.303972000	-1.342812000	-2.137303000
C	-5.793633000	-2.408588000	-1.377832000
C	-5.141891000	-2.747896000	-0.192967000
O	-1.372362000	0.732517000	-1.874298000
N	-2.633554000	0.905247000	1.764394000
C	-2.529369000	0.222700000	2.924224000
C	-3.121248000	0.670804000	4.104112000
C	-3.832851000	1.872605000	4.092934000
C	-3.937405000	2.579358000	2.895210000
C	-3.325286000	2.053731000	1.757309000
C	-1.713728000	-1.053748000	2.881486000
N	3.920908000	0.225251000	-0.955222000
C	4.851293000	0.319609000	0.008769000
C	6.174300000	-0.074025000	-0.194564000
C	6.546511000	-0.572074000	-1.443846000
C	5.577673000	-0.675742000	-2.444056000
C	4.276414000	-0.275711000	-2.147955000
C	4.413585000	0.942344000	1.317138000
O	1.150736000	0.334989000	-2.083200000
H	-0.379653000	0.663403000	-2.088669000
H	3.952400000	-3.027862000	2.964900000
H	3.917623000	-5.034316000	1.463779000
H	2.825013000	-4.836133000	-0.792471000
H	1.840353000	-2.620436000	-1.448726000
H	2.534089000	4.613012000	2.569577000
H	2.167036000	6.311511000	0.762468000
H	1.630870000	5.509547000	-1.558532000
H	1.485478000	3.029979000	-1.956202000
H	6.896390000	0.012264000	0.611966000
H	7.570790000	-0.881095000	-1.629690000
H	5.818857000	-1.066067000	-3.427230000
H	3.476609000	-0.377441000	-2.875104000
H	3.515047000	-0.628310000	3.256825000
H	1.344962000	1.536023000	2.572745000
H	2.901781000	2.211158000	3.150451000
H	5.069676000	0.612225000	2.134861000
H	4.542131000	2.027272000	1.225265000
H	1.789907000	-0.532429000	2.822866000
H	-0.382773000	-5.681595000	-2.333479000
H	-0.657861000	-5.275953000	0.126837000
H	-0.457756000	-3.713102000	-3.894643000
H	-0.845487000	-1.428032000	-2.911480000
H	0.022050000	-2.377856000	1.621729000
H	-1.109169000	-3.720531000	1.941369000
H	-1.918734000	-1.667991000	3.771290000
H	-0.653359000	-0.779199000	2.869039000
H	-3.948374000	-1.828922000	2.320723000
H	-3.375314000	-3.381957000	1.727410000
H	-3.729843000	0.145774000	-2.240201000
H	-3.389322000	2.564376000	0.804644000
H	-5.489613000	-3.574909000	0.419281000
H	-5.775863000	-1.049312000	-3.069123000
H	-3.028294000	0.082773000	5.012209000
H	-4.487757000	3.512491000	2.834723000
H	-6.663489000	-2.969513000	-1.706457000
H	-4.304316000	2.241606000	4.998957000
H	-1.705528000	1.574538000	-2.235540000
H	1.712792000	0.784208000	-2.730856000
C	-3.205644000	2.925014000	-3.186243000
C	-2.098626000	3.612537000	-3.502041000
C	-1.652160000	4.506251000	-2.364851000
C	-2.442912000	3.943652000	-1.155431000
C	-3.676463000	3.232734000	-1.778889000
H	-3.752006000	2.278009000	-3.867767000
H	-1.616647000	3.602669000	-4.476078000
H	-1.928586000	5.549067000	-2.579966000
H	-0.568799000	4.494845000	-2.195488000
H	-4.553405000	3.895787000	-1.809598000
H	-3.980314000	2.333702000	-1.225626000
H	-2.715380000	4.714259000	-0.427770000
H	-1.817867000	3.200978000	-0.642023000

Ib-⁸P_{2Hhs-is}

C	-0.329840000	-2.259379000	-2.382386000
N	-0.519955000	-2.214816000	-1.056320000

C	-0.228523000	-3.293633000	-0.301446000
C	0.250684000	-4.471903000	-0.867472000
C	0.447189000	-4.527063000	-2.250150000
C	0.159165000	-3.400251000	-3.020708000
Fe	-1.378118000	-0.622533000	0.048800000
O	0.076099000	-0.159092000	0.717298000
Fe	1.723267000	0.527955000	-0.343772000
N	1.169792000	2.581869000	0.319177000
C	1.307863000	2.841085000	1.632009000
C	1.004074000	4.090323000	2.172223000
C	0.520465000	5.092232000	1.327294000
C	0.361197000	4.812572000	-0.031159000
C	0.704799000	3.541756000	-0.489841000
C	1.760058000	1.676816000	2.489884000
N	2.708939000	0.820508000	1.749447000
C	2.829104000	-0.529846000	2.328198000
C	3.254168000	-1.560965000	1.301220000
N	2.682442000	-1.450332000	0.087746000
C	2.956415000	-2.364589000	-0.851317000
C	3.810682000	-3.442763000	-0.621169000
C	4.410753000	-3.559558000	0.633620000
C	4.127948000	-2.602045000	1.611472000
C	-0.416141000	-3.130061000	1.194882000
N	-1.639294000	-2.353686000	1.471270000
C	-2.880839000	-3.091754000	1.167325000
C	-3.796406000	-2.366324000	0.199355000
N	-3.276838000	-1.359181000	-0.528762000
C	-4.042835000	-0.758847000	-1.460190000
C	-5.363290000	-1.127178000	-1.691080000
C	-5.914283000	-2.156848000	-0.924339000
C	-5.116974000	-2.785224000	0.030739000
O	-1.370682000	0.602962000	-1.712107000
N	-2.491266000	0.309168000	1.604737000
C	-2.540275000	-0.429461000	2.732524000
C	-3.304350000	-0.035022000	3.829242000
C	-4.022118000	1.161549000	3.763597000
C	-3.954315000	1.926793000	2.598665000
C	-3.177912000	1.457768000	1.540389000
C	-1.666660000	-1.671261000	2.773411000
N	3.870139000	0.989605000	-0.807881000
C	4.685099000	1.150046000	0.249524000
C	6.072778000	1.082288000	0.129920000
C	6.632363000	0.855982000	-1.129056000
C	5.784447000	0.690888000	-2.226036000
C	4.408690000	0.754569000	-2.013816000
C	4.018296000	1.485456000	1.567952000
O	1.109298000	0.577905000	-2.194014000
H	-0.377900000	0.675252000	-2.001124000
H	4.579786000	-2.656970000	2.597387000
H	5.092793000	-4.377165000	0.847604000
H	4.005823000	-4.162530000	-1.409366000
H	2.468151000	-2.214983000	-1.809700000
H	1.147345000	4.272016000	3.233212000
H	0.280851000	6.075165000	1.721923000
H	-0.012038000	5.560156000	-0.722732000
H	0.605875000	3.264266000	-1.535597000
H	6.700002000	1.209152000	1.007278000
H	7.710323000	0.803801000	-1.249480000
H	6.176361000	0.507383000	-3.221008000
H	3.697008000	0.595608000	-2.819035000
H	3.513853000	-0.542667000	3.189635000
H	0.877691000	1.064430000	2.700718000
H	2.181620000	2.037153000	3.440190000
H	4.692867000	1.258300000	2.406441000
H	3.843521000	2.567769000	1.579682000
H	1.830933000	-0.812703000	2.681600000
H	0.811836000	-5.437787000	-2.716248000
H	0.463020000	-5.328019000	-0.234463000
H	0.293567000	-3.401874000	-4.097298000
H	-0.573396000	-1.353468000	-2.922372000
H	0.427234000	-2.541490000	1.569164000
H	-0.423327000	-4.111337000	1.690811000
H	-1.997005000	-2.339260000	3.582358000
H	-0.642449000	-1.346982000	2.984935000
H	-3.428540000	-3.325018000	2.090325000

H	-2.615401000	-4.055041000	0.713344000
H	-3.558343000	0.025480000	-2.027441000
H	-3.098608000	2.006389000	0.610205000
H	-5.506527000	-3.596202000	0.638909000
H	-5.943365000	-0.616114000	-2.452139000
H	-3.333429000	-0.657659000	4.718314000
H	-4.496372000	2.861678000	2.502680000
H	-6.944543000	-2.467263000	-1.070353000
H	-4.626030000	1.486365000	4.605594000
H	-1.801669000	1.449682000	-1.917966000
H	1.477330000	1.254660000	-2.780574000
C	-3.551353000	2.523826000	-3.132958000
C	-2.506511000	3.234183000	-3.579121000
C	-2.144849000	4.350545000	-2.622754000
C	-2.869128000	3.926846000	-1.319896000
C	-4.051297000	3.042816000	-1.799346000
H	-4.039467000	1.724184000	-3.684285000
H	-2.019914000	3.093406000	-4.540293000
H	-2.529044000	5.308341000	-3.003846000
H	-1.064017000	4.477603000	-2.487715000
H	-4.962963000	3.641594000	-1.942211000
H	-4.313730000	2.244010000	-1.092353000
H	-3.186594000	4.774375000	-0.704888000
H	-2.172476000	3.323024000	-0.721081000

Ib-⁴P_{2Hs-is}

Fe	1.434732000	-0.660498000	0.076749000
O	1.538549000	0.651280000	-1.698937000
Fe	-1.614585000	0.438882000	-0.249914000
O	-1.013176000	0.457966000	-2.081912000
H	-1.478948000	1.039841000	-2.700022000
O	-0.242563000	-0.078804000	0.746941000
N	0.568989000	-2.184809000	-0.907262000
N	2.375171000	0.450144000	1.452804000
N	3.289892000	-1.522993000	-0.405797000
C	0.282590000	-3.245283000	-0.115434000
C	-0.161508000	-4.452867000	-0.647188000
H	-0.366869000	-5.288066000	0.015264000
C	-0.329668000	-4.569240000	-2.029633000
H	-0.664519000	-5.505644000	-2.466129000
C	-0.047671000	-3.467218000	-2.837181000
H	-0.156907000	-3.513052000	-3.915651000
C	0.406448000	-2.293334000	-2.235421000
H	0.646628000	-1.408805000	-2.811192000
C	2.376934000	-0.101566000	2.689707000
C	3.070925000	0.482930000	3.746547000
H	3.065815000	0.005624000	4.721761000
C	3.766232000	1.675604000	3.532421000
H	4.314846000	2.145546000	4.343094000
C	3.750902000	2.243072000	2.258152000
H	4.279686000	3.165340000	2.042247000
C	3.048481000	1.591964000	1.246348000
H	3.016537000	1.982852000	0.237021000
C	3.755083000	-2.499622000	0.389939000
C	4.992252000	-3.106331000	0.161504000
H	5.338724000	-3.892444000	0.826562000
C	5.763121000	-2.692109000	-0.922253000
H	6.728398000	-3.149525000	-1.117386000
C	5.268939000	-1.683329000	-1.754302000
H	5.830672000	-1.333715000	-2.614053000
C	4.028539000	-1.127943000	-1.462043000
H	3.581624000	-0.351656000	-2.072140000
C	0.423683000	-3.026046000	1.380354000
H	0.422934000	-3.991841000	1.906995000
C	1.541382000	-1.357244000	2.873960000
H	0.497938000	-1.043262000	2.970446000
H	1.842921000	-1.880755000	3.793234000
C	2.891408000	-2.952579000	1.559592000
H	2.690860000	-4.026487000	1.448095000
H	3.470932000	-2.845336000	2.485822000
N	1.619962000	-2.222164000	1.685050000
H	-0.445069000	-2.443786000	1.702919000
H	-5.081807000	-4.365286000	1.099453000
C	-4.414075000	-3.548129000	0.843072000
C	-4.202809000	-2.501236000	1.745157000

C	-3.760337000	-3.524238000	-0.389640000
C	-3.345441000	-1.464190000	1.383390000
H	-4.695346000	-2.486527000	2.712668000
H	-3.896964000	-3.17640000	-1.116854000
C	-2.926805000	-2.444275000	-0.679568000
N	-2.728118000	-1.443692000	0.186887000
C	-2.987177000	-0.336925000	2.330930000
H	-2.395218000	-2.367955000	-1.623331000
H	-2.000462000	-0.561562000	2.750507000
H	-3.712081000	-0.282180000	3.156172000
N	-2.864319000	0.954706000	1.629099000
N	-3.792260000	0.851251000	-1.010450000
N	-1.351124000	2.607888000	0.113062000
C	-1.992423000	1.916418000	2.337956000
C	-4.175477000	1.549664000	1.287330000
C	-4.705202000	1.095670000	-0.056257000
C	-4.215642000	0.496551000	-2.232845000
C	-1.555394000	3.006738000	1.382559000
C	-0.915235000	3.489066000	-0.795396000
H	-2.480519000	2.344443000	3.225339000
H	-1.098826000	1.363373000	2.646137000
H	-4.048886000	2.637679000	1.241154000
H	-4.912696000	1.347263000	2.077123000
C	-6.075876000	1.002382000	-0.298220000
C	-5.564417000	0.396735000	-2.568052000
H	-3.437096000	0.264753000	-2.953654000
C	-1.342142000	4.325883000	1.777528000
C	-0.665874000	4.824038000	-0.481170000
H	-0.760528000	3.092786000	-1.793350000
H	-6.783449000	1.202262000	0.500993000
C	-6.513728000	0.654967000	-1.577191000
H	-5.858297000	0.115022000	-3.573761000
H	-1.532412000	4.623465000	2.804201000
C	-0.887145000	5.248055000	0.830891000
H	-0.314167000	5.508223000	-1.246176000
H	-7.575272000	0.580088000	-1.793333000
H	-0.717228000	6.282947000	1.112764000
H	0.558026000	0.654661000	-1.960503000
H	1.775875000	1.585177000	-1.549350000
C	2.736792000	4.032570000	-1.313778000
H	2.162377000	4.591048000	-0.579268000
C	2.250072000	3.548545000	-2.465978000
H	1.226445000	3.671180000	-2.811542000
C	3.326126000	2.887485000	-3.303157000
H	3.607964000	3.541852000	-4.140841000
H	3.002354000	1.932341000	-3.733027000
C	4.232467000	3.809807000	-1.210729000
H	4.759844000	4.745970000	-1.446061000
H	4.572854000	3.504187000	-0.213590000
C	4.489328000	2.726542000	-2.289444000
H	5.476042000	2.812384000	-2.752859000
H	4.423661000	1.735508000	-1.820855000

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C	0.572325000	-2.642556000	2.252175000
N	0.757617000	-2.375817000	0.951796000
C	0.499431000	-3.334729000	0.045489000
C	0.060851000	-4.605234000	0.411819000
C	-0.133723000	-4.885111000	1.766482000
C	0.121084000	-3.884038000	2.704544000
Fe	1.556231000	-0.476274000	0.126154000
O	-0.158044000	0.055614000	-0.476184000
Fe	-1.655923000	0.415258000	0.221930000
N	-1.550393000	2.664731000	-0.351434000
C	-1.585478000	2.796214000	-1.690392000
C	-1.438454000	4.034175000	-2.316413000
C	-1.227943000	5.168317000	-1.528499000
C	-1.183972000	5.028367000	-0.140459000
C	-1.356871000	3.754351000	0.400086000
C	-1.753408000	1.517726000	-2.489951000
N	-2.598595000	0.544557000	-1.758161000
C	-2.518147000	-0.813953000	-2.334780000
C	-2.910785000	-1.882963000	-1.330937000
N	-2.455572000	-1.708112000	-0.077314000
C	-2.718166000	-2.631705000	0.851423000

C	-3.445521000	-3.789914000	0.570335000
C	-3.921499000	-3.976956000	-0.727489000
C	-3.650209000	-3.006147000	-1.697042000
C	0.681923000	-2.931836000	-1.401862000
N	1.821658000	-2.008286000	-1.536851000
C	3.120347000	-2.672147000	-1.291685000
C	4.038503000	-1.894232000	-0.369981000
N	3.476624000	-0.996637000	0.467748000
C	4.263917000	-0.361881000	1.358375000
C	5.632410000	-0.589116000	1.451237000
C	6.218727000	-1.506228000	0.576567000
C	5.406879000	-2.164067000	-0.346062000
O	1.299117000	0.291990000	2.019592000
N	2.426461000	0.715866000	-1.470354000
C	2.547911000	0.078839000	-2.650473000
C	3.260653000	0.626606000	-3.716118000
C	3.850878000	1.882971000	-3.562925000
C	3.705691000	2.549533000	-2.345728000
C	2.989700000	1.923783000	-1.326196000
C	1.797447000	-1.230619000	-2.783051000
N	-3.700746000	0.675171000	0.744540000
C	-4.581486000	0.783612000	-0.267908000
C	-5.957573000	0.735468000	-0.052446000
C	-6.432661000	0.580765000	1.250406000
C	-5.514550000	0.466465000	2.296710000
C	-4.155542000	0.508337000	1.999296000
C	-4.001759000	1.023395000	-1.640463000
O	-1.214059000	0.555088000	2.090810000
H	0.284627000	0.438209000	2.134747000
H	-4.010157000	-3.115417000	-2.715891000
H	-4.500928000	-4.859217000	-0.983166000
H	-3.636515000	-4.517961000	1.351835000
H	-2.322985000	-2.430874000	1.842583000
H	-1.491579000	4.106364000	-3.398740000
H	-1.111918000	6.144169000	-1.990620000
H	-1.032308000	5.883223000	0.510369000
H	-1.335764000	3.599185000	1.475204000
H	-6.640480000	0.819672000	-0.892369000
H	-7.500556000	0.542955000	1.443667000
H	-5.840822000	0.336442000	3.323106000
H	-3.382707000	0.390405000	2.751684000
H	-3.128670000	-0.897721000	-3.245038000
H	-0.768304000	1.052499000	-2.595335000
H	-2.162635000	1.736541000	-3.486489000
H	-4.633839000	0.563555000	-2.411528000
H	-4.011995000	2.103772000	-1.825208000
H	-1.470220000	-0.967881000	-2.611205000
H	-0.467185000	-5.869419000	2.082182000
H	-0.120257000	-5.357131000	-0.350453000
H	-0.008182000	-4.060043000	3.767534000
H	0.800776000	-1.827610000	2.929594000
H	-0.212395000	-2.383511000	-1.707858000
H	0.787394000	-3.821054000	-2.041608000
H	2.186248000	-1.808448000	-3.635191000
H	0.748773000	-0.988073000	-2.990266000
H	3.635904000	-2.888171000	-2.238047000
H	2.924761000	-3.639980000	-0.814062000
H	3.767598000	0.350818000	2.005617000
H	2.857534000	2.396889000	-0.360780000
H	5.823252000	-2.886423000	-1.041770000
H	6.221404000	-0.053269000	2.187988000
H	3.348372000	0.075188000	-4.647541000
H	4.144847000	3.527787000	-2.180016000
H	7.285594000	-1.704551000	0.611837000
H	4.414316000	2.329346000	-4.376825000
H	1.784678000	0.941460000	2.557608000
H	-1.373532000	1.481472000	2.338213000
C	3.197076000	2.591998000	3.517180000
C	1.970379000	2.637623000	4.055568000
C	1.002366000	3.409182000	3.184378000
C	1.765497000	3.544334000	1.837572000
C	3.263308000	3.336435000	2.200189000
H	4.068801000	2.151982000	3.994971000
H	1.697728000	2.232144000	5.025959000
H	0.783979000	4.387345000	3.636570000

H	0.041003000	2.891551000	3.068203000
H	3.782374000	4.296056000	2.337268000
H	3.823948000	2.789380000	1.430267000
H	1.580210000	4.498934000	1.336725000
H	1.428960000	2.743586000	1.168724000

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C	0.572310000	-2.642604000	2.252203000
N	0.757609000	-2.375803000	0.951803000
C	0.499412000	-3.334704000	0.045503000
C	0.060916000	-4.605205000	0.411803000
C	-0.133683000	-4.885106000	1.766503000
C	0.121114000	-3.884005000	2.704503000
Fe	1.556203000	-0.476300000	0.126203000
O	-0.157999000	0.055594000	-0.476197000
Fe	-1.655900000	0.415289000	0.221903000
N	-1.550408000	2.664689000	-0.351397000
C	-1.585508000	2.796189000	-1.690397000
C	-1.438512000	4.034190000	-2.316397000
C	-1.227916000	5.168290000	-1.528497000
C	-1.184016000	5.028391000	-0.140497000
C	-1.356912000	3.754390000	0.400103000
C	-1.753404000	1.517689000	-2.489997000
N	-2.598601000	0.544586000	-1.758197000
C	-2.518096000	-0.814014000	-2.334797000
C	-2.910793000	-1.883015000	-1.330897000
N	-2.455593000	-1.708114000	-0.077297000
C	-2.718190000	-2.631714000	0.851403000
C	-3.445486000	-3.789917000	0.570303000
C	-3.921486000	-3.977018000	-0.727497000
C	-3.650189000	-3.006118000	-1.696997000
C	0.681911000	-2.931803000	-1.401897000
N	1.821708000	-2.008299000	-1.536897000
C	3.120310000	-2.672095000	-1.291697000
C	4.038507000	-1.894192000	-0.369997000
N	3.476604000	-0.996594000	0.467703000
C	4.263902000	-0.361891000	1.358403000
C	5.632403000	-0.589087000	1.451203000
C	6.218706000	-1.506185000	0.576603000
C	5.406908000	-2.164087000	-0.346097000
O	1.299100000	0.291999000	2.019603000
N	2.426499000	0.715903000	-1.470397000
C	2.547901000	0.078803000	-2.650497000
C	3.260699000	0.626605000	-3.716097000
C	3.850895000	1.883007000	-3.562897000
C	3.705692000	2.549507000	-2.345697000
C	2.989695000	1.923805000	-1.326197000
C	1.797405000	-1.230599000	-2.783097000
N	-3.700701000	0.675182000	0.744503000
C	-4.581502000	0.783579000	-0.267897000
C	-5.957602000	0.735475000	-0.052397000
C	-6.432701000	0.580773000	1.250403000
C	-5.514501000	0.466476000	2.296703000
C	-4.155501000	0.508281000	1.999303000
C	-4.001802000	1.023381000	-1.640497000
O	-1.214101000	0.555091000	2.090803000
H	0.284599000	0.438196000	2.134703000
H	-4.010189000	-3.115419000	-2.715897000
H	-4.500883000	-4.859220000	-0.983197000
H	-3.636484000	-4.518018000	1.351803000
H	-2.322991000	-2.430913000	1.842603000
H	-1.491613000	4.106390000	-3.398697000
H	-1.111920000	6.144191000	-1.990597000
H	-1.032319000	5.883191000	0.510403000
H	-1.335811000	3.599190000	1.475203000
H	-6.640502000	0.819672000	-0.892397000
H	-7.500601000	0.542970000	1.443703000
H	-5.840800000	0.336375000	3.323103000
H	-3.382700000	0.390383000	2.751703000
H	-3.128696000	-0.897716000	-3.244997000
H	-0.768303000	1.052492000	-2.595297000
H	-2.162605000	1.736487000	-3.486497000
H	-4.633801000	0.563579000	-2.411497000
H	-4.012006000	2.103781000	-1.825197000
H	-1.470196000	-0.967910000	-2.611197000

H	-0.467180000	-5.869407000	2.082203000
H	-0.120281000	-5.357106000	-0.350497000
H	-0.008186000	-4.060005000	3.767503000
H	0.800807000	-1.827603000	2.929603000
H	-0.212391000	-2.383506000	-1.707897000
H	0.787414000	-3.821103000	-2.041597000
H	2.186207000	-1.808398000	-3.635197000
H	0.748804000	-0.988103000	-2.990297000
H	3.635911000	-2.888193000	-2.237997000
H	2.924813000	-3.639996000	-0.814097000
H	3.767600000	0.350807000	2.005603000
H	2.857493000	2.396904000	-0.360797000
H	5.823311000	-2.886386000	-1.041797000
H	6.221401000	-0.053285000	2.188003000
H	3.348401000	0.075206000	-4.647497000
H	4.144789000	3.527808000	-2.179997000
H	7.285607000	-1.704581000	0.611803000
H	4.414293000	2.329309000	-4.376797000
H	1.784698000	0.941501000	2.557603000
H	-1.373504000	1.481490000	2.338203000
C	3.197092000	2.592005000	3.517203000
C	1.970392000	2.637601000	4.055603000
C	1.002390000	3.409198000	3.184403000
C	1.765489000	3.544300000	1.837603000
C	3.263290000	3.336405000	2.200203000
H	4.068794000	2.152008000	3.995003000
H	1.697694000	2.232100000	5.026003000
H	0.783986000	4.387297000	3.636603000
H	0.040991000	2.891595000	3.068203000
H	3.782387000	4.296107000	2.337303000
H	3.823892000	2.789407000	1.430303000
H	1.580186000	4.498900000	1.336703000
H	1.428992000	2.743599000	1.168703000

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Fe	1.603348000	-0.459348000	-0.240455000
O	1.405682000	0.632397000	1.437029000
Fe	-1.599365000	0.289561000	0.116564000
O	-0.963992000	-0.019645000	1.968348000
H	-1.277566000	0.714645000	2.522261000
O	-0.221598000	-0.089717000	-0.763639000
N	2.128545000	1.075632000	-1.375795000
N	1.010535000	-2.198948000	0.533681000
N	3.573095000	-0.810137000	-0.013357000
C	2.171500000	0.768977000	-2.689682000
C	2.594115000	1.693092000	-3.641833000
H	2.634235000	1.415049000	-4.690728000
C	2.961007000	2.974588000	-3.220598000
H	3.298356000	3.712126000	-3.942691000
C	2.890672000	3.288861000	-1.862280000
H	3.161316000	4.273883000	-1.497215000
C	2.475253000	2.304300000	-0.967539000
H	2.395817000	2.471955000	0.100636000
C	0.647059000	-3.090237000	-0.417459000
C	0.193504000	-4.365347000	-0.095549000
H	-0.072686000	-5.060520000	-0.885746000
C	0.090645000	-4.726413000	1.250864000
H	-0.254572000	-5.717742000	1.529020000
C	0.449155000	-3.797612000	2.228324000
H	0.386558000	-4.036015000	3.284792000
C	0.908598000	-2.544550000	1.825093000
H	1.199638000	-1.786868000	2.541240000
C	4.118388000	-1.536690000	-1.011706000
C	5.494911000	-1.702860000	-1.147058000
H	5.890063000	-2.289056000	-1.971256000
C	6.344082000	-1.111516000	-0.211538000
H	7.420406000	-1.227803000	-0.292730000
C	5.781367000	-0.363503000	0.824070000
H	6.400527000	0.119436000	1.572703000
C	4.397201000	-0.230829000	0.879502000
H	3.925940000	0.362021000	1.653519000
C	1.631280000	-0.599289000	-3.055870000
H	2.081581000	-0.972373000	-3.985113000
C	0.715485000	-2.577239000	-1.839499000
H	-0.223941000	-2.059728000	-2.046606000

H	0.854797000	-3.395841000	-2.558283000
C	3.142663000	-2.222135000	-1.936950000
H	3.543354000	-2.285146000	-2.956138000
H	3.009752000	-3.250928000	-1.582061000
N	1.803113000	-1.562693000	-1.935761000
H	0.553865000	-0.492307000	-3.214214000
H	0.138073000	6.057612000	-0.839261000
C	-0.192573000	5.051862000	-0.596889000
C	-0.766206000	4.242077000	-1.579637000
C	-0.058700000	4.552742000	0.700276000
C	-1.185718000	2.957931000	-1.232201000
H	-0.885653000	4.596675000	-2.599155000
H	0.380364000	5.149063000	1.493487000
C	-0.522112000	3.264241000	0.963963000
N	-1.078989000	2.491667000	0.024519000
C	-1.705353000	1.987238000	-2.279660000
H	-0.436826000	2.825198000	1.953305000
H	-0.846105000	1.416807000	-2.645184000
H	-2.158541000	2.532788000	-3.119913000
N	-2.645307000	1.007497000	-1.692283000
N	-3.557670000	0.638961000	0.872829000
N	-2.631915000	-1.582217000	-0.541735000
C	-2.836645000	-0.192715000	-2.533951000
C	-3.925378000	1.648405000	-1.304006000
C	-4.468030000	1.105695000	-0.003878000
C	-3.972009000	0.174765000	2.065149000
C	-3.234943000	-1.423858000	-1.733007000
C	-2.863911000	-2.683858000	0.179506000
H	-3.566023000	-0.007744000	-3.335462000
H	-1.868592000	-0.404889000	-3.001065000
H	-4.670921000	1.552312000	-2.105214000
H	-3.738263000	2.719920000	-1.166535000
C	-5.828466000	1.136586000	0.296416000
C	-5.310804000	0.187882000	2.445419000
H	-3.191639000	-0.232572000	2.699217000
C	-4.113166000	-2.379811000	-2.241471000
C	-3.718212000	-3.695837000	-0.261401000
H	-2.343875000	-2.738701000	1.131857000
H	-6.535700000	1.514164000	-0.435732000
C	-6.256996000	0.678691000	1.543174000
H	-5.601380000	-0.189721000	3.419992000
H	-4.594883000	-2.223567000	-3.202181000
C	-4.357470000	-3.534710000	-1.492053000
H	-3.884824000	-4.577354000	0.349130000
H	-7.311661000	0.695967000	1.801049000
H	-5.040547000	-4.293054000	-1.863218000
H	0.426451000	0.393192000	1.718117000
H	1.955283000	0.377337000	2.201535000
C	2.992698000	1.092336000	4.136825000
H	4.056696000	1.198134000	3.937349000
C	2.385327000	-0.058973000	4.457134000
H	2.889196000	-1.018347000	4.551961000
C	0.906568000	0.120192000	4.725349000
H	0.634996000	-0.265905000	5.716133000
H	0.285976000	-0.417925000	3.995262000
C	2.037781000	2.265031000	4.104291000
H	2.390148000	3.092138000	4.732814000
H	1.941762000	2.657513000	3.081801000
C	0.697171000	1.662703000	4.624389000
H	0.455614000	2.076747000	5.607182000
H	-0.139139000	1.909990000	3.959726000

Ib-²P_{2Hls-is}

Fe	1.490008000	-0.148674000	-0.228227000
O	1.108181000	-0.046473000	1.793568000
Fe	-1.756886000	0.319743000	0.116788000
O	-1.276592000	-0.762950000	1.658121000
H	-1.678617000	-0.378857000	2.453223000
O	-0.261019000	0.125921000	-0.787873000
N	2.133634000	1.734738000	-1.014538000
N	1.006768000	-2.318201000	-0.404511000
N	3.488178000	-0.423267000	0.073770000
C	2.519555000	1.717524000	-2.303422000
C	3.194927000	2.793269000	-2.879067000
H	3.506342000	2.745125000	-3.918352000

C	3.460220000	3.921474000	-2.098926000
H	3.988779000	4.769717000	-2.523658000
C	3.042540000	3.937896000	-0.766367000
H	3.231278000	4.793552000	-0.126307000
C	2.387465000	2.815340000	-0.262954000
H	2.051047000	2.759223000	0.768526000
C	0.831251000	-2.737895000	-1.669079000
C	0.379096000	-4.023115000	-1.965721000
H	0.272211000	-4.335429000	-3.000428000
C	0.074969000	-4.890270000	-0.913990000
H	-0.271751000	-5.899424000	-1.116950000
C	0.235038000	-4.442122000	0.398195000
H	0.013545000	-5.082576000	1.245875000
C	0.708500000	-3.146148000	0.603342000
H	0.850006000	-2.746450000	1.599598000
C	4.214614000	-0.842298000	-0.985651000
C	5.608473000	-0.880193000	-0.952569000
H	6.157306000	-1.215853000	-1.827384000
C	6.276431000	-0.487767000	0.206991000
H	7.360861000	-0.513267000	0.253596000
C	5.523572000	-0.052600000	1.299696000
H	5.997953000	0.273778000	2.219280000
C	4.137454000	-0.028246000	1.185861000
H	3.508465000	0.328822000	1.993336000
C	2.101737000	0.503121000	-3.116293000
H	2.725942000	0.421925000	-4.018927000
C	1.092389000	-1.715600000	-2.758682000
H	0.162895000	-1.154599000	-2.899019000
H	1.357185000	-2.217553000	-3.701921000
C	3.454416000	-1.339511000	-2.199423000
H	4.051891000	-1.179262000	-3.108651000
H	3.330751000	-2.423149000	-2.087909000
N	2.110335000	-0.741280000	-2.333795000
H	1.069701000	0.672393000	-3.445393000
H	0.012911000	5.681669000	1.724555000
C	-0.297183000	4.670863000	1.476793000
C	-0.685984000	4.350532000	0.173286000
C	-0.323408000	3.675803000	2.454475000
C	-1.085022000	3.048245000	-0.110627000
H	-0.680110000	5.097182000	-0.614554000
H	-0.031701000	3.881119000	3.478944000
C	-0.751160000	2.398040000	2.097016000
N	-1.127644000	2.092307000	0.848029000
C	-1.443495000	2.585484000	-1.505530000
H	-0.785355000	1.588432000	2.814210000
H	-0.551326000	2.126267000	-1.939102000
H	-1.782134000	3.421243000	-2.131881000
N	-2.472365000	1.513343000	-1.404644000
N	-3.729132000	0.547800000	0.823073000
N	-2.528185000	-1.161152000	-0.937862000
C	-2.532863000	0.614600000	-2.587601000
C	-3.799281000	2.093631000	-1.040753000
C	-4.514165000	1.283852000	0.012847000
C	-4.306766000	-0.174617000	1.798259000
C	-2.908156000	-0.795791000	-2.179644000
C	-2.711825000	-2.417609000	-0.513058000
H	-3.211768000	1.004548000	-3.356712000
H	-1.520894000	0.574324000	-2.999599000
H	-4.424276000	2.213271000	-1.934076000
H	-3.625748000	3.097417000	-0.635714000
C	-5.897857000	1.340072000	0.167738000
C	-5.678966000	-0.160215000	2.032074000
H	-3.642550000	-0.805049000	2.378175000
C	-3.518614000	-1.701089000	-3.042839000
C	-3.299464000	-3.382963000	-1.329005000
H	-2.361856000	-2.612529000	0.494729000
H	-6.495765000	1.941215000	-0.510561000
C	-6.490945000	0.614603000	1.201664000
H	-6.097488000	-0.755187000	2.836858000
H	-3.830486000	-1.384284000	-4.033389000
C	-3.716848000	-3.015856000	-2.609399000
H	-3.432602000	-4.394779000	-0.961571000
H	-7.566500000	0.643461000	1.347210000
H	-4.193498000	-3.739688000	-3.263666000
H	0.121055000	-0.394137000	1.810046000

H	1.623560000	-0.641580000	2.371301000
C	2.607379000	-1.317765000	4.354803000
H	3.687509000	-1.266723000	4.240957000
C	1.844286000	-2.340140000	3.943527000
H	2.222551000	-3.233713000	3.452780000
C	0.388859000	-2.161362000	4.324508000
H	0.109459000	-2.891586000	5.097050000
H	-0.297166000	-2.307964000	3.479111000
C	1.808745000	-0.269341000	5.097353000
H	2.071402000	-0.284031000	6.164429000
H	2.007911000	0.749691000	4.739651000
C	0.332841000	-0.700145000	4.858617000
H	-0.275763000	-0.611483000	5.762721000
H	-0.108551000	-0.055177000	4.091103000

Ib-²P_{2Hls-ls}

C	-0.851712000	2.321888000	2.099944000
N	-0.956503000	2.151495000	0.774307000
C	-0.660616000	3.185326000	-0.047427000
C	-0.275098000	4.428653000	0.443085000
C	-0.168405000	4.606695000	1.825202000
C	-0.456771000	3.532684000	2.667388000
Fe	-1.465278000	0.499395000	-0.232895000
O	0.323906000	0.330994000	-0.783429000
Fe	1.758405000	-0.306439000	0.040709000
N	1.128472000	-2.198876000	-0.204790000
C	1.177545000	-2.587766000	-1.500686000
C	0.776945000	-3.859125000	-1.898349000
C	0.291053000	-4.747798000	-0.935183000
C	0.227202000	-4.334270000	0.395893000
C	0.661459000	-3.050050000	0.718344000
C	1.645856000	-1.528218000	-2.475015000
N	2.636794000	-0.655096000	-1.789697000
C	2.796929000	0.691108000	-2.397303000
C	3.090141000	1.735986000	-1.337629000
N	2.569859000	1.487504000	-0.117431000
C	2.674231000	2.394888000	0.861884000
C	3.322118000	3.612748000	0.661761000
C	3.884434000	3.875996000	-0.588725000
C	3.765738000	2.923239000	-1.605823000
C	-0.725650000	2.870801000	-1.526756000
N	-1.764555000	1.828975000	-1.751378000
C	-3.132739000	2.414650000	-1.638573000
C	-4.062221000	1.551791000	-0.819453000
N	-3.468605000	0.715004000	0.056053000
C	-4.249677000	-0.046638000	0.843475000
C	-5.639601000	0.014386000	0.812793000
C	-6.252816000	0.885345000	-0.089711000
C	-5.447508000	1.660141000	-0.925128000
O	-1.237622000	-0.774347000	1.294200000
N	-1.968207000	-0.875345000	-1.564984000
C	-2.070236000	-0.380738000	-2.818538000
C	-2.526676000	-1.162861000	-3.876106000
C	-2.873122000	-2.495152000	-3.630064000
C	-2.749571000	-3.000238000	-2.334491000
C	-2.296512000	-2.152462000	-1.325069000
C	-1.572726000	1.040301000	-2.995325000
N	3.654724000	-0.847421000	0.740394000
C	4.530206000	-1.142167000	-0.240742000
C	5.896412000	-1.277900000	-0.002574000
C	6.374994000	-1.109261000	1.297369000
C	5.470268000	-0.788392000	2.311149000
C	4.123460000	-0.654704000	1.985112000
C	3.933949000	-1.370665000	-1.608404000
O	1.064123000	-0.086023000	1.859603000
H	-0.247340000	-0.510154000	1.596640000
H	4.189548000	3.098641000	-2.589995000
H	4.411145000	4.807585000	-0.772782000
H	3.389951000	4.330497000	1.472284000
H	2.210662000	2.104398000	1.798580000
H	0.844525000	-4.144836000	-2.943365000
H	-0.023098000	-5.747595000	-1.219687000
H	-0.142483000	-4.990299000	1.176714000
H	0.622729000	-2.674655000	1.732767000
H	6.569406000	-1.510403000	-0.822335000

H	7.434387000	-1.212902000	1.511292000
H	5.799017000	-0.629478000	3.332692000
H	3.391572000	-0.351043000	2.725055000
H	3.563253000	0.693617000	-3.183235000
H	0.787368000	-0.896082000	-2.714325000
H	2.052371000	-1.975583000	-3.391830000
H	4.643093000	-1.090184000	-2.397078000
H	3.742189000	-2.444286000	-1.718663000
H	1.835150000	0.947628000	-2.851000000
H	0.124513000	5.568960000	2.234538000
H	-0.062955000	5.240262000	-0.246116000
H	-0.390526000	3.628097000	3.746146000
H	-1.083540000	1.456334000	2.708030000
H	0.231089000	2.427127000	-1.811128000
H	-0.911346000	3.773688000	-2.124135000
H	-2.042846000	1.523077000	-3.862353000
H	-0.493710000	0.991857000	-3.169313000
H	-3.553454000	2.611338000	-2.632657000
H	-3.041650000	3.383339000	-1.133531000
H	-3.737565000	-0.736013000	1.502407000
H	-2.175005000	-2.469861000	-0.295283000
H	-5.883781000	2.341786000	-1.649128000
H	-6.223342000	-0.617180000	1.474288000
H	-2.612498000	-0.736281000	-4.870974000
H	-3.006693000	-4.028836000	-2.104348000
H	-7.334704000	0.953598000	-0.149207000
H	-3.238336000	-3.123487000	-4.436854000
H	-1.783495000	-0.575702000	2.076908000
H	1.448355000	-0.776847000	2.421207000
C	-3.063921000	-0.909150000	4.095455000
C	-1.782630000	-0.675693000	4.413176000
C	-0.935238000	-1.925825000	4.313859000
C	-1.864349000	-2.931783000	3.578517000
C	-3.301895000	-2.363005000	3.743615000
H	-3.864063000	-0.175736000	4.158302000
H	-1.392967000	0.272868000	4.774592000
H	-0.661294000	-2.278074000	5.318471000
H	0.005302000	-1.749670000	3.773793000
H	-3.845814000	-2.857440000	4.561180000
H	-3.912833000	-2.501447000	2.840594000
H	-1.772121000	-3.949345000	3.968880000
H	-1.606059000	-2.943404000	2.514802000

Ic-²TS_{2Hhs-hs}

Fe	-1.684512000	0.406817000	-0.525231000
O	-1.119354000	0.949223000	-2.253353000
Fe	1.445020000	-0.369975000	-0.297326000
O	0.985171000	-0.735958000	-2.036935000
H	0.242022000	-0.138693000	-2.322652000
O	0.033905000	0.589281000	0.395855000
N	-2.745655000	2.167740000	0.339913000
N	-1.595540000	-1.862416000	-0.542770000
N	-3.801254000	-0.249473000	-1.228809000
C	-3.013156000	2.105139000	1.659319000
C	-3.658104000	3.139981000	2.329922000
H	-3.864210000	3.055782000	3.392629000
C	-4.042603000	4.273558000	1.605198000
H	-4.549726000	5.095272000	2.102046000
C	-3.786201000	4.322120000	0.234577000
H	-4.085216000	5.174777000	-0.365985000
C	-3.133632000	3.240906000	-0.358889000
H	-2.891539000	3.226918000	-1.416508000
C	-2.075934000	-2.455206000	0.564865000
C	-2.446492000	-3.797157000	0.585151000
H	-2.838916000	-4.238637000	1.496157000
C	-2.304700000	-4.550607000	-0.583552000
H	-2.594829000	-5.597182000	-0.601635000
C	-1.790586000	-3.935412000	-1.726436000
H	-1.663686000	-4.484283000	-2.653918000
C	-1.451676000	-2.582272000	-1.662817000
H	-1.030361000	-2.053304000	-2.509887000
C	-4.625504000	-0.750976000	-0.295232000
C	-5.796576000	-1.435145000	-0.626943000
H	-6.432743000	-1.832329000	0.158697000
C	-6.131259000	-1.593826000	-1.971285000

H	-7.038637000	-2.118558000	-2.255013000	O	0.841585000	-1.094606000	-1.946778000
C	-5.273928000	-1.073383000	-2.942884000	H	0.140415000	-0.430037000	-2.261649000
H	-5.486993000	-1.177266000	-4.001626000	O	0.076175000	0.518322000	0.447669000
C	-4.118805000	-0.420328000	-2.521215000	N	-2.352753000	2.397576000	0.236069000
H	-3.405962000	-0.030902000	-3.240302000	N	-1.922928000	-1.810248000	-0.512697000
C	-2.569790000	0.821306000	2.330010000	N	-3.946186000	0.090370000	-1.280842000
H	-3.069696000	0.694450000	3.301734000	C	-2.644828000	2.407833000	1.552344000
C	-2.162368000	-1.551663000	1.774681000	C	-3.041247000	3.569140000	2.210452000
H	-1.144672000	-1.292942000	2.083780000	H	-3.278050000	3.540190000	3.269784000
H	-2.671568000	-2.058821000	2.608119000	C	-3.132883000	4.758794000	1.481455000
C	-4.280880000	-0.488464000	1.157219000	H	-3.438539000	5.679101000	1.969974000
H	-4.807766000	0.423278000	1.461169000	C	-2.842574000	4.741067000	0.117139000
H	-4.674471000	-1.299492000	1.786088000	H	-2.912978000	5.639490000	-0.486949000
N	-2.834261000	-0.296271000	1.403862000	C	-2.458824000	3.533377000	-0.465952000
H	-1.484772000	0.848873000	2.484074000	H	-2.210392000	3.458228000	-1.520046000
H	5.673532000	3.748716000	-1.512450000	C	-2.493935000	-2.295725000	0.603926000
C	4.861486000	3.058930000	-1.302288000	C	-2.990801000	-3.594907000	0.679632000
C	4.539123000	2.731872000	0.018623000	H	-3.453329000	-3.946654000	1.596917000
C	4.140449000	2.473605000	-2.344767000	C	-2.879571000	-4.423482000	-0.440073000
C	3.497199000	1.838537000	0.253002000	H	-3.263368000	-5.439266000	-0.413597000
H	5.095012000	3.149953000	0.852429000	C	-2.275900000	-3.920756000	-1.594738000
H	4.370184000	2.692608000	-3.382160000	H	-2.171988000	-4.528738000	-2.487534000
C	3.112453000	1.585785000	-2.028278000	C	-1.819036000	-2.601901000	-1.589179000
N	2.798032000	1.293645000	-0.758429000	H	-1.339359000	-2.156591000	-2.453295000
C	3.077071000	1.388026000	1.636669000	C	-4.805015000	-0.274448000	-0.313108000
H	2.518645000	1.073845000	-2.778349000	C	-6.045459000	-0.844882000	-0.600287000
H	2.135906000	1.877013000	1.898677000	H	-6.709114000	-1.134585000	0.209111000
H	3.834131000	1.674087000	2.382126000	C	-6.415771000	-1.025432000	-1.933448000
N	2.828474000	-0.060671000	1.630880000	H	-7.378032000	-1.462577000	-2.182659000
N	3.434497000	-1.438602000	-0.716854000	C	-5.527823000	-0.636425000	-2.938344000
N	1.202829000	-2.142250000	1.041044000	H	-5.772906000	-0.756344000	-3.988416000
C	1.911174000	-0.521304000	2.689151000	C	-4.301935000	-0.092997000	-2.561427000
C	4.079026000	-0.849708000	1.570499000	H	-3.565641000	0.202098000	-3.303368000
C	4.423780000	-1.358436000	0.183274000	C	-2.498579000	1.073646000	2.256040000
C	3.691577000	-1.940653000	-1.936919000	H	-3.042566000	1.079166000	3.212377000
C	1.468950000	-1.927948000	2.346265000	C	-2.500678000	-1.342853000	1.778733000
C	0.900894000	-3.378938000	0.626457000	H	-1.469798000	-1.243124000	2.136282000
H	2.368123000	-0.494327000	3.689512000	H	-3.116968000	-1.739816000	2.599754000
H	1.045177000	0.149558000	2.667364000	C	-4.408981000	0.046283000	1.114544000
H	3.976823000	-1.720325000	2.229598000	H	-4.750029000	1.066857000	1.323812000
H	4.919789000	-0.264132000	1.966841000	H	-4.942430000	-0.614631000	1.812815000
C	5.722532000	-1.779427000	-0.108071000	N	-2.949012000	-0.005966000	1.357040000
C	4.954740000	-2.400653000	-2.301140000	H	-1.436137000	0.894291000	2.453097000
H	2.847825000	-1.939667000	-2.619164000	H	5.906614000	2.947552000	-2.042833000
C	1.397439000	-2.952709000	3.286678000	C	5.022004000	2.402095000	-1.727984000
C	0.819867000	-4.460621000	1.502727000	C	4.793622000	2.153234000	-0.371026000
H	0.711781000	-3.491068000	-0.435145000	C	4.099353000	1.943148000	-2.669907000
H	6.504122000	-1.690872000	0.641071000	C	3.653360000	1.446716000	-0.001501000
C	5.990961000	-2.314250000	-1.368046000	H	5.487773000	2.498342000	0.388660000
H	5.121763000	-2.804029000	-3.294423000	H	4.238867000	2.122466000	-3.730640000
H	1.625466000	-2.748298000	4.328286000	C	2.988187000	1.229302000	-2.222925000
C	1.059968000	-4.240452000	2.858928000	N	2.779203000	0.989154000	-0.919149000
H	0.575284000	-5.446953000	1.123873000	C	3.284782000	1.147245000	1.434599000
H	6.992442000	-2.651311000	-1.618780000	H	2.247113000	0.812449000	-2.896304000
H	1.007772000	-5.058616000	3.571168000	H	2.438890000	1.790228000	1.702708000
H	-1.707039000	1.083997000	-3.008426000	H	4.120533000	1.384208000	2.108530000
H	-0.773856000	3.299657000	1.413311000	N	2.859815000	-0.259142000	1.565039000
C	0.116547000	3.331825000	0.775061000	N	3.331208000	-1.798726000	-0.699938000
H	0.317996000	2.164237000	0.677765000	N	0.982158000	-2.176566000	1.194672000
C	1.191151000	4.091794000	1.350920000	C	1.933756000	-0.508810000	2.684955000
H	1.434313000	4.095622000	2.411575000	C	4.006645000	-1.195168000	1.565142000
C	1.867113000	4.975636000	0.363302000	C	4.331091000	-1.751991000	0.194671000
H	2.962528000	4.969912000	0.432591000	C	3.545019000	-2.354279000	-1.906293000
H	1.559580000	6.015818000	0.581718000	C	1.265245000	-1.852286000	2.475368000
C	-0.067338000	3.882705000	-0.660564000	C	0.436236000	-3.369464000	0.918175000
H	-0.364212000	3.098242000	-1.363133000	H	2.436451000	-0.480373000	3.662633000
H	-0.842070000	4.659496000	-0.651935000	H	1.173239000	0.277462000	2.649781000
C	1.306149000	4.504234000	-0.998381000	H	3.762616000	-2.043838000	2.215562000
H	1.966946000	3.742638000	-1.414669000	H	4.896314000	-0.717337000	1.997768000
H	1.234239000	5.318506000	-1.724939000	C	5.597505000	-2.260860000	-0.092430000
Ic-²P_{2Hhs-hs}				C	4.774804000	-2.902055000	-2.261524000
Fe	-1.806236000	0.439686000	-0.648399000	H	2.696071000	-2.327684000	-2.581146000
O	-0.967567000	0.731412000	-2.347028000	C	0.978536000	-2.720490000	3.525813000
Fe	1.455266000	-0.646867000	-0.305639000	C	0.124987000	-4.292897000	1.914777000
				H	0.237303000	-3.570480000	-0.128849000

H	6.388578000	-2.198840000	0.649001000
C	5.821374000	-2.849707000	-1.337685000
H	4.908580000	-3.346996000	-3.241885000
H	1.227616000	-2.437707000	4.543974000
C	0.393148000	-3.958072000	3.242171000
H	-0.314523000	-5.247599000	1.648494000
H	6.797968000	-3.255813000	-1.584057000
H	0.169130000	-4.654287000	4.045001000
H	-1.440415000	0.806559000	-3.186727000
H	-0.250113000	3.396195000	1.468217000
C	0.622762000	3.802343000	0.966097000
H	0.332735000	1.456743000	0.425683000
C	1.712713000	4.259854000	1.593618000
H	1.854682000	4.262864000	2.672185000
C	2.712255000	4.869549000	0.639355000
H	3.728084000	4.476386000	0.781711000
H	2.778025000	5.954468000	0.803424000
C	0.686993000	4.019667000	-0.531753000
H	0.455373000	3.114883000	-1.112095000
H	-0.053745000	4.773416000	-0.831903000
C	2.139277000	4.523575000	-0.765201000
H	2.734756000	3.734388000	-1.226304000
H	2.166947000	5.383904000	-1.439617000

II-²RC_{hs-hs}

Fe	1.596161000	-0.596549000	-0.651756000
O	1.247972000	-0.627620000	-2.256267000
Fe	-1.569268000	-0.383469000	-0.725121000
O	-1.306301000	-1.646280000	-2.025589000
H	-0.395323000	-1.514665000	-2.371896000
O	0.097943000	0.035487000	0.011653000
N	1.072725000	-2.691041000	-0.012596000
N	2.792136000	1.251604000	-0.343929000
N	3.551207000	-1.376386000	-1.009269000
C	1.068359000	-2.871145000	1.320030000
C	0.759839000	-4.103038000	1.892495000
H	0.782142000	-4.223918000	2.971228000
C	0.429459000	-5.168868000	1.050412000
H	0.194100000	-6.143690000	1.467600000
C	0.416350000	-4.967605000	-0.331214000
H	0.168053000	-5.770760000	-1.017041000
C	0.750261000	-3.705037000	-0.824085000
H	0.760588000	-3.486682000	-1.885947000
C	3.182945000	1.444119000	0.929245000
C	4.111602000	2.422669000	1.269848000
H	4.417447000	2.547730000	2.303840000
C	4.627919000	3.238178000	0.258008000
H	5.353802000	4.010404000	0.494720000
C	4.200827000	3.046179000	-1.056788000
H	4.577263000	3.660818000	-1.867663000
C	3.282700000	2.027931000	-1.317106000
H	2.927153000	1.809587000	-2.319710000
C	4.356557000	-1.590419000	0.045263000
C	5.697970000	-1.934246000	-0.118807000
H	6.327121000	-2.094953000	0.751573000
C	6.206799000	-2.072068000	-1.410409000
H	7.247901000	-2.340344000	-1.563017000
C	5.359286000	-1.859751000	-2.500855000
H	5.714678000	-1.958809000	-3.520935000
C	4.036309000	-1.505635000	-2.256672000
H	3.321009000	-1.306673000	-3.047976000
C	1.386432000	-1.635549000	2.133138000
H	1.711768000	-1.900237000	3.148719000
C	2.495595000	0.555530000	1.939494000
H	1.470226000	0.915314000	2.060503000
H	3.001800000	0.591950000	2.913815000
C	3.731922000	-1.511069000	1.419106000
H	3.598502000	-2.535495000	1.786635000
H	4.417316000	-1.015293000	2.118098000
N	2.407868000	-0.829620000	1.424760000
H	0.483125000	-1.020582000	2.190872000
H	-3.560121000	-3.126372000	4.272539000
C	-3.151562000	-2.660867000	3.380464000
C	-2.992578000	-1.272520000	3.321284000
C	-2.789267000	-3.436279000	2.277913000

C	-2.476561000	-0.703821000	2.159468000
H	-3.271028000	-0.639694000	4.158354000
H	-2.901833000	-4.515192000	2.284557000
C	-2.285634000	-2.792239000	1.148350000
N	-2.134448000	-1.462646000	1.099778000
C	-2.215758000	0.781861000	2.011030000
H	-1.990426000	-3.331587000	0.253552000
H	-1.141492000	0.953376000	2.140920000
H	-2.752855000	1.346550000	2.787108000
N	-2.562084000	1.240783000	0.654761000
N	-3.788079000	-0.596046000	-1.030253000
N	-1.668126000	1.409406000	-1.921930000
C	-1.857872000	2.473505000	0.242423000
C	-4.023050000	1.338452000	0.437009000
C	-4.618789000	0.145863000	-0.283550000
C	-4.281296000	-1.607377000	-1.766470000
C	-1.848997000	2.573536000	-1.268801000
C	-1.581248000	1.390752000	-3.259741000
H	-2.296833000	3.372881000	0.693253000
H	-0.823488000	2.387965000	0.584618000
H	-4.217411000	2.223845000	-0.180748000
H	-4.544929000	1.503400000	1.389553000
C	-5.989332000	-0.109530000	-0.232964000
C	-5.638787000	-1.917480000	-1.782998000
H	-3.544488000	-2.160981000	-2.339348000
C	-1.982470000	3.775866000	-1.958248000
C	-1.682488000	2.556697000	-4.017431000
H	-1.435656000	0.411644000	-3.703804000
H	-6.635368000	0.506395000	0.385839000
C	-6.507094000	-1.157172000	-0.995602000
H	-6.002288000	-2.736824000	-2.394206000
H	-2.153950000	4.698194000	-1.413109000
C	-1.893244000	3.766511000	-3.353813000
H	-1.610854000	2.510352000	-5.098840000
H	-7.570785000	-1.375246000	-0.976120000
H	-1.995564000	4.691540000	-3.913415000
H	0.533341000	6.142818000	0.730280000
H	-0.979783000	6.314437000	2.579365000
C	0.063329000	5.186626000	0.981573000
H	-0.617717000	4.946972000	0.158697000
C	-0.682619000	5.289512000	2.337085000
H	-1.598640000	4.681153000	2.317599000
C	0.296925000	4.686604000	3.359255000
H	-0.183812000	4.388478000	4.297359000
H	1.080358000	5.416393000	3.601328000
C	1.149714000	4.084185000	1.170221000
H	1.113953000	3.314998000	0.390168000
H	2.148180000	4.530473000	1.123706000
C	0.912523000	3.510477000	2.585361000
H	0.183230000	2.686387000	2.545201000
H	1.827238000	3.119313000	3.045823000

II-²TS_{Hhs-hs}

Fe	-1.729607000	0.122244000	-0.476052000
O	-1.314573000	0.574399000	-1.996047000
Fe	1.610808000	-0.016566000	-0.303168000
O	1.204358000	-0.306982000	-2.043243000
H	0.270809000	0.019323000	-2.215197000
O	-0.048277000	0.697783000	0.405146000
N	-3.113350000	1.664088000	0.558109000
N	-1.168158000	-2.068258000	-0.590529000
N	-3.562759000	-0.677725000	-1.120376000
C	-3.184817000	1.508339000	1.893670000
C	-3.960269000	2.337390000	2.699454000
H	-3.994523000	2.180202000	3.773336000
C	-4.705297000	3.353661000	2.092698000
H	-5.318393000	4.018222000	2.694037000
C	-4.674975000	3.476349000	0.703654000
H	-5.264279000	4.228758000	0.190213000
C	-3.864693000	2.604649000	-0.025329000
H	-3.802589000	2.661718000	-1.106253000
C	-1.478129000	-2.770320000	0.512894000
C	-1.645052000	-4.151700000	0.489928000
H	-1.905121000	-4.687569000	1.397759000
C	-1.477521000	-4.822731000	-0.726132000

H	-1.610053000	-5.899403000	-0.780848000
C	-1.152470000	-4.089226000	-1.868916000
H	-1.023925000	-4.573888000	-2.831401000
C	-1.013697000	-2.703695000	-1.756865000
H	-0.770997000	-2.070280000	-2.603993000
C	-4.332946000	-1.312037000	-0.219427000
C	-5.498887000	-1.979763000	-0.594679000
H	-6.095700000	-2.490992000	0.154956000
C	-5.881912000	-1.970531000	-1.935807000
H	-6.787798000	-2.479725000	-2.250900000
C	-5.081709000	-1.299364000	-2.863789000
H	-5.342894000	-1.266973000	-3.916237000
C	-3.923020000	-0.671960000	-2.415942000
H	-3.235952000	-0.150504000	-3.074470000
C	-2.413535000	0.320725000	2.425883000
H	-2.791672000	0.017678000	3.412770000
C	-1.637804000	-1.917205000	1.749518000
H	-0.666081000	-1.502303000	2.025094000
H	-2.026371000	-2.502665000	2.595174000
C	-3.927487000	-1.221883000	1.235528000
H	-4.596168000	-0.508035000	1.728930000
H	-4.088856000	-2.188552000	1.729679000
N	-2.517039000	-0.774237000	1.432032000
H	-1.349292000	0.567288000	2.504822000
H	5.251083000	4.800048000	-0.616293000
C	4.553649000	3.968902000	-0.572097000
C	4.193645000	3.416282000	0.662284000
C	4.015921000	3.431312000	-1.741877000
C	3.299971000	2.351349000	0.681967000
H	4.602351000	3.801329000	1.591390000
H	4.277913000	3.826346000	-2.717643000
C	3.125952000	2.362376000	-1.637512000
N	2.773666000	1.848119000	-0.451882000
C	2.828158000	1.674350000	1.951030000
H	2.672909000	1.891162000	-2.503445000
H	1.794458000	1.973383000	2.158922000
C	3.454298000	1.966634000	2.806418000
N	2.829921000	0.219509000	1.731130000
N	3.719051000	-0.744399000	-0.736145000
N	1.624469000	-1.968951000	0.747720000
C	1.978962000	-0.546844000	2.660222000
C	4.206099000	-0.326787000	1.635361000
C	4.649891000	-0.672909000	0.224482000
C	4.077293000	-1.091123000	-1.985029000
C	1.824972000	-1.937378000	2.080759000
C	1.617646000	-3.145538000	0.107605000
H	2.393979000	-0.593799000	3.677489000
H	1.008206000	-0.038613000	2.693143000
H	4.271080000	-1.237561000	2.242876000
H	4.920788000	0.381729000	2.073901000
C	5.994143000	-0.948428000	-0.034461000
C	5.393622000	-1.394283000	-2.321301000
H	3.268434000	-1.103300000	-2.708499000
C	1.961321000	-3.104134000	2.828185000
C	1.762418000	-4.356894000	0.780861000
H	1.485011000	-3.097518000	-0.966600000
H	6.727962000	-0.874570000	0.763089000
C	6.370927000	-1.318192000	-1.325202000
H	5.645095000	-1.672997000	-3.339227000
H	2.125019000	-3.045745000	3.899856000
C	1.920006000	-4.335879000	2.167342000
H	1.752448000	-5.289049000	0.226781000
H	7.410141000	-1.538189000	-1.550943000
H	2.035087000	-5.260510000	2.725191000
H	0.372252000	2.428416000	-1.814065000
C	0.162683000	3.381914000	-1.320650000
C	0.115358000	3.262878000	0.200152000
H	1.068758000	3.383258000	0.713280000
C	-1.001129000	4.162704000	0.729203000
H	-0.604873000	4.880841000	1.458345000
H	-1.773686000	3.595050000	1.253934000
C	-1.213488000	3.941423000	-1.705473000
H	-1.201470000	4.465874000	-2.666503000
H	-1.903727000	3.098065000	-1.792482000
C	-1.577340000	4.865986000	-0.529361000

H	-1.077204000	5.833139000	-0.661080000
H	-2.650593000	5.061477000	-0.444078000
H	0.962761000	4.089097000	-1.589770000
H	-0.071279000	1.956737000	0.404018000

II-²Int_{hs-hs}

Fe	-1.683432000	0.025642000	-0.574915000
O	-1.159679000	0.491528000	-2.144571000
Fe	1.698583000	-0.324521000	-0.324815000
O	1.161725000	-0.630491000	-2.012038000
H	0.268934000	-0.178720000	-2.240374000
O	0.068577000	0.362738000	0.593869000
N	-2.718164000	1.728522000	0.323700000
N	-1.289857000	-2.161333000	-0.498415000
N	-3.685387000	-0.726100000	-1.134453000
C	-3.118082000	1.618571000	1.607124000
C	-4.011961000	2.524056000	2.171923000
H	-4.323277000	2.406701000	3.205364000
C	-4.510423000	3.564614000	1.379972000
H	-5.216650000	4.277718000	1.794640000
C	-4.096286000	3.666417000	0.052119000
H	-4.463012000	4.455095000	-0.596037000
C	-3.194022000	2.722034000	-0.438601000
H	-2.835757000	2.733908000	-1.462821000
C	-1.644308000	-2.798764000	0.633333000
C	-1.821815000	-4.178874000	0.669310000
H	-2.115345000	-4.664633000	1.594820000
C	-1.632100000	-4.913155000	-0.506080000
H	-1.781142000	-5.989163000	-0.509517000
C	-1.262480000	-4.244759000	-1.674451000
H	-1.114393000	-4.778103000	-2.607788000
C	-1.102413000	-2.858804000	-1.626916000
H	-0.814880000	-2.273265000	-2.493818000
C	-4.474392000	-1.313461000	-0.223098000
C	-5.638770000	-1.989055000	-0.592171000
H	-6.256296000	-2.462358000	0.165844000
C	-5.992320000	-2.037205000	-1.940950000
H	-6.895506000	-2.554120000	-2.251725000
C	-5.168908000	-1.415296000	-2.883881000
H	-5.409241000	-1.431483000	-3.941702000
C	-4.016134000	-0.775296000	-2.438046000
H	-3.310053000	-0.290453000	-3.105807000
C	-2.570145000	0.413741000	2.346044000
H	-3.084311000	0.286373000	3.310329000
C	-1.837876000	-1.901148000	1.838371000
H	-0.863882000	-1.489803000	2.121995000
H	-2.243810000	-2.475838000	2.685166000
C	-4.101993000	-1.161856000	1.242637000
H	-4.756500000	-0.392128000	1.670167000
H	-4.334429000	-2.093063000	1.778226000
N	-2.696940000	-0.766642000	1.472175000
H	-1.500555000	0.559742000	2.529318000
H	4.717111000	4.824926000	-0.957362000
C	4.102515000	3.937274000	-0.840730000
C	3.958420000	3.342308000	0.417535000
C	3.456863000	3.372504000	-1.941432000
C	3.172332000	2.200700000	0.532617000
H	4.454059000	3.751912000	1.292195000
H	3.547947000	3.803322000	-2.932822000
C	2.681879000	2.230284000	-1.745638000
N	2.544831000	1.669100000	-0.535064000
C	2.929100000	1.490379000	1.849754000
H	2.155983000	1.730518000	-2.552563000
H	1.932357000	1.756722000	2.218271000
H	3.661461000	1.814914000	2.602781000
N	2.947448000	0.029564000	1.658715000
N	3.799419000	-0.843489000	-0.847130000
N	1.692571000	-2.205106000	0.787951000
C	2.147829000	-0.719819000	2.648733000
C	4.321068000	-0.506066000	1.516059000
C	4.760573000	-0.683395000	0.076237000
C	4.137852000	-1.084028000	-2.126746000
C	1.909339000	-2.118517000	2.117359000
C	1.555772000	-3.408845000	0.213747000
H	2.629298000	-0.761472000	3.636325000

H	1.188460000	-0.199881000	2.738952000
H	4.359510000	-1.491224000	1.996470000
H	5.040546000	0.127736000	2.051938000
C	6.113444000	-0.751679000	-0.255503000
C	5.465677000	-1.186632000	-2.533205000
H	3.303617000	-1.175442000	-2.814807000
C	1.953049000	-3.253970000	2.922632000
C	1.595819000	-4.590300000	0.950694000
H	1.404614000	-3.405232000	-0.859349000
H	6.868956000	-0.608116000	0.511333000
C	6.471355000	-1.011331000	-1.579395000
H	5.701724000	-1.386982000	-3.572940000
H	2.137930000	-3.155301000	3.987886000
C	1.786539000	-4.509506000	2.330970000
H	1.484849000	-5.545598000	0.449800000
H	7.518246000	-1.071223000	-1.861794000
H	1.827859000	-5.409617000	2.937190000
H	0.075204000	1.340363000	0.638709000
H	-0.084881000	3.209191000	-1.405471000
C	0.107769000	4.072423000	-0.748242000
C	0.050072000	3.730655000	0.716219000
H	0.867375000	3.222356000	1.217569000
C	-0.893700000	4.633445000	1.457696000
H	-0.508361000	4.947333000	2.436440000
H	-1.856411000	4.133581000	1.647652000
C	-0.941467000	5.201131000	-0.923823000
H	-0.635542000	5.937570000	-1.673256000
H	-1.894468000	4.779537000	-1.256622000
C	-1.098372000	5.819619000	0.481482000
H	-0.310045000	6.563261000	0.648679000
H	-2.062107000	6.321471000	0.619267000
H	1.112658000	4.437647000	-1.010174000

II-²TS_{Rebhs-hs}

Fe	-1.887225000	0.242943000	-0.442999000
O	-1.472438000	0.885536000	-1.882802000
Fe	1.661402000	-0.081260000	-0.232825000
O	1.102412000	-0.152243000	-1.985403000
H	0.192923000	0.209761000	-2.115873000
O	-0.056312000	0.746343000	0.522604000
N	-3.058527000	1.773314000	0.735000000
N	-1.289580000	-1.907876000	-0.737219000
N	-3.706800000	-0.500979000	-1.197237000
C	-3.217710000	1.493453000	2.042830000
C	-3.938439000	2.325228000	2.897213000
H	-4.053530000	2.065944000	3.945483000
C	-4.529085000	3.477953000	2.369684000
H	-5.099823000	4.143513000	3.010311000
C	-4.401754000	3.740310000	1.004813000
H	-4.871608000	4.606562000	0.550801000
C	-3.657109000	2.856696000	0.222627000
H	-3.516267000	3.013004000	-0.841141000
C	-1.704756000	-2.714309000	0.255478000
C	-1.890457000	-4.082096000	0.077313000
H	-2.233732000	-4.699284000	0.902020000
C	-1.616989000	-4.633658000	-1.178363000
H	-1.755520000	-5.696557000	-1.353857000
C	-1.169261000	-3.796714000	-2.202364000
H	-0.945981000	-4.186272000	-3.190296000
C	-1.028545000	-2.431074000	-1.941371000
H	-0.685167000	-1.729041000	-2.692310000
C	-4.486620000	-1.214446000	-0.366355000
C	-5.601302000	-1.915495000	-0.824097000
H	-6.205283000	-2.490484000	-0.128455000
C	-5.924868000	-1.854975000	-2.180298000
H	-6.790271000	-2.388665000	-2.561660000
C	-5.118781000	-1.100597000	-3.035677000
H	-5.335662000	-1.026455000	-4.096081000
C	-4.010580000	-0.444924000	-2.505257000
H	-3.319604000	0.138383000	-3.105205000
C	-2.619072000	0.170822000	2.487926000
H	-3.121790000	-0.193602000	3.395524000
C	-1.901440000	-2.006945000	1.575221000
H	-0.920833000	-1.675668000	1.931263000
H	-2.348235000	-2.672562000	2.327366000

C	-4.150001000	-1.147720000	1.105518000
H	-4.783912000	-0.375740000	1.555620000
H	-4.403875000	-2.093095000	1.602828000
N	-2.723406000	-0.793816000	1.370401000
H	-1.553572000	0.277719000	2.721826000
H	5.836617000	4.280403000	-1.002181000
C	5.035565000	3.561226000	-0.859516000
C	4.718863000	3.103500000	0.424147000
C	4.320736000	3.067577000	-1.951775000
C	3.689122000	2.178358000	0.565976000
H	5.265914000	3.450269000	1.295684000
H	4.547787000	3.385864000	-2.963970000
C	3.303169000	2.140115000	-1.721721000
N	2.989691000	1.720033000	-0.488046000
C	3.266917000	1.601223000	1.901291000
H	2.713772000	1.695530000	-2.517864000
H	2.321301000	2.057045000	2.223135000
H	4.017508000	1.823435000	2.674744000
N	3.034991000	0.156665000	1.754145000
N	3.623926000	-1.012236000	-0.739649000
N	1.492710000	-1.954941000	1.059079000
C	2.183948000	-0.427685000	2.803819000
C	4.307702000	-0.588508000	1.578455000
C	4.632945000	-0.957639000	0.141549000
C	3.870905000	-1.388261000	-2.006898000
C	1.785046000	-1.822726000	2.369344000
C	1.260100000	-3.179759000	0.570047000
H	2.678955000	-0.460404000	3.786245000
H	1.295766000	0.210451000	2.895199000
H	4.251589000	-1.519221000	2.155374000
H	5.142504000	-0.016113000	2.004988000
C	5.941738000	-1.283420000	-0.217998000
C	5.144764000	-1.747135000	-2.440345000
H	3.009018000	-1.366276000	-2.666493000
C	1.799960000	-2.909485000	3.240053000
C	1.268437000	-4.323145000	1.370087000
H	1.054460000	-3.236671000	-0.493178000
H	6.739928000	-1.219380000	0.516019000
C	6.200507000	-1.690433000	-1.527112000
H	5.304656000	-2.050028000	-3.469848000
H	2.046944000	-2.762409000	4.287111000
C	1.526613000	-4.183819000	2.733004000
H	1.077538000	-5.294179000	0.926345000
H	7.210147000	-1.951203000	-1.830442000
H	1.541747000	-5.050364000	3.387399000
H	-0.154804000	1.127405000	1.406497000
H	0.458286000	2.309224000	-1.774103000
C	0.359832000	3.320606000	-1.358884000
C	0.348462000	3.309611000	0.111152000
H	1.147112000	2.877329000	0.692366000
C	-0.671506000	4.225683000	0.678685000
H	-0.241771000	4.880877000	1.451542000
H	-1.453937000	3.644308000	1.189170000
C	-0.934644000	4.058340000	-1.756422000
H	-0.830875000	4.615016000	-2.692114000
H	-1.711837000	3.302150000	-1.893623000
C	-1.233933000	4.983449000	-0.554241000
H	-0.696546000	5.932047000	-0.665877000
H	-2.296586000	5.218847000	-0.445094000
H	1.266743000	3.871499000	-1.679506000

II-²P_{Rebhs-hs}

Fe	-3.074326000	0.279092000	0.532009000
O	-1.730252000	1.314676000	0.685455000
N	-4.651302000	1.650563000	0.029123000
N	-2.741538000	-1.363981000	1.877706000
N	-2.600902000	-1.144612000	-1.017410000
C	-5.935790000	1.239349000	-0.002834000
C	-6.956951000	2.067970000	-0.459729000
H	-7.979869000	1.704922000	-0.484232000
C	-6.640408000	3.364809000	-0.872269000
H	-7.420856000	4.030428000	-1.228658000
C	-5.311640000	3.791344000	-0.821391000
H	-5.027120000	4.791377000	-1.130355000
C	-4.343084000	2.901198000	-0.366561000

H	-3.292176000	3.157843000	-0.303902000
C	-3.612069000	-2.391205000	1.888893000
C	-3.285135000	-3.618330000	2.463800000
H	-4.007016000	-4.429644000	2.455016000
C	-2.026489000	-3.780147000	3.044249000
H	-1.753594000	-4.726566000	3.501975000
C	-1.122965000	-2.716036000	3.013695000
H	-0.127653000	-2.807692000	3.435210000
C	-1.513328000	-1.523003000	2.412649000
H	-0.832358000	-0.688099000	2.291357000
C	-3.605570000	-1.919317000	-1.472305000
C	-3.362915000	-3.023331000	-2.285632000
H	-4.190134000	-3.631922000	-2.637278000
C	-2.042622000	-3.328379000	-2.630131000
H	-1.830059000	-4.182902000	-3.266132000
C	-1.007913000	-2.536603000	-2.129421000
H	0.032467000	-2.756452000	-2.347000000
C	-1.324702000	-1.451070000	-1.312371000
H	-0.561277000	-0.838618000	-0.827405000
C	-6.211052000	-0.141449000	0.555857000
H	-7.139839000	-0.548127000	0.128865000
C	-4.996343000	-2.161665000	1.305338000
H	-5.674874000	-1.947796000	2.139694000
H	-5.357183000	-3.093360000	0.847994000
C	-5.000361000	-1.493343000	-1.067250000
H	-5.295740000	-0.642972000	-1.694503000
H	-5.718175000	-2.306284000	-1.250363000
N	-5.059765000	-1.041339000	0.343080000
H	-6.365717000	-0.043075000	1.636783000
O	2.585819000	2.690171000	0.193715000
H	2.830543000	2.922299000	1.104357000
H	0.420302000	1.906161000	-1.012856000
C	0.635565000	2.940642000	-1.296990000
C	1.484029000	3.560322000	-0.190259000
H	1.918512000	4.512421000	-0.521793000
C	0.476709000	3.784320000	0.937393000
H	0.849908000	4.450271000	1.725168000
H	0.228913000	2.808624000	1.371476000
C	-0.669097000	3.770147000	-1.250609000
H	-0.639994000	4.584805000	-1.982234000
H	-1.524351000	3.133556000	-1.495397000
C	-0.758945000	4.342530000	0.201406000
H	-0.736585000	5.437436000	0.181143000
H	-1.670372000	4.032483000	0.718469000
H	1.127154000	2.944604000	-2.274544000
Fe	2.422992000	0.453018000	0.200259000
O	0.658399000	-0.019411000	0.631665000
H	-0.088995000	0.617977000	0.683570000
C	3.374597000	-0.311572000	-5.757126000
C	3.165732000	-0.091912000	-4.714248000
C	4.188659000	0.326818000	-3.861547000
C	1.873150000	-0.221286000	-4.202345000
C	3.885703000	0.602585000	-2.528447000
H	5.206546000	0.444440000	-4.220643000
H	1.046230000	-0.537388000	-4.829919000
C	1.660695000	0.066978000	-2.855645000
N	2.641120000	0.468621000	-2.035550000
C	4.917532000	1.143576000	-1.563105000
H	0.677312000	-0.014871000	-2.405735000
H	4.731536000	2.217541000	-1.452158000
H	5.931721000	1.010206000	-1.969079000
N	4.779674000	0.535653000	-0.228095000
N	3.022171000	-1.671386000	-0.099125000
N	3.439751000	0.698595000	2.161901000
C	5.362507000	1.366415000	0.842849000
C	5.305372000	-0.846565000	-0.179048000
C	4.277556000	-1.910959000	-0.508044000
C	2.085364000	-2.618836000	-0.256486000
C	4.751252000	1.006487000	2.184255000
C	2.811491000	0.412121000	3.312730000
H	6.458509000	1.281507000	0.886985000
H	5.122194000	2.410387000	0.613188000
H	5.640609000	-1.038087000	0.847779000
H	6.186948000	-0.952665000	-0.828114000
C	4.638433000	-3.114369000	-1.116236000

C	2.365742000	-3.854754000	-0.836684000
H	1.095778000	-2.340445000	0.093639000
C	5.482093000	1.026505000	3.371036000
C	3.466534000	0.422227000	4.543111000
H	1.757390000	0.168749000	3.211285000
H	5.661120000	-3.272567000	-1.445421000
C	3.666925000	-4.102516000	-1.282311000
H	1.584437000	-4.601621000	-0.937888000
H	6.540593000	1.267909000	3.352979000
C	4.827734000	0.733820000	4.570564000
H	2.924366000	0.188133000	5.453355000
H	3.922607000	-5.049269000	-1.749216000
H	5.373767000	0.744217000	5.509050000

III-²TS_{Hhs-hs}

Fe	1.638886000	-0.466271000	0.069676000
O	1.098243000	-0.933226000	1.571814000
Fe	-1.549269000	0.315550000	0.009495000
O	-1.012566000	0.557248000	1.935896000
H	-0.164709000	0.005500000	1.935743000
O	0.162529000	-0.142443000	-0.753938000
N	2.084401000	1.700040000	0.495505000
N	2.079251000	-2.291853000	-1.115696000
N	3.680121000	-0.629708000	0.715508000
C	2.518930000	2.396800000	-0.566770000
C	2.986507000	3.703518000	-0.444001000
H	3.340715000	4.241835000	-1.317820000
C	2.997497000	4.293366000	0.823571000
H	3.367474000	5.306402000	0.951856000
C	2.538059000	3.562524000	1.920710000
H	2.537203000	3.985868000	2.919860000
C	2.089023000	2.258425000	1.709902000
H	1.724074000	1.630355000	2.516665000
C	2.353440000	-2.061088000	-2.412469000
C	2.639449000	-3.099310000	-3.295991000
H	2.874327000	-2.884268000	-4.334125000
C	2.621343000	-4.412508000	-2.815992000
H	2.842438000	-5.241198000	-3.482046000
C	2.327332000	-4.643162000	-1.470820000
H	2.309963000	-5.647767000	-1.061514000
C	2.065021000	-3.546450000	-0.649283000
H	1.837925000	-3.654973000	0.407212000
C	4.656603000	-0.236203000	-0.118015000
C	5.988037000	-0.173657000	0.293668000
H	6.755583000	0.156007000	-0.400324000
C	6.309321000	-0.544492000	1.599195000
H	7.339121000	-0.506812000	1.941665000
C	5.287919000	-0.960476000	2.457471000
H	5.494981000	-1.256043000	3.480495000
C	3.982368000	-0.980526000	1.977380000
H	3.128996000	-1.265011000	2.584534000
C	2.412858000	1.668544000	-1.888963000
H	3.010173000	2.167224000	-2.665110000
C	2.296226000	-0.606410000	-2.832777000
H	1.248221000	-0.330925000	-2.986902000
H	2.852758000	-0.442629000	-3.766159000
C	4.267590000	0.082460000	-1.544285000
H	4.799021000	0.979986000	-1.885440000
H	4.611475000	-0.742316000	-2.180095000
N	2.801350000	0.248933000	-1.734703000
H	1.361706000	1.676877000	-2.188672000
H	-0.299363000	6.111008000	-1.396824000
C	-0.532889000	5.090222000	-1.108476000
C	-0.871778000	4.144328000	-2.079673000
C	-0.514064000	4.708621000	0.234089000
C	-1.174523000	2.845017000	-1.673908000
H	-0.910543000	4.409579000	-3.132179000
H	-0.261090000	5.414917000	1.017463000
C	-0.840198000	3.391548000	0.556490000
N	-1.160800000	2.486448000	-0.377356000
C	-1.492079000	1.744640000	-2.671202000
H	-0.844322000	3.022598000	1.576860000
H	-0.566014000	1.209393000	-2.904836000
H	-1.881572000	2.176149000	-3.605618000
N	-2.413924000	0.758321000	-2.082937000

N	-3.701168000	0.745715000	0.410597000
N	-2.454444000	-1.663545000	-0.596383000
C	-2.369240000	-0.550838000	-2.759536000
C	-3.787341000	1.294026000	-1.964410000
C	-4.481294000	0.917186000	-0.670906000
C	-4.276964000	0.518406000	1.601986000
C	-2.884313000	-1.667688000	-1.875036000
C	-2.800957000	-2.681481000	0.203415000
H	-2.920174000	-0.532954000	-3.711899000
H	-1.315376000	-0.763659000	-2.971905000
H	-4.399731000	0.992754000	-2.826254000
H	-3.724021000	2.388807000	-1.987838000
C	-5.871918000	0.844099000	-0.595396000
C	-5.657813000	0.446183000	1.767594000
H	-3.596995000	0.387822000	2.435686000
C	-3.694808000	-2.682139000	-2.379660000
C	-3.598861000	-3.742802000	-0.225553000
H	-2.420846000	-2.641734000	1.216611000
H	-6.471723000	0.978325000	-1.490611000
C	-6.470005000	0.604979000	0.642807000
H	-6.081031000	0.263914000	2.749766000
H	-4.028564000	-2.644551000	-3.412177000
C	-4.061318000	-3.738061000	-1.540857000
H	-3.852076000	-4.543777000	0.461126000
H	-7.550981000	0.544960000	0.727403000
H	-4.694687000	-4.539232000	-1.910017000
H	-1.522726000	0.108259000	2.966787000
C	-1.806129000	-0.443649000	4.142989000
H	-2.472040000	0.292233000	4.605938000
C	-0.424032000	-0.639777000	4.768222000
H	-0.438070000	-0.389614000	5.836912000
C	-0.076920000	-2.135833000	4.524350000
H	-0.209795000	-2.700922000	5.453997000
H	0.955495000	-2.274067000	4.189506000
C	-2.363309000	-1.816243000	3.813811000
H	-2.844437000	-2.240216000	4.710605000
H	-3.124346000	-1.799341000	3.023187000
C	-1.094918000	-2.620063000	3.470823000
H	-1.250652000	-3.704172000	3.494584000
H	-0.731163000	-2.337140000	2.474633000
H	0.315106000	0.025979000	4.301953000

III-²Int_{hs-hs}

Fe	1.665961000	-0.442094000	0.058022000
O	1.093975000	-1.045932000	1.508841000
Fe	-1.537635000	0.341140000	-0.070469000
O	-0.972611000	0.378426000	1.983688000
H	-0.137713000	-0.209080000	1.923998000
O	0.217358000	-0.059694000	-0.774653000
N	2.075217000	1.687469000	0.673926000
N	2.182937000	-2.151228000	-1.272658000
N	3.696740000	-0.662956000	0.718178000
C	2.489835000	2.487454000	-0.321598000
C	2.910830000	3.793926000	-0.083697000
H	3.251467000	4.416417000	-0.905427000
C	2.894140000	4.273627000	1.229568000
H	3.227897000	5.284120000	1.446695000
C	2.454950000	3.436293000	2.256720000
H	2.434370000	3.772043000	3.288412000
C	2.053271000	2.140060000	1.931528000
H	1.705228000	1.433061000	2.678168000
C	2.517007000	-1.802353000	-2.528011000
C	2.893097000	-2.750899000	-3.476195000
H	3.173141000	-2.440253000	-4.478284000
C	2.904719000	-4.099522000	-3.107564000
H	3.195639000	-4.860240000	-3.825840000
C	2.548260000	-4.453516000	-1.805026000
H	2.550460000	-5.489075000	-1.481491000
C	2.196360000	-3.440300000	-0.912567000
H	1.917620000	-3.645846000	0.116835000
C	4.691008000	-0.205939000	-0.058687000
C	6.022370000	-0.249086000	0.357759000
H	6.805906000	0.132902000	-0.290151000
C	6.322439000	-0.790307000	1.607025000
H	7.351334000	-0.836868000	1.951150000

C	5.280952000	-1.267841000	2.407641000
H	5.471251000	-1.695072000	3.386460000
C	3.978873000	-1.180268000	1.926923000
H	3.111893000	-1.510704000	2.489899000
C	2.422985000	1.868678000	-1.700704000
H	3.010715000	2.449897000	-2.425162000
C	2.419797000	-0.321440000	-2.828550000
H	1.366687000	-0.069996000	-2.990355000
H	2.994575000	-0.061969000	-3.728681000
C	4.329066000	0.330910000	-1.426870000
H	4.815696000	1.302882000	-1.577456000
H	4.748321000	-0.344326000	-2.182814000
N	2.863916000	0.456995000	-1.650988000
H	1.375364000	1.860202000	-2.015341000
H	-0.401969000	6.240688000	-0.952138000
C	-0.615080000	5.194745000	-0.751460000
C	-0.949931000	4.331371000	-1.798214000
C	-0.572604000	4.698268000	0.552445000
C	-1.226169000	2.996537000	-1.504967000
H	-1.004935000	4.686939000	-2.822935000
H	-0.320341000	5.337445000	1.391631000
C	-0.874467000	3.352889000	0.761736000
N	-1.192273000	2.527288000	-0.243802000
C	-1.535635000	1.980125000	-2.591854000
H	-0.858427000	2.897291000	1.746477000
H	-0.601857000	1.480282000	-2.872903000
H	-1.934064000	2.485248000	-3.484761000
N	-2.442155000	0.934013000	-2.087099000
N	-3.711130000	0.668818000	0.419812000
N	-2.411665000	-1.600776000	-0.813738000
C	-2.399222000	-0.310792000	-2.876859000
C	-3.817884000	1.440518000	-1.893860000
C	-4.495554000	0.904443000	-0.647942000
C	-4.285347000	0.289836000	1.572583000
C	-2.873405000	-1.508838000	-2.077038000
C	-2.724922000	-2.680891000	-0.086026000
H	-2.978549000	-0.220269000	-3.807929000
H	-1.349754000	-0.487185000	-3.139909000
H	-4.437005000	1.237191000	-2.779372000
H	-3.762090000	2.530724000	-1.788091000
C	-5.880641000	0.749107000	-0.596755000
C	-5.661200000	0.125196000	1.714517000
H	-3.613992000	0.108848000	2.405548000
C	-3.681967000	-2.493101000	-2.641108000
C	-3.518963000	-3.717534000	-0.577972000
H	-2.322662000	-2.708803000	0.920015000
H	-6.480339000	0.940162000	-1.481634000
C	-6.474248000	0.353720000	0.602922000
H	-6.078529000	-0.179902000	2.668362000
H	-4.042636000	-2.380924000	-3.659098000
C	-4.011937000	-3.616970000	-1.878706000
H	-3.746340000	-4.573468000	0.048874000
H	-7.550797000	0.226882000	0.667696000
H	-4.642491000	-4.397056000	-2.294878000
H	-1.520563000	-0.018996000	2.695244000
C	-2.165623000	-0.998751000	4.367978000
H	-2.905389000	-0.303702000	4.760072000
C	-0.748519000	-1.056176000	4.879568000
H	-0.696271000	-0.897165000	5.965800000
C	-0.247822000	-2.463086000	4.456209000
H	-0.391992000	-3.166219000	5.284753000
H	0.812417000	-2.467358000	4.185199000
C	-2.528707000	-2.271291000	3.655929000
H	-3.051286000	-2.955915000	4.348239000
H	-3.209757000	-2.123794000	2.805417000
C	-1.152857000	-2.862117000	3.272313000
H	-1.184169000	-3.944543000	3.107191000
H	-0.772002000	-2.384494000	2.360561000
H	-0.124979000	-0.265076000	4.430309000

III-²TS_{2H_{hs}-hs}

Fe	-1.536905000	0.040302000	-0.088702000
O	-1.217907000	-0.574199000	-1.673402000
Fe	1.747795000	0.170093000	-0.295102000
O	1.129895000	-0.030706000	-2.342802000

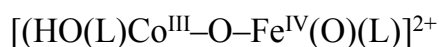
H	0.113894000	-0.214903000	-2.154502000
O	0.041595000	0.074998000	0.577398000
N	-1.627799000	2.216802000	-0.739802000
N	-2.258610000	-1.572196000	1.363198000
N	-3.615805000	0.171708000	-0.552002000
C	-1.813496000	3.068403000	0.280898000
C	-2.053893000	4.424903000	0.071598000
H	-2.211091000	5.089904000	0.915498000
C	-2.096291000	4.901204000	-1.242302000
H	-2.290588000	5.952004000	-1.437002000
C	-1.898794000	4.009403000	-2.298102000
H	-1.933193000	4.341403000	-3.330702000
C	-1.671398000	2.665002000	-1.998302000
H	-1.524800000	1.911602000	-2.767002000
C	-2.293408000	-1.141196000	2.636498000
C	-2.658811000	-1.977895000	3.690098000
H	-2.692910000	-1.593595000	4.705298000
C	-2.985215000	-3.307494000	3.409798000
H	-3.274617000	-3.981393000	4.210698000
C	-2.951516000	-3.748594000	2.085898000
H	-3.212019000	-4.768993000	1.823998000
C	-2.587213000	-2.840195000	1.092098000
H	-2.558214000	-3.120795000	0.046798000
C	-4.423003000	0.799410000	0.318198000
C	-5.771502000	1.020814000	0.035598000
H	-6.398501000	1.539316000	0.754998000
C	-6.291704000	0.564116000	-1.174802000
H	-7.338603000	0.722719000	-1.415702000
C	-5.445705000	-0.093887000	-2.071902000
H	-5.810006000	-0.460886000	-3.025602000
C	-4.109106000	-0.261691000	-1.725302000
H	-3.378507000	-0.731093000	-2.376202000
C	-1.694698000	2.448602000	1.656398000
H	-2.106796000	3.115104000	2.427198000
C	-1.894504000	0.305003000	2.843898000
H	-0.802304000	0.368000000	2.860298000
H	-2.293703000	0.689904000	3.793098000
C	-3.831102000	1.220709000	1.644598000
H	-4.146599000	2.244609000	1.881898000
H	-4.254404000	0.577710000	2.425498000
N	-2.345702000	1.118404000	1.692798000
H	-0.633399000	2.285499000	1.859998000
H	1.692412000	6.170893000	0.687998000
C	1.699509000	5.108593000	0.462098000
C	1.955207000	4.175792000	1.471298000
C	1.469808000	4.656793000	-0.838302000
C	1.964803000	2.819292000	1.147098000
H	2.152408000	4.493492000	2.490998000
H	1.272710000	5.348394000	-1.650202000
C	1.510804000	3.283493000	-1.079602000
N	1.748302000	2.391093000	-0.111102000
C	2.168300000	1.744691000	2.204598000
H	1.346303000	2.867894000	-2.069202000
H	1.184499000	1.379694000	2.517098000
H	2.673601000	2.170190000	3.084898000
N	2.887196000	0.585189000	1.650398000
N	3.892196000	0.371487000	-0.959302000
N	2.507789000	-1.878009000	0.302598000
C	2.678493000	-0.663410000	2.405998000
C	4.314397000	0.873985000	1.397998000
C	4.802196000	0.443484000	0.026598000
C	4.307495000	0.120085000	-2.211802000
C	2.996189000	-1.882511000	1.559798000
C	2.720386000	-2.946010000	-0.475902000
H	3.268193000	-0.682512000	3.335198000
H	1.614393000	-0.704907000	2.664598000
H	4.945596000	0.426284000	2.178398000
H	4.460100000	1.959485000	1.463898000
C	6.161395000	0.229080000	-0.207002000
C	5.645695000	-0.087118000	-2.535102000
H	3.528495000	0.098488000	-2.967502000
C	3.715586000	-2.963113000	2.067798000
C	3.419483000	-4.073712000	-0.044802000
H	2.310787000	-2.892709000	-1.480102000
H	6.868496000	0.283878000	0.615498000

C	6.590095000	-0.042521000	-1.506302000
H	5.936594000	-0.281419000	-3.562102000
H	4.101286000	-2.928014000	3.082198000
C	3.928883000	-4.078914000	1.254198000
H	3.565081000	-4.915612000	-0.713702000
H	7.642694000	-0.211224000	-1.713202000
H	4.487781000	-4.932115000	1.626898000
H	1.431792000	-0.829906000	-2.801602000
C	-0.513917000	-4.200601000	-1.285602000
H	0.250382000	-4.333903000	-0.525602000
C	-0.495614000	-3.159201000	-2.297002000
H	0.495886000	-2.926704000	-2.714702000
C	-1.569715000	-3.572298000	-3.327502000
H	-1.134817000	-4.241499000	-4.080502000
H	-2.003913000	-2.711497000	-3.845902000
C	-1.712620000	-5.085397000	-1.430502000
H	-1.397122000	-6.063898000	-1.834702000
H	-2.221520000	-5.306896000	-0.481702000
C	-2.592618000	-4.338895000	-2.464302000
H	-3.230019000	-5.012793000	-3.043702000
H	-3.245415000	-3.621093000	-1.948202000
H	-0.832411000	-2.139700000	-1.843602000

III- $^{212}\text{Pb}_{\text{hs-hs}}$

Fe	1.574956000	0.107638000	-0.004391000
O	1.374663000	1.065906000	-1.669164000
Fe	-1.678172000	-0.117279000	-0.134961000
O	-0.994099000	0.159361000	-2.211144000
H	-0.024384000	0.474033000	-2.088966000
O	-0.039733000	0.073592000	0.742428000
N	1.437696000	-1.922336000	-0.886321000
N	2.499780000	1.389800000	1.512132000
N	3.741775000	-0.324078000	-0.592204000
C	1.589862000	-2.938045000	-0.017173000
C	1.694794000	-4.257026000	-0.450252000
H	1.827599000	-5.056455000	0.272060000
C	1.633348000	-4.523276000	-1.821326000
H	1.721943000	-5.542620000	-2.185627000
C	1.471477000	-3.462619000	-2.714336000
H	1.430094000	-3.627098000	-3.786000000
C	1.385891000	-2.167950000	-2.200857000
H	1.280512000	-1.296804000	-2.839206000
C	2.603960000	0.842789000	2.739691000
C	3.163620000	1.545620000	3.804043000
H	3.249453000	1.075631000	4.778952000
C	3.617283000	2.850240000	3.589041000
H	4.058541000	3.417448000	4.403116000
C	3.513279000	3.404807000	2.312190000
H	3.868147000	4.407927000	2.100370000
C	2.950209000	2.632849000	1.297320000
H	2.857465000	3.002080000	0.281714000
C	4.436086000	-1.197230000	0.150925000
C	5.668581000	-1.703861000	-0.264782000
H	6.202679000	-2.416277000	0.357407000
C	6.196644000	-1.274700000	-1.482642000
H	7.155436000	-1.650672000	-1.827309000
C	5.471078000	-0.361769000	-2.251930000
H	5.844153000	-0.007135000	-3.207106000
C	4.240583000	0.080747000	-1.772518000
H	3.602665000	0.760541000	-2.328293000
C	1.603018000	-2.541490000	1.443876000
H	1.955893000	-3.374714000	2.069282000
C	2.078902000	-0.573455000	2.866126000
H	0.986330000	-0.534140000	2.922981000
H	2.474002000	-1.054443000	3.772571000
C	3.867455000	-1.571747000	1.507633000
H	4.101135000	-2.621517000	1.731953000
H	4.389072000	-0.971477000	2.263101000
N	2.413788000	-1.326002000	1.639837000
H	0.576765000	-2.290273000	1.728332000
H	-2.367589000	-6.094373000	0.876445000
C	-2.192044000	-5.046306000	0.652122000
C	-2.340818000	-4.077112000	1.648933000
C	-1.831567000	-4.644470000	-0.634310000
C	-2.119595000	-2.739106000	1.326082000

H	-2.635193000	-4.351360000	2.657600000
H	-1.714429000	-5.362958000	-1.438716000
C	-1.629842000	-3.284511000	-0.872927000
N	-1.765349000	-2.357557000	0.082095000
C	-2.249794000	-1.624989000	2.351259000
H	-1.343441000	-2.913975000	-1.852115000
H	-1.246118000	-1.293494000	2.640119000
H	-2.770741000	-1.991525000	3.248491000
N	-2.918218000	-0.455921000	1.751529000
N	-3.782272000	-0.378145000	-0.915592000
N	-2.515724000	1.939962000	0.340078000
C	-2.689975000	0.804294000	2.482803000
C	-4.345006000	-0.700145000	1.456330000
C	-4.747447000	-0.421872000	0.017200000
C	-4.132320000	-0.249470000	-2.207251000
C	-2.992855000	2.000102000	1.599694000
C	-2.724022000	2.976842000	-0.479113000
H	-3.282625000	0.853983000	3.408775000
H	-1.624766000	0.832559000	2.738076000
H	-4.983360000	-0.118006000	2.134635000
H	-4.568115000	-1.756243000	1.655406000
C	-6.099016000	-0.300873000	-0.314449000
C	-5.454811000	-0.137688000	-2.624753000
H	-3.312328000	-0.250691000	-2.918672000
C	-3.696529000	2.007982000	2.069781000
C	-3.409324000	4.127849000	-0.089849000
H	-2.319589000	2.881172000	-1.482295000
H	-6.853002000	-0.330044000	0.466908000
C	-6.459082000	-0.153046000	-1.652785000
H	-5.689157000	-0.039472000	-3.679517000
H	-4.073676000	3.118320000	3.087915000
C	-3.905798000	4.191608000	1.212774000
H	-3.551330000	4.943317000	-0.791419000
H	-7.503668000	-0.057435000	-1.933721000
H	-4.452264000	5.065386000	1.555022000
H	-1.430101000	0.898001000	-2.664063000
C	0.281168000	4.425246000	-1.382054000
H	-0.526894000	4.553957000	-0.667626000
C	0.177489000	3.809518000	-2.568146000
H	-0.734136000	3.371706000	-2.971168000
C	1.470664000	3.870752000	-3.355613000
H	1.388173000	4.613577000	-4.162463000
H	1.733948000	2.913097000	-3.819188000
C	1.655410000	5.033326000	-1.196159000
H	1.609254000	6.116057000	-1.386004000
H	2.051662000	4.916278000	-0.179734000
C	2.497855000	4.308625000	-2.278011000
H	3.303101000	4.929875000	-2.679836000
H	2.949897000	3.404962000	-1.846783000
H	1.072736000	1.990397000	-1.589589000



⁵R_{ls-hs}

Fe	-1.474201000	0.034899000	-0.454803000
Co	1.763600000	-0.254791000	-0.257703000
O	-1.096899000	-0.639700000	-1.905203000
O	1.432497000	0.517308000	-1.891903000
H	0.534598000	0.209205000	-2.126903000
O	0.027899000	-0.083496000	0.415897000
N	-1.150409000	2.219900000	-0.827603000
N	-2.468496000	-1.591404000	0.738697000
N	-3.506602000	0.330492000	-1.046703000
C	-1.155311000	2.982200000	0.278097000
C	-0.866015000	4.344501000	0.232597000
H	-0.899417000	4.940401000	1.139697000
C	-0.537217000	4.917002000	-0.999403000
H	-0.314821000	5.978003000	-1.068203000
C	-0.509315000	4.111702000	-2.139903000
H	-0.260416000	4.520303000	-3.113703000
C	-0.827710000	2.759401000	-2.008503000
H	-0.826808000	2.080701000	-2.854503000

C	-2.874497000	-1.211906000	1.963397000
C	-3.673195000	-2.031908000	2.757697000
H	-3.995796000	-1.696409000	3.738697000
C	-4.048391000	-3.284810000	2.262997000
H	-4.673788000	-3.943112000	2.858497000
C	-3.617489000	-3.673208000	0.992897000
H	-3.894286000	-4.635109000	0.573997000
C	-2.829992000	-2.786506000	0.257297000
H	-2.476991000	-3.016204000	-0.744003000
C	-4.348404000	0.918589000	-0.179403000
C	-5.722404000	0.965385000	-0.411003000
H	-6.378606000	1.441083000	0.311697000
C	-6.229003000	0.401583000	-1.582603000
H	-7.295303000	0.427480000	-1.786203000
C	-5.345801000	-0.193914000	-2.486503000
H	-5.698199000	-0.639515000	-3.410603000
C	-3.989201000	-0.215109000	-2.176403000
H	-3.242299000	-0.673307000	-2.816403000
C	-1.429809000	2.244499000	1.571797000
H	-1.808811000	2.927498000	2.345197000
C	-2.349902000	0.130896000	2.428197000
H	-1.302401000	0.001099000	2.721197000
H	-2.912603000	0.491494000	3.300797000
C	-3.730907000	1.604091000	1.017597000
H	-3.671010000	2.674892000	0.789597000
H	-4.384406000	1.504889000	1.894197000
N	-2.360605000	1.119296000	1.329397000
H	-0.487007000	1.805402000	1.911497000
H	3.213884000	4.530914000	2.639297000
C	2.912387000	3.657513000	2.068697000
C	2.785891000	2.416213000	2.702297000
C	2.649686000	3.759812000	0.701597000
C	2.405894000	1.314211000	1.942697000
H	2.978191000	2.306413000	3.765097000
H	2.729583000	4.708313000	0.181897000
C	2.288790000	2.611511000	-0.001603000
N	2.181894000	1.430011000	0.617297000
C	2.111699000	-0.051489000	2.531097000
H	2.060790000	2.583310000	-1.062203000
H	1.049699000	-0.075093000	2.792197000
H	2.698299000	-0.234088000	3.439697000
N	2.328602000	-1.115489000	1.514397000
N	3.682900000	-0.424784000	-0.719303000
N	1.393006000	-2.082992000	-0.780303000
C	1.405606000	-2.282092000	1.627897000
C	3.756604000	-1.553384000	1.425397000
C	4.468702000	-0.951882000	0.236197000
C	4.222399000	0.057317000	-1.852103000
C	1.279708000	-2.930092000	0.265997000
C	1.238107000	-2.518992000	-2.036203000
H	1.743708000	-2.995691000	2.389497000
H	0.423705000	-1.887895000	1.900297000
H	3.771907000	-2.644184000	1.316397000
H	4.285103000	-1.320482000	2.357197000
C	5.853302000	-1.002577000	0.093697000
C	5.596999000	0.026922000	-2.069603000
H	3.499297000	0.459915000	-2.553803000
C	1.016013000	-4.280693000	0.070097000
C	0.962011000	-3.858893000	-2.305303000
H	1.341704000	-1.759692000	-2.801303000
H	6.466703000	-1.428775000	0.881697000
C	6.425600000	-0.505475000	-1.078703000
H	6.005597000	0.419023000	-2.994803000
H	0.945815000	-4.950393000	0.921597000
C	0.851614000	-4.750494000	-1.237803000
H	0.844612000	-4.189294000	-3.331603000
H	7.502300000	-0.534372000	-1.215603000
H	0.650818000	-5.802394000	-1.417703000

³R_{ls-is}

Fe	1.593454000	0.134681000	-0.334681000
Co	-1.664675000	0.056704000	-0.276517000
O	1.273653000	0.646775000	-1.852856000
O	-1.156611000	-0.668046000	-1.885401000
H	-0.305657000	-0.231535000	-2.084627000

O	0.009889000	0.206112000	0.521361000
N	1.401353000	-1.835382000	-0.588195000
N	2.018858000	1.921257000	0.452254000
N	3.629149000	-0.199695000	-0.831367000
C	1.564721000	-2.563404000	0.537117000
C	1.552931000	-3.954729000	0.504453000
H	1.698395000	-4.516397000	1.421770000
C	1.360074000	-4.601863000	-0.718818000
H	1.356185000	-5.686646000	-0.770157000
C	1.190064000	-3.836037000	-1.872691000
H	1.048291000	-4.298525000	-2.843561000
C	1.223029000	-2.446880000	-1.767106000
H	1.115711000	-1.793677000	-2.622545000
C	2.238196000	1.927221000	1.785888000
C	2.571432000	3.101675000	2.454387000
H	2.763586000	3.080207000	3.522741000
C	2.657658000	4.293954000	1.728823000
H	2.920600000	5.220835000	2.229712000
C	2.413015000	4.273300000	0.355216000
H	2.474377000	5.176165000	-0.242906000
C	2.100848000	3.058147000	-0.252331000
H	1.904574000	2.955843000	-1.313864000
C	4.437109000	-0.688366000	0.121794000
C	5.734780000	-1.115239000	-0.158579000
H	6.360291000	-1.512605000	0.635280000
C	6.207029000	-1.014661000	-1.467192000
H	7.213916000	-1.338402000	-1.713011000
C	5.365377000	-0.493075000	-2.453264000
H	5.694187000	-0.396066000	-3.482481000
C	4.078522000	-0.103134000	-2.094813000
H	3.360298000	0.291323000	-2.805724000
C	1.688389000	-1.776485000	1.822984000
H	2.164933000	-2.376893000	2.608971000
C	2.036995000	0.602092000	2.491638000
H	0.970895000	0.493749000	2.699598000
H	2.592186000	0.568628000	3.438046000
C	3.894300000	-0.683541000	1.532112000
H	4.187885000	-1.598954000	2.061013000
H	4.360399000	0.150774000	2.070301000
N	2.417932000	-0.506277000	1.583537000
H	0.675534000	-1.508153000	2.131839000
H	-2.699906000	-4.845060000	2.606701000
C	-2.470880000	-3.946988000	2.040775000
C	-2.525733000	-2.694263000	2.661058000
C	-2.128592000	-4.027933000	0.689813000
C	-2.236076000	-1.561043000	1.907062000
H	-2.792533000	-2.598096000	3.709029000
H	-2.078167000	-4.983050000	0.178256000
C	-1.863650000	-2.850405000	-0.007938000
N	-1.919925000	-1.659382000	0.599108000
C	-2.163652000	-0.163046000	2.488596000
H	-1.592423000	-2.804857000	-1.057275000
H	-1.132305000	0.010403000	2.805759000
H	-2.819335000	-0.058247000	3.362101000
N	-2.469656000	0.850276000	1.445535000
N	-3.583365000	-0.035749000	-0.854947000
N	-1.508255000	1.921616000	-0.803021000
C	-1.741707000	2.141813000	1.597727000
C	-3.938407000	1.073003000	1.269209000
C	-4.488981000	0.370143000	0.050328000
C	-3.986526000	-0.589516000	-2.011228000
C	-1.596993000	2.783003000	0.234154000
C	-1.306691000	2.370555000	-2.047608000
H	-2.243240000	2.809589000	2.309446000
H	-0.737970000	1.903259000	1.953203000
H	-4.106506000	2.149193000	1.144740000
H	-4.480116000	0.770899000	2.173311000
C	-5.857076000	0.217859000	-0.164535000
C	-5.336851000	-0.760807000	-2.303242000
H	-3.176332000	-0.882637000	-2.670832000
C	-1.499460000	4.156082000	0.037797000
C	-1.181656000	3.733630000	-2.315142000
H	-1.251158000	1.602534000	-2.809294000
H	-6.567503000	0.549517000	0.586690000
C	-6.286875000	-0.357135000	-1.361719000

H	-5.633429000	-1.206809000	-3.246588000
H	-1.593100000	4.832985000	0.881270000
C	-1.283807000	4.638012000	-1.257639000
H	-1.022412000	4.070810000	-3.333754000
H	-7.347361000	-0.486341000	-1.556019000
H	-1.209568000	5.706511000	-1.437124000

¹R_{ls}-ls

Fe	1.555887000	0.182545000	-0.308325000
O	1.281248000	0.695356000	-1.859809000
Co	-1.646193000	0.050603000	-0.259563000
O	-1.110154000	-0.660111000	-1.861487000
H	-0.236963000	-0.256031000	-2.057438000
O	0.028577000	0.304282000	0.536816000
N	1.341454000	-1.823784000	-0.576437000
N	2.025094000	1.970237000	0.422915000
N	3.541438000	-0.260358000	-0.829363000
C	1.530053000	-2.524167000	0.561172000
C	1.564368000	-3.916257000	0.558587000
H	1.726388000	-4.455730000	1.486597000
C	1.400116000	-4.593069000	-0.653218000
H	1.431850000	-5.678285000	-0.683067000
C	1.219347000	-3.855578000	-1.824266000
H	1.107715000	-4.342813000	-2.787147000
C	1.204806000	-2.463595000	-1.743041000
H	1.093042000	-1.826778000	-2.611630000
C	2.252533000	1.993749000	1.754595000
C	2.607411000	3.173388000	2.402425000
H	2.806637000	3.168550000	3.469778000
C	2.706498000	4.351740000	1.654800000
H	2.986906000	5.282772000	2.138359000
C	2.452746000	4.312365000	0.283213000
H	2.524652000	5.205250000	-0.328789000
C	2.117385000	3.091656000	-0.302166000
H	1.906848000	2.962350000	-1.358697000
C	4.371111000	-0.727846000	0.115420000
C	5.648725000	-1.196939000	-0.185770000
H	6.288668000	-1.572990000	0.606820000
C	6.080853000	-1.166466000	-1.511123000
H	7.071649000	-1.524355000	-1.774237000
C	5.217971000	-0.668853000	-2.490919000
H	5.513037000	-0.624584000	-3.533871000
C	3.953638000	-0.230254000	-2.111765000
H	3.224292000	0.151697000	-2.817142000
C	1.653361000	-1.711639000	1.836486000
H	2.125738000	-2.305206000	2.630449000
C	2.041672000	0.679433000	2.483855000
H	0.979321000	0.585802000	2.716649000
H	2.612837000	0.651907000	3.420927000
C	3.865946000	-0.646807000	1.533404000
H	4.157928000	-1.537099000	2.104622000
H	4.348873000	0.211158000	2.016360000
N	2.396031000	-0.448613000	1.586221000
H	0.645238000	-1.430085000	2.148964000
H	-2.646985000	-4.842998000	2.641848000
C	-2.421457000	-3.945671000	2.073378000
C	-2.485874000	-2.691044000	2.689357000
C	-2.075160000	-4.029719000	0.723720000
C	-2.200258000	-1.558982000	1.932732000
H	-2.757558000	-2.592753000	3.735824000
H	-2.017785000	-4.986135000	0.215549000
C	-1.812969000	-2.853712000	0.022749000
N	-1.875827000	-1.660962000	0.626122000
C	-2.147608000	-0.156053000	2.504149000
H	-1.539170000	-2.810960000	-1.025897000
H	-1.118473000	0.040933000	2.815829000
H	-2.801088000	-0.055420000	3.379698000
N	-2.477772000	0.840816000	1.451733000
N	-3.542753000	-0.068121000	-0.862121000
N	-1.505147000	1.915144000	-0.795419000
C	-1.790552000	2.155908000	1.600918000
C	-3.952168000	1.017127000	1.267404000
C	-4.468969000	0.325776000	0.027721000
C	-3.919242000	-0.614718000	-2.031872000
C	-1.624278000	2.783906000	0.233301000

C	-1.261024000	2.354017000	-2.036281000
H	-2.330769000	2.818138000	2.288783000
H	-0.791208000	1.956943000	1.991581000
H	-4.159488000	2.089251000	1.171103000
H	-4.489248000	0.670898000	2.158283000
C	-5.831369000	0.168009000	-0.217490000
C	-5.262095000	-0.791305000	-2.351803000
H	-3.094523000	-0.895966000	-2.677861000
C	-1.525627000	4.154974000	0.029347000
C	-1.130539000	3.716018000	-2.309045000
H	-1.180768000	1.581225000	-2.790306000
H	-6.558603000	0.490773000	0.521417000
C	-6.233643000	-0.399949000	-1.427152000
H	-5.536215000	-1.231258000	-3.304694000
H	-1.645117000	4.838324000	0.864287000
C	-1.270705000	4.627397000	-1.263107000
H	-0.935867000	4.045293000	-3.324002000
H	-7.289207000	-0.532791000	-1.644327000
H	-1.193439000	5.694741000	-1.447965000

⁵TS_{Hls-hs}

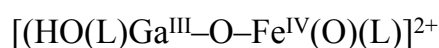
Fe	1.296477000	-0.180062000	0.035384000
Co	-1.956174000	0.185763000	-0.121041000
O	1.244002000	0.905959000	-1.361049000
O	-1.323607000	-0.029181000	-1.836626000
H	-0.417344000	0.345692000	-1.847316000
O	-0.341437000	-0.124982000	0.756094000
N	0.911704000	-2.195388000	-0.816367000
N	2.257765000	0.997409000	1.625055000
N	3.407076000	-0.965262000	-0.502795000
C	0.919077000	-3.215316000	0.057876000
C	0.786022000	-4.537477000	-0.362237000
H	0.808105000	-5.344041000	0.364320000
C	0.630633000	-4.796949000	-1.726717000
H	0.535763000	-5.818820000	-2.082605000
C	0.607940000	-3.728048000	-2.624643000
H	0.490981000	-3.888810000	-3.691356000
C	0.756943000	-2.434619000	-2.123149000
H	0.743877000	-1.558471000	-2.761621000
C	2.279700000	0.442766000	2.852183000
C	2.840203000	1.105316000	3.942274000
H	2.860931000	0.627171000	4.916926000
C	3.378953000	2.381521000	3.752360000
H	3.826073000	2.916144000	4.585184000
C	3.345147000	2.951006000	2.478269000
H	3.758340000	3.936113000	2.288050000
C	2.774499000	2.219038000	1.437819000
H	2.720442000	2.600679000	0.425621000
C	3.929658000	-1.933198000	0.265189000
C	5.005719000	-2.715144000	-0.156010000
H	5.398354000	-3.493748000	0.491382000
C	5.562537000	-2.475010000	-1.412900000
H	6.402495000	-3.066998000	-1.764047000
C	5.015076000	-1.469413000	-2.212041000
H	5.410572000	-1.254128000	-3.199232000
C	3.929920000	-0.748067000	-1.719282000
H	3.440275000	0.020484000	-2.303980000
C	0.994939000	-2.826544000	1.520012000
H	1.261894000	-3.696951000	2.138088000
C	1.638258000	-0.927182000	2.957245000
H	0.552552000	-0.794816000	3.001959000
H	1.972922000	-1.443950000	3.868859000
C	3.341680000	-2.096105000	1.650672000
H	3.480310000	-3.127977000	2.003334000
H	3.914386000	-1.452767000	2.329664000
N	1.920033000	-1.700000000	1.733914000
H	-0.001553000	-2.478007000	1.810335000
H	-3.484081000	-5.291014000	0.926868000
C	-3.170953000	-4.276409000	0.699274000
C	-3.197784000	-3.294529000	1.695432000
C	-2.747303000	-3.936970000	-0.586871000
C	-2.795871000	-2.002167000	1.371093000
H	-3.526613000	-3.526380000	2.703765000
H	-2.712543000	-4.673775000	-1.381666000
C	-2.373685000	-2.619163000	-0.844990000

N	-2.400882000	-1.692329000	0.119261000
C	-2.679682000	-0.878101000	2.379629000
H	-2.028637000	-2.254767000	-1.806077000
H	-1.660524000	-0.892707000	2.773704000
H	-3.383760000	-1.007335000	3.210970000
N	-2.859836000	0.434939000	1.704988000
N	-3.795973000	0.467168000	-0.831828000
N	-1.657485000	2.095818000	-0.005832000
C	-2.080793000	1.553695000	2.308595000
C	-4.299274000	0.799583000	1.521116000
C	-4.758160000	0.648608000	0.088273000
C	-4.111674000	0.388341000	-2.136084000
C	-1.820987000	2.592964000	1.239849000
C	-1.356171000	2.900607000	-1.030654000
H	-2.590971000	1.982448000	3.180045000
H	-1.114713000	1.140558000	2.607877000
H	-4.431801000	1.846370000	1.818948000
H	-4.928163000	0.200690000	2.190219000
C	-6.100865000	0.747094000	-0.271510000
C	-5.429868000	0.489081000	-2.570744000
H	-3.258914000	0.241027000	-2.791065000
C	-1.702996000	3.955770000	1.489207000
C	-1.209566000	4.274776000	-0.850094000
H	-1.239036000	2.400512000	-1.984313000
H	-6.860408000	0.888925000	0.491439000
C	-6.440879000	0.666170000	-1.622563000
H	-5.656177000	0.424719000	-3.629690000
H	-1.854542000	4.339948000	2.493067000
C	-1.390582000	4.809382000	0.425646000
H	-0.957844000	4.904706000	-1.695516000
H	-7.479709000	0.740744000	-1.929727000
H	-1.296189000	5.877958000	0.593808000
H	0.615063000	3.435426000	-3.076010000
H	1.902412000	1.616029000	-2.149187000
C	1.680501000	3.664512000	-2.958256000
H	1.982272000	4.280112000	-3.819875000
C	2.548315000	2.415565000	-2.896740000
H	2.673441000	1.853476000	-3.827756000
C	3.819249000	2.770807000	-2.115528000
H	4.702695000	2.761433000	-2.765993000
H	4.010732000	2.034430000	-1.323832000
C	2.027618000	4.387752000	-1.646081000
H	1.738565000	5.444226000	-1.640112000
H	1.507132000	3.887620000	-0.819629000
C	3.552067000	4.185940000	-1.529429000
H	4.065405000	4.938885000	-2.137624000
H	3.922002000	4.294818000	-0.503162000

⁵Int_{Is-hs}

Fe	1.245299000	-0.213101000	0.079998000
Co	-1.978001000	0.220195000	-0.133702000
O	1.219998000	0.973599000	-1.349102000
O	-1.305801000	-0.042804000	-1.830602000
H	-0.409402000	0.353797000	-1.852002000
O	-0.404401000	-0.146803000	0.799898000
N	0.858201000	-2.207702000	-0.802502000
N	2.197998000	0.944200000	1.684698000
N	3.391300000	-1.021299000	-0.471102000
C	0.839902000	-3.237902000	0.059498000
C	0.682304000	-4.552402000	-0.375602000
H	0.683005000	-5.366802000	0.342398000
C	0.529904000	-4.793702000	-1.743502000
H	0.415605000	-5.809402000	-2.111402000
C	0.535403000	-3.714602000	-2.629602000
H	0.421903000	-3.861002000	-3.698702000
C	0.707002000	-2.430202000	-2.113202000
H	0.712301000	-1.548102000	-2.742902000
C	2.205498000	0.377300000	2.906498000
C	2.754298000	1.027300000	4.009698000
H	2.762898000	0.539000000	4.979398000
C	3.296696000	2.304701000	3.839198000
H	3.735396000	2.829901000	4.682398000
C	3.276496000	2.887901000	2.571098000
H	3.692395000	3.874601000	2.395598000
C	2.716196000	2.168300000	1.516598000

H	2.670996000	2.562900000	0.509198000
C	3.857201000	-2.020699000	0.295698000
C	4.889802000	-2.860897000	-0.121502000
H	5.233603000	-3.661497000	0.526898000
C	5.468602000	-2.650197000	-1.373602000
H	6.275702000	-3.287996000	-1.721402000
C	4.985901000	-1.610797000	-2.170102000
H	5.401200000	-1.411097000	-3.152402000
C	3.940200000	-0.830798000	-1.680502000
H	3.517499000	-0.028799000	-2.274202000
C	0.912602000	-2.867002000	1.525798000
H	1.173803000	-3.744802000	2.135498000
C	1.558500000	-0.990901000	2.989598000
H	0.473200000	-0.855302000	3.031298000
H	1.888401000	-1.523601000	3.893598000
C	3.263001000	-2.152999000	1.681198000
H	3.394602000	-3.178299000	2.054998000
H	3.836700000	-1.497699000	2.347698000
N	1.843501000	-1.747101000	1.755298000
H	-0.083098000	-2.515903000	1.816598000
H	-3.710095000	-5.194307000	0.914298000
C	-3.359797000	-4.191907000	0.686998000
C	-3.388298000	-3.199207000	1.672298000
C	-2.885497000	-3.878806000	-0.588302000
C	-2.937599000	-1.922806000	1.348598000
H	-3.754397000	-3.410707000	2.672198000
H	-2.847596000	-4.624906000	-1.374302000
C	-2.465098000	-2.575406000	-0.847202000
N	-2.495899000	-1.637706000	0.106598000
C	-2.813000000	-0.794606000	2.351098000
H	-2.078799000	-2.231505000	-1.800102000
H	-1.807000000	-0.842605000	2.775198000
H	-3.546100000	-0.891507000	3.161398000
N	-2.924802000	0.518494000	1.661798000
N	-3.783002000	0.571793000	-0.900802000
N	-1.606504000	2.119395000	-0.025402000
C	-2.119803000	1.610995000	2.279598000
C	-4.343202000	0.937192000	1.434698000
C	-4.763102000	0.805392000	-0.012002000
C	-4.061502000	0.500693000	-2.213702000
C	-1.784204000	2.630595000	1.212998000
C	-1.239604000	2.905396000	-1.044002000
H	-2.638203000	2.067194000	3.131998000
H	-1.180902000	1.161696000	2.611298000
H	-4.446803000	1.987292000	1.732098000
H	-5.014002000	0.359992000	2.081698000
C	-6.087302000	0.968690000	-0.414302000
C	-5.358802000	0.663991000	-2.690202000
H	-3.195802000	0.307794000	-2.839202000
C	-1.610606000	3.987495000	1.460898000
C	-1.034906000	4.272296000	-0.863702000
H	-1.116904000	2.400196000	-1.993402000
H	-6.862402000	1.152490000	0.323598000
C	-6.388702000	0.897090000	-1.775102000
H	-5.554802000	0.604491000	-3.755502000
H	-1.774406000	4.382995000	2.458498000
C	-1.226707000	4.820696000	0.404398000
H	-0.733107000	4.886196000	-1.704702000
H	-7.412502000	1.021789000	-2.114902000
H	-1.087808000	5.884496000	0.571798000
H	1.949697000	1.278699000	-1.923302000
H	1.188295000	3.125399000	-3.342602000
C	2.188695000	3.517000000	-3.110802000
H	2.437894000	4.237800000	-3.908902000
C	3.241196000	2.446101000	-3.031702000
H	3.465997000	1.780401000	-3.861702000
C	4.198696000	2.704702000	-1.897802000
H	5.249796000	2.682003000	-2.216602000
H	4.106597000	1.936502000	-1.109502000
C	2.270494000	4.194900000	-1.725402000
H	1.905193000	5.227299000	-1.727702000
H	1.661595000	3.614799000	-1.021902000
C	3.765594000	4.093201000	-1.361002000
H	4.324093000	4.876302000	-1.886502000
H	3.961394000	4.216202000	-0.289202000



⁵ R _{ls-hs}			
Fe	1.568322000	-0.000993000	-0.419691000
O	1.182267000	0.684213000	-1.863549000
O	-1.358232000	-0.494323000	-2.086458000
H	-0.466411000	-0.239171000	-2.384593000
O	0.060747000	0.169145000	0.457405000
N	1.165708000	-2.189149000	-0.782069000
N	2.650392000	1.590994000	0.721761000
N	3.564961000	-0.398311000	-1.051155000
C	1.163537000	-2.935330000	0.335890000
C	0.857598000	-4.294389000	0.311885000
H	0.884037000	-4.875736000	1.228574000
C	0.523163000	-4.883604000	-0.910835000
H	0.287768000	-5.942719000	-0.962203000
C	0.507863000	-4.097266000	-2.064261000
H	0.256629000	-4.518195000	-3.032094000
C	0.841150000	-2.746625000	-1.954271000
H	0.848213000	-2.085753000	-2.813573000
C	3.030926000	1.220410000	1.957391000
C	3.859600000	2.020904000	2.740175000
H	4.160055000	1.692609000	3.703680000
C	4.292769000	3.245291000	2.221988000
H	4.941762000	3.888561000	2.808752000
C	3.889100000	3.624444000	0.940326000
H	4.210413000	4.564128000	0.503338000
C	3.068482000	2.757807000	0.217326000
H	2.733789000	2.981072000	-0.791556000
C	4.396653000	-1.007821000	-0.188780000
C	5.759845000	-1.132067000	-0.453676000
H	6.409612000	-1.622872000	0.264712000
C	6.264003000	-0.624726000	-1.651660000
H	7.321951000	-0.711335000	-1.880638000
C	5.390013000	-0.005324000	-2.548622000
H	5.741180000	0.399357000	-3.491803000
C	4.045065000	0.094228000	-2.206090000
H	3.306400000	0.576538000	-2.837982000
C	1.457877000	-2.183272000	1.615692000
H	1.817348000	-2.862421000	2.401365000
C	2.445938000	-0.089235000	2.440998000
H	1.402306000	0.089014000	2.720849000
H	2.988031000	-0.463154000	3.320677000
C	3.778851000	-1.623882000	1.045351000
H	3.693318000	-2.702991000	0.870445000
H	4.445752000	-1.497523000	1.907922000
N	2.423582000	-1.091747000	1.352762000
H	0.529541000	-1.707140000	1.944838000
H	-3.485373000	-4.427582000	2.778040000
C	-3.107250000	-3.601473000	2.183108000
C	-2.958015000	-2.334560000	2.756803000
C	-2.771658000	-3.790137000	0.840881000
C	-2.478227000	-1.293711000	1.966701000
H	-3.210262000	-2.156783000	3.797707000
H	-2.874497000	-4.759249000	0.364839000
C	-2.312490000	-2.697024000	0.109686000
N	-2.176641000	-1.485455000	0.669283000
C	-2.175908000	0.089548000	2.514385000
H	-2.038300000	-2.752315000	-0.939659000
H	-1.110293000	0.116669000	2.763555000
H	-2.753091000	0.277574000	3.429536000
N	-2.407196000	1.134414000	1.495957000
N	-3.722522000	0.357542000	-0.797299000
N	-1.432953000	2.283363000	-0.755083000
C	-1.556447000	2.336135000	1.663574000
C	-3.839223000	1.494057000	1.357010000
C	-4.516917000	0.822313000	0.179602000
C	-4.271573000	-0.163956000	-1.912813000
C	-1.443459000	3.067412000	0.339930000
C	-1.259718000	2.819509000	-1.973265000
H	-1.937619000	3.003679000	2.447540000
H	-0.556154000	1.988638000	1.936940000
H	-3.906928000	2.577467000	1.201428000

H	-4.385496000	1.275755000	2.283464000
C	-5.906282000	0.767328000	0.085280000
C	-5.649912000	-0.239853000	-2.086501000
H	-3.556327000	-0.517815000	-2.647632000
C	-1.305653000	4.448132000	0.241015000
C	-1.102794000	4.191805000	-2.150266000
H	-1.251624000	2.110688000	-2.794261000
H	-6.521743000	1.146229000	0.895766000
C	-6.481479000	0.228994000	-1.066398000
H	-6.058973000	-0.661628000	-2.998260000
H	-1.336772000	5.063097000	1.135137000
C	-1.131061000	5.017274000	-1.024458000
H	-0.971472000	4.600421000	-3.146320000
H	-7.561627000	0.176628000	-1.165282000
H	-1.026170000	6.093191000	-1.128380000
Ga	-1.584101000	0.213450000	-0.454409000

³R_{Is-is}

Fe	1.692539000	0.062242000	-0.314106000
O	1.343564000	0.559563000	-1.830638000
O	-1.144719000	-0.681705000	-2.103643000
H	-0.271475000	-0.342120000	-2.368862000
O	0.084697000	0.093511000	0.529122000
N	1.499899000	-1.906214000	-0.571393000
N	2.073304000	1.850385000	0.467768000
N	3.717149000	-0.226635000	-0.802111000
C	1.639575000	-2.633889000	0.558162000
C	1.584290000	-4.024157000	0.530797000
H	1.712654000	-4.586832000	1.450140000
C	1.367465000	-4.670452000	-0.689143000
H	1.325432000	-5.754646000	-0.734418000
C	1.222672000	-3.905545000	-1.846742000
H	1.062491000	-4.367042000	-2.815146000
C	1.302817000	-2.518098000	-1.747558000
H	1.213884000	-1.866851000	-2.606513000
C	2.282434000	1.860685000	1.802847000
C	2.582605000	3.042963000	2.473329000
H	2.767549000	3.025756000	3.542981000
C	2.642881000	4.237116000	1.748793000
H	2.879148000	5.170086000	2.251664000
C	2.405561000	4.211473000	0.373908000
H	2.445227000	5.116094000	-0.223195000
C	2.129444000	2.989414000	-0.236210000
H	1.940077000	2.883135000	-1.298382000
C	4.531663000	-0.701690000	0.153272000
C	5.843976000	-1.084925000	-0.122231000
H	6.475116000	-1.471913000	0.672252000
C	6.323033000	-0.955943000	-1.425652000
H	7.341187000	-1.246273000	-1.666668000
C	5.473430000	-0.450114000	-2.413197000
H	5.806736000	-0.332730000	-3.438801000
C	4.172965000	-0.103081000	-2.061483000
H	3.448910000	0.276990000	-2.774102000
C	1.775928000	-1.847177000	1.842275000
H	2.261715000	-2.445992000	2.623486000
C	2.098095000	0.533461000	2.506832000
H	1.031420000	0.412733000	2.705563000
H	2.649381000	0.506097000	3.455518000
C	3.977227000	-0.737239000	1.558764000
H	4.271743000	-1.665808000	2.063189000
H	4.434252000	0.083082000	2.125450000
N	2.498406000	-0.571896000	1.600689000
H	0.764324000	-1.584165000	2.159811000
H	-3.365534000	-4.722685000	2.674439000
C	-2.993197000	-3.883239000	2.094770000
C	-2.924771000	-2.609587000	2.668050000
C	-2.587542000	-4.061132000	0.770157000
C	-2.449057000	-1.551605000	1.897804000
H	-3.236791000	-2.438962000	3.693880000
H	-2.632730000	-5.034300000	0.293069000
C	-2.138867000	-2.951215000	0.057754000
N	-2.075470000	-1.734145000	0.618213000
C	-2.237327000	-0.154678000	2.455735000
H	-1.820554000	-2.995988000	-0.979814000
H	-1.185701000	-0.077364000	2.748150000

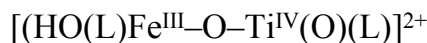
H	-2.861977000	0.001955000	3.345723000
N	-2.473762000	0.878526000	1.428665000
N	-3.602608000	0.041267000	-0.938977000
N	-1.443954000	2.085732000	-0.772681000
C	-1.705347000	2.125876000	1.637891000
C	-3.912855000	1.151316000	1.210399000
C	-4.478794000	0.461857000	-0.014878000
C	-4.056869000	-0.494019000	-2.089817000
C	-1.548852000	2.862564000	0.321308000
C	-1.223139000	2.635167000	-1.976159000
H	-2.169949000	2.774131000	2.393221000
H	-0.704534000	1.835038000	1.966390000
H	-4.041489000	2.231406000	1.070172000
H	-4.497935000	0.880932000	2.099047000
C	-5.856071000	0.346177000	-0.197695000
C	-5.416455000	-0.630418000	-2.352617000
H	-3.281245000	-0.807967000	-2.780029000
C	-1.457280000	4.248881000	0.234732000
C	-1.103727000	4.013444000	-2.140543000
H	-1.147074000	1.931261000	-2.798355000
H	-6.537902000	0.690820000	0.574169000
C	-6.332350000	-0.207957000	-1.385986000
H	-5.746695000	-1.062454000	-3.291198000
H	-1.566088000	4.857339000	1.127301000
C	-1.228745000	4.831459000	-1.015462000
H	-0.933062000	4.432095000	-3.126634000
H	-7.400544000	-0.307816000	-1.554161000
H	-1.160281000	5.911294000	-1.109986000
Ga	-1.455602000	-0.015189000	-0.463412000

⁵TS_{Hls-hs}

Fe	1.458207000	-0.097430000	0.020977000
O	1.335934000	0.845738000	-1.463045000
O	-1.277979000	0.099838000	-2.013463000
H	-0.342755000	0.382211000	-2.086160000
O	-0.187300000	-0.030563000	0.753077000
N	1.101788000	-2.133184000	-0.777550000
N	2.413776000	1.160122000	1.538494000
N	3.579296000	-0.780603000	-0.497586000
C	1.140307000	-3.128475000	0.125669000
C	1.052973000	-4.464301000	-0.259297000
H	1.101429000	-5.250166000	0.488250000
C	0.908999000	-4.764929000	-1.617023000
H	0.849849000	-5.798691000	-1.945155000
C	0.850526000	-3.722631000	-2.543674000
H	0.739200000	-3.916083000	-3.605523000
C	0.955502000	-2.411329000	-2.077978000
H	0.915027000	-1.552060000	-2.738592000
C	2.475578000	0.638111000	2.778944000
C	3.055381000	1.337513000	3.835080000
H	3.108168000	0.886689000	4.821396000
C	3.569152000	2.615833000	3.596969000
H	4.029802000	3.179194000	4.403016000
C	3.491659000	3.151657000	2.310313000
H	3.882882000	4.138154000	2.084470000
C	2.905450000	2.384083000	1.304820000
H	2.817088000	2.740712000	0.284978000
C	4.157028000	-1.708514000	0.279030000
C	5.307460000	-2.392503000	-0.116813000
H	5.743680000	-3.144589000	0.534144000
C	5.882169000	-2.087633000	-1.350816000
H	6.779104000	-2.603069000	-1.681150000
C	5.282321000	-1.114712000	-2.153899000
H	5.694127000	-0.848724000	-3.121797000
C	4.124358000	-0.495282000	-1.691005000
H	3.591610000	0.244030000	-2.276963000
C	1.212907000	-2.691247000	1.574035000
H	1.490601000	-3.536915000	2.220721000
C	1.850541000	-0.733769000	2.939398000
H	0.764212000	-0.607925000	2.987371000
H	2.199959000	-1.214646000	3.864638000
C	3.553774000	-1.934218000	1.650277000
H	3.693546000	-2.980316000	1.956106000
H	4.120879000	-1.323827000	2.363845000
N	2.129047000	-1.549060000	1.741189000

H	0.215388000	-2.339996000	1.855200000	H	-1.154162000	-1.149517000	2.712747000
H	-3.219518000	-5.527083000	0.957848000	C	-2.195197000	0.636579000	-2.820912000
C	-2.928955000	-4.508244000	0.719131000	C	-2.623742000	1.400227000	-3.902621000
C	-2.951902000	-3.521520000	1.709678000	H	-2.616527000	0.973639000	-4.901015000
C	-2.541955000	-4.166816000	-0.578260000	C	-3.067728000	2.706313000	-3.678735000
C	-2.581034000	-2.222940000	1.370908000	H	-3.408237000	3.320162000	-4.507138000
H	-3.257905000	-3.752619000	2.725469000	C	-3.085585000	3.196970000	-2.373614000
H	-2.517842000	-4.904992000	-1.372345000	H	-3.437584000	4.198591000	-2.150619000
C	-2.197842000	-2.843367000	-0.843041000	C	-2.655186000	2.366734000	-1.339323000
N	-2.215179000	-1.906336000	0.115495000	H	-2.668224000	2.685352000	-0.307094000
C	-2.496126000	-1.094663000	2.381206000	C	-4.201210000	-1.577639000	-0.524109000
H	-1.893972000	-2.491020000	-1.823440000	C	-5.469547000	-2.079894000	-0.235304000
H	-1.453007000	-1.012321000	2.701022000	H	-5.932400000	-2.802974000	-0.900326000
H	-3.119946000	-1.314567000	3.258394000	C	-6.124778000	-1.631304000	0.911364000
N	-2.854476000	0.192948000	1.757266000	H	-7.114077000	-2.004116000	1.159013000
N	-3.828282000	0.205923000	-0.825337000	C	-5.487513000	-0.698460000	1.733626000
N	-1.939416000	2.192891000	0.163163000	H	-5.961898000	-0.323350000	2.634251000
C	-2.242493000	1.368811000	2.415930000	C	-4.214537000	-0.257902000	1.385266000
C	-4.315269000	0.353835000	1.570405000	H	-3.644815000	0.443831000	1.983372000
C	-4.769100000	0.202461000	0.129711000	C	-1.129851000	-2.697703000	-1.482523000
C	-4.193530000	0.138793000	-2.121988000	H	-1.408365000	-3.587938000	-2.061394000
C	-2.201237000	2.528476000	1.440976000	C	-1.667269000	-0.772854000	-2.973565000
C	-1.830947000	3.142012000	-0.777790000	H	-0.578053000	-0.724669000	-2.999618000
H	-2.772905000	1.649630000	3.335606000	H	-2.040460000	-1.241741000	-3.893423000
H	-1.209946000	1.098492000	2.655794000	C	-3.472065000	-1.948471000	-1.793445000
H	-4.605403000	1.355686000	1.909742000	H	-3.569224000	-3.021991000	-1.997075000
H	-4.861903000	-0.356603000	2.203459000	H	-3.955056000	-1.425688000	-2.627541000
C	-6.127217000	0.118849000	-0.177237000	N	-2.034438000	-1.554485000	-1.765705000
C	-5.527681000	0.063356000	-2.507216000	H	-0.125112000	-2.378066000	-1.764079000
H	-3.366908000	0.143796000	-2.824368000	H	3.444104000	-5.522014000	-0.514965000
C	-2.380347000	3.855959000	1.817100000	C	3.074081000	-4.511115000	-0.371507000
C	-1.986298000	4.492778000	-0.476247000	C	3.066656000	-3.607482000	-1.439017000
H	-1.617479000	2.778469000	-1.777567000	C	2.615830000	-4.093901000	0.879365000
H	-6.864962000	0.113308000	0.619821000	C	2.596794000	-2.315194000	-1.220628000
C	-6.512242000	0.048996000	-1.515514000	H	3.428709000	-3.895985000	-2.421148000
H	-5.786666000	0.013014000	-3.559360000	H	2.615644000	-4.764453000	1.731958000
H	-2.606326000	4.102479000	2.849924000	C	2.167953000	-2.782090000	1.020467000
C	-2.267972000	4.853060000	0.842596000	N	2.156785000	-1.925426000	-0.009967000
H	-1.894086000	5.238393000	-1.258166000	C	2.497056000	-1.273940000	-2.320093000
H	-7.563488000	-0.015797000	-1.780055000	H	1.805643000	-2.376495000	1.960043000
H	-2.407098000	5.896044000	1.111064000	H	1.466580000	-1.261943000	-2.686131000
H	0.100440000	2.989776000	-3.168938000	H	3.160969000	-1.534929000	-3.156136000
H	1.841363000	1.598054000	-2.343076000	N	2.777504000	0.071057000	-1.790822000
C	1.073992000	3.487339000	-3.093211000	N	3.677678000	0.265808000	0.813935000
H	1.159138000	4.186607000	-3.939502000	N	1.823171000	2.165240000	-0.379451000
C	2.232224000	2.500645000	-3.123046000	C	2.146079000	1.166785000	-2.558071000
H	2.429479000	1.984067000	-4.067636000	C	4.222488000	0.306480000	-1.569835000
C	3.421438000	3.157513000	-2.413271000	C	4.642043000	0.206590000	-0.115371000
H	4.225956000	3.394381000	-3.120415000	C	4.012470000	0.262786000	2.119695000
H	3.855773000	2.478014000	-1.666797000	C	2.062833000	2.401051000	-1.683186000
C	1.307223000	4.229750000	-1.765708000	C	1.714177000	3.186875000	0.481826000
H	0.750447000	5.169171000	-1.684469000	H	2.685662000	1.385286000	-3.489763000
H	1.004139000	3.574065000	-0.938847000	H	1.124236000	0.849659000	-2.783411000
C	2.835434000	4.439202000	-1.755450000	H	4.467621000	1.317424000	-1.917293000
H	3.085870000	5.311839000	-2.369134000	H	4.822676000	-0.383286000	-2.177426000
H	3.238204000	4.626902000	-0.753303000	C	5.991611000	0.124416000	0.227406000
Ga	-1.716621000	0.133592000	-0.275986000	C	5.336690000	0.196534000	2.541267000
⁵TS_{Hls-ls}				H	3.170515000	0.310274000	2.801764000
Fe	-1.602144000	-0.213930000	-0.177119000	C	2.202680000	3.696971000	-2.171019000
O	-1.496349000	0.740356000	1.308556000	C	1.827360000	4.512023000	0.067415000
O	1.115460000	0.229742000	1.949936000	H	1.532134000	2.905898000	1.512536000
H	0.152999000	0.417713000	1.960983000	H	6.747617000	0.070766000	-0.550526000
O	0.082939000	-0.078910000	-0.842630000	C	6.344417000	0.120175000	1.576548000
N	-1.165032000	-1.910055000	0.806467000	H	5.569718000	0.199478000	3.600709000
N	-2.209095000	1.122607000	-1.558312000	H	2.413712000	3.861555000	-3.223228000
N	-3.588612000	-0.690308000	0.276257000	C	2.074891000	4.769114000	-1.282373000
C	-1.102595000	-2.991879000	0.000104000	H	1.735573000	5.317587000	0.788180000
C	-0.962446000	-4.276568000	0.515098000	H	7.388258000	0.058270000	1.869640000
H	-0.927176000	-5.128104000	-0.157062000	H	2.182084000	5.789286000	-1.638897000
C	-0.873979000	-4.442685000	1.899908000	H	-1.412618000	1.962952000	1.371918000
H	-0.773696000	-5.436076000	2.327225000	H	-3.617010000	2.942889000	1.592690000
C	-0.930944000	-3.317881000	2.722733000	C	-2.870249000	3.396409000	2.257818000
H	-0.873913000	-3.403811000	3.802684000	H	-3.101185000	4.471072000	2.324550000
C	-1.083958000	-2.062473000	2.135153000	C	-1.431716000	3.204895000	1.786140000
				H	-1.094043000	3.789643000	0.924537000

C	-0.533069000	3.207895000	3.029732000
H	0.153325000	4.065466000	3.025616000
H	0.088664000	2.303424000	3.058446000
C	-2.854721000	2.778094000	3.666987000
H	-3.711963000	3.076263000	4.278839000
H	-2.850082000	1.683197000	3.582916000
C	-1.506850000	3.256753000	4.237380000
H	-1.608911000	4.290548000	4.588316000
H	-1.160249000	2.652510000	5.081394000
Ga	1.556580000	0.131568000	0.214261000



⁶R_{hs-ls}

Ti	1.640646000	0.203033000	-0.540579000
O	1.393110000	0.651066000	-2.120963000
Fe	-1.579301000	0.229251000	-0.474219000
O	-1.244966000	-0.274723000	-2.204662000
H	-0.349594000	0.020720000	-2.486971000
O	0.086708000	0.433420000	0.375857000
N	1.327876000	-1.959960000	-0.656534000
N	2.689477000	1.832555000	0.450402000
N	3.790907000	-0.379778000	-0.968652000
C	1.398817000	-2.660320000	0.496995000
C	1.248016000	-4.043585000	0.516069000
H	1.325804000	-4.582860000	1.454871000
C	1.003894000	-4.715464000	-0.685315000
H	0.894590000	-5.796025000	-0.695706000
C	0.912691000	-3.982001000	-1.869134000
H	0.727383000	-4.465501000	-2.822385000
C	1.083645000	-2.599504000	-1.812498000
H	1.027257000	-1.971337000	-2.694077000
C	3.016624000	1.650182000	1.750506000
C	3.771140000	2.590000000	2.445835000
H	4.029973000	2.413780000	3.485204000
C	4.186191000	3.750732000	1.785791000
H	4.777962000	4.495621000	2.309409000
C	3.838550000	3.934285000	0.446722000
H	4.145141000	4.818843000	-0.101136000
C	3.091328000	2.944939000	-0.189138000
H	2.799372000	3.018846000	-1.231873000
C	4.586823000	-0.880428000	-0.010360000
C	5.946425000	-1.110257000	-0.225791000
H	6.562442000	-1.511439000	0.573846000
C	6.490852000	-0.822210000	-1.476591000
H	7.545839000	-0.994074000	-1.668454000
C	5.658356000	-0.310516000	-2.475789000
H	6.040020000	-0.075076000	-3.463586000
C	4.315854000	-0.100161000	-2.179881000
H	3.613351000	0.302703000	-2.901728000
C	1.608822000	-1.836869000	1.749750000
H	1.928399000	-2.476398000	2.585351000
C	2.469132000	0.395299000	2.398829000
H	1.403464000	0.556760000	2.595168000
H	2.979203000	0.201627000	3.353676000
C	3.953206000	-1.244753000	1.318404000
H	3.951851000	-2.338913000	1.403505000
H	4.584042000	-0.876627000	2.138484000
N	2.568174000	-0.749693000	1.473691000
H	0.652970000	-1.367234000	2.002771000
H	-3.032912000	-4.759525000	2.602921000
C	-2.724109000	-3.883972000	2.039456000
C	-2.685432000	-2.628870000	2.654942000
C	-2.374675000	-3.993324000	0.692512000
C	-2.296403000	-1.522574000	1.903244000
H	-2.960943000	-2.507028000	3.698001000
H	-2.399341000	-4.948176000	0.178319000
C	-2.003817000	-2.838288000	0.005486000
N	-1.963353000	-1.640387000	0.603147000
C	-2.171242000	-0.130420000	2.490098000
H	-1.729102000	-2.847873000	-1.044445000
H	-1.109619000	0.062383000	2.680414000

H	-2.713982000	-0.066941000	3.444541000
N	-2.624888000	0.888635000	1.528085000
N	-3.773688000	0.016821000	-0.849207000
N	-1.900972000	2.358358000	-0.663030000
C	-2.035839000	2.226747000	1.750964000
C	-4.098097000	0.939152000	1.393363000
C	-4.631685000	0.241252000	0.156494000
C	-4.222642000	-0.513333000	-2.001454000
C	-2.120694000	3.042504000	0.476716000
C	-1.902980000	2.994555000	-1.843661000
H	-2.515279000	2.757413000	2.585788000
H	-0.977200000	2.075075000	1.985319000
H	-4.402850000	1.991370000	1.333519000
H	-4.581070000	0.528777000	2.290475000
C	-5.986101000	-0.077065000	0.050793000
C	-5.561831000	-0.842979000	-2.191427000
H	-3.464930000	-0.665689000	-2.763169000
C	-2.371001000	4.411833000	0.462945000
C	-2.132684000	4.366600000	-1.936992000
H	-1.716408000	2.370156000	-2.711636000
H	-6.655729000	0.111048000	0.885046000
C	-6.458244000	-0.626149000	-1.141650000
H	-5.889828000	-1.262848000	-3.136457000
H	-2.561468000	4.939183000	1.392655000
C	-2.373826000	5.083742000	-0.763744000
H	-2.130704000	4.853384000	-2.906410000
H	-7.508762000	-0.879241000	-1.249835000
H	-2.569674000	6.151250000	-0.801083000

⁴R_{is-ls}

Ti	1.635944000	0.382024000	-0.570500000
O	1.432322000	0.801103000	-2.165591000
Fe	-1.635730000	0.158881000	-0.449672000
O	-1.138251000	-0.247382000	-2.116608000
H	-0.281022000	0.186802000	-2.344750000
O	0.031375000	0.469182000	0.266600000
N	1.468078000	-1.801682000	-0.642274000
N	2.514171000	2.102861000	0.426767000
N	3.795558000	-0.232728000	-0.953934000
C	1.642306000	-2.476221000	0.513309000
C	1.636708000	-3.867765000	0.550047000
H	1.794507000	-4.383987000	1.491736000
C	1.427376000	-4.575677000	-0.636862000
H	1.429731000	-5.661794000	-0.634716000
C	1.220818000	-3.868839000	-1.822657000
H	1.053847000	-4.380191000	-2.764740000
C	1.253965000	-2.475350000	-1.783906000
H	1.106318000	-1.865817000	-2.667994000
C	2.717742000	2.006621000	1.761475000
C	3.290713000	3.048565000	2.483838000
H	3.457244000	2.939769000	3.550998000
C	3.649702000	4.222187000	1.813239000
H	4.101932000	5.046050000	2.357306000
C	3.430888000	4.315910000	0.438068000
H	3.701468000	5.206916000	-0.118210000
C	2.862036000	3.228647000	-0.222211000
H	2.671524000	3.232229000	-1.290637000
C	4.542864000	-0.784298000	0.016721000
C	5.788558000	-1.355227000	-0.243696000
H	6.361484000	-1.800836000	0.564262000
C	6.280776000	-1.335120000	-1.548740000
H	7.249296000	-1.770404000	-1.776477000
C	5.508258000	-0.749560000	-2.554665000
H	5.853028000	-0.712484000	-3.582587000
C	4.267810000	-0.216971000	-2.216877000
H	3.604436000	0.230643000	-2.949405000
C	1.758903000	-1.627147000	1.761186000
H	2.156935000	-2.221206000	2.597029000
C	2.258557000	0.712994000	2.403754000
H	1.168703000	0.749904000	2.507713000
H	2.707261000	0.596521000	3.400982000
C	4.016044000	-0.697796000	1.434520000
H	4.263778000	-1.615834000	1.984780000
H	4.552261000	0.116942000	1.937244000
N	2.565659000	-0.419813000	1.507913000

H	0.747229000	-1.292791000	2.014127000
H	-2.639436000	-4.705931000	3.101087000
C	-2.391040000	-3.873322000	2.449597000
C	-2.451983000	-2.561015000	2.929962000
C	-2.016993000	-4.096886000	1.123262000
C	-2.135287000	-1.518831000	2.061133000
H	-2.743612000	-2.351080000	3.954653000
H	-1.961932000	-5.100565000	0.714898000
C	-1.726088000	-2.994467000	0.318663000
N	-1.784281000	-1.742085000	0.783182000
C	-2.097907000	-0.066538000	2.485797000
H	-1.436846000	-3.100669000	-0.722722000
H	-1.053249000	0.211381000	2.661142000
H	-2.662994000	0.089353000	3.414843000
N	-2.591157000	0.815829000	1.403396000
N	-3.575864000	-0.363939000	-0.895933000
N	-2.140297000	2.284039000	-0.808518000
C	-2.151563000	2.221933000	1.596608000
C	-4.073553000	0.721497000	1.237329000
C	-4.496515000	-0.127686000	0.058393000
C	-3.917796000	-1.031816000	-2.011588000
C	-2.341018000	2.999530000	0.311381000
C	-2.224077000	2.875652000	-2.006398000
H	-2.680196000	2.696662000	2.434529000
H	-1.080928000	2.182281000	1.821850000
H	-4.463934000	1.732945000	1.074575000
H	-4.537077000	0.350113000	2.159854000
C	-5.807744000	-0.581552000	-0.071593000
C	-5.211247000	-1.502223000	-2.216486000
H	-3.111971000	-1.165085000	-2.725999000
C	-2.658585000	4.354401000	0.270131000
C	-2.522908000	4.232503000	-2.136309000
H	-2.042753000	2.229339000	-2.859925000
H	-6.531194000	-0.383467000	0.713501000
C	-6.170197000	-1.278628000	-1.225295000
H	-5.456691000	-2.033266000	-3.129935000
H	-2.833529000	4.906095000	1.188926000
C	-2.747025000	4.979749000	-0.978209000
H	-2.585069000	4.685637000	-3.120054000
H	-7.187132000	-1.638809000	-1.349003000
H	-2.994802000	6.035062000	-1.043356000

²R_{ls-ls}

Ti	1.480986000	0.221393000	-0.456613000
O	1.181606000	0.711527000	-2.022443000
Fe	-1.744469000	0.129611000	-0.316340000
O	-1.257208000	-0.603227000	-1.884053000
H	-0.474737000	-0.113086000	-2.222359000
O	-0.044522000	0.257084000	0.485210000
N	1.420989000	-1.966452000	-0.547244000
N	2.339071000	1.972112000	0.518181000
N	3.657218000	-0.265080000	-0.956987000
C	1.640715000	-2.638876000	0.601830000
C	1.638303000	-4.030838000	0.641388000
H	1.831109000	-4.545286000	1.577641000
C	1.388713000	-4.741359000	-0.535935000
H	1.390563000	-5.827465000	-0.530984000
C	1.148386000	-4.037110000	-1.716883000
H	0.955100000	-4.550562000	-2.652767000
C	1.177573000	-2.644129000	-1.680528000
H	0.998807000	-2.038520000	-2.561116000
C	2.636454000	1.869346000	1.833607000
C	3.208759000	2.928442000	2.532407000
H	3.452129000	2.814316000	3.584173000
C	3.467490000	4.125500000	1.857544000
H	3.918779000	4.962414000	2.382176000
C	3.150480000	4.225480000	0.501959000
H	3.343362000	5.134515000	-0.057665000
C	2.588623000	3.120557000	-0.134802000
H	2.325244000	3.125375000	-1.187613000
C	4.472883000	-0.812461000	-0.041842000
C	5.727882000	-1.320162000	-0.379091000
H	6.358015000	-1.764391000	0.385985000
C	6.154157000	-1.240370000	-1.704762000
H	7.127689000	-1.626461000	-1.992073000

C	5.309006000	-0.659540000	-2.653673000
H	5.601035000	-0.577616000	-3.695275000
C	4.065747000	-0.191111000	-2.239490000
H	3.348494000	0.250013000	-2.923731000
C	1.802248000	-1.792016000	1.846525000
H	2.260215000	-2.379645000	2.655812000
C	2.275158000	0.550529000	2.487189000
H	1.194994000	0.543940000	2.668826000
H	2.795895000	0.441721000	3.449729000
C	4.012791000	-0.797450000	1.401994000
H	4.308538000	-1.731538000	1.898614000
H	4.555302000	0.007275000	1.914368000
N	2.561331000	-0.560907000	1.559586000
H	0.797663000	-1.484018000	2.156144000
H	-2.841324000	-4.719296000	2.709079000
C	-2.601341000	-3.839841000	2.119036000
C	-2.657749000	-2.568840000	2.699489000
C	-2.241996000	-3.963344000	0.775357000
C	-2.350413000	-1.460041000	1.915667000
H	-2.935348000	-2.439692000	3.741082000
H	-2.189509000	-4.933517000	0.293170000
C	-1.964912000	-2.807889000	0.047009000
N	-2.021116000	-1.596287000	0.614301000
C	-2.263627000	-0.050443000	2.468691000
H	-1.688189000	-2.804600000	-1.001514000
H	-1.227737000	0.115336000	2.777107000
H	-2.914878000	0.076406000	3.342498000
N	-2.562203000	0.959924000	1.415985000
N	-3.702267000	-0.016446000	-0.830108000
N	-1.590556000	2.042333000	-0.828962000
C	-1.827887000	2.246977000	1.574195000
C	-4.026926000	1.194300000	1.239640000
C	-4.594785000	0.411541000	0.081066000
C	-4.129767000	-0.637111000	-1.944136000
C	-1.689571000	2.898171000	0.214166000
C	-1.402406000	2.515159000	-2.068880000
H	-2.324245000	2.912332000	2.291979000
H	-0.826333000	2.003096000	1.935417000
H	-4.174567000	2.260343000	1.030404000
H	-4.565471000	0.974151000	2.169197000
C	-5.963712000	0.215047000	-0.084255000
C	-5.483147000	-0.854195000	-2.186765000
H	-3.340211000	-0.950105000	-2.618404000
C	-1.618185000	4.274658000	0.031751000
C	-1.305444000	3.882357000	-2.325023000
H	-1.327265000	1.768168000	-2.848714000
H	-6.658813000	0.566512000	0.672168000
C	-6.415419000	-0.427665000	-1.238094000
H	-5.794484000	-1.353338000	-3.098135000
H	-1.720321000	4.940731000	0.882950000
C	-1.418925000	4.774927000	-1.259395000
H	-1.154310000	4.230279000	-3.341134000
H	-7.477539000	-0.591247000	-1.393353000
H	-1.364367000	5.846279000	-1.428052000

[(N4Py)Fe^{IV}(O)]²⁺

⁵R_{hs}

Fe	0.103197000	0.000005000	-0.765939000
O	0.267535000	0.000007000	-2.401099000
N	-0.087048000	0.000006000	1.315376000
N	-1.479070000	-1.415693000	-0.521198000
N	1.522815000	-1.474085000	-0.350540000
N	1.522851000	1.474065000	-0.350530000
N	-1.479045000	1.415712000	-0.521208000
C	1.612958000	-1.815345000	0.963701000
C	-2.117403000	-1.227217000	0.666905000
C	-2.928910000	-3.249882000	-1.025104000
H	-3.232333000	-4.029396000	-1.712786000
C	-3.171884000	-2.043924000	1.063635000
H	-3.669171000	-1.886994000	2.014007000

C	-1.870029000	-2.399982000	-1.360168000
H	-1.329485000	-2.485631000	-2.294197000
C	2.600545000	2.695802000	1.408441000
H	2.670019000	2.955733000	2.458695000
C	0.545171000	-1.257889000	1.878144000
H	0.949724000	-1.057292000	2.875243000
H	-0.242584000	-2.008735000	2.000552000
C	1.612994000	1.815322000	0.963711000
C	2.384753000	-1.998611000	-1.258236000
C	0.545187000	1.257891000	1.878146000
H	0.949724000	1.057293000	2.875251000
H	-0.242557000	2.008752000	2.000539000
C	3.380932000	-2.894287000	-0.874171000
C	3.493511000	3.242898000	0.477887000
H	4.265277000	3.930345000	0.804672000
C	3.381004000	2.894224000	-0.874149000
C	-1.615841000	0.000017000	1.418839000
H	-1.947295000	0.000023000	2.462216000
C	2.384807000	1.998572000	-1.258221000
C	2.600492000	-2.695847000	1.408424000
H	2.669965000	-2.955780000	2.458677000
C	-2.117385000	1.227252000	0.666896000
C	-3.581210000	-3.073915000	0.199848000
H	-4.400933000	-3.724496000	0.482138000
C	3.493439000	-3.242964000	0.477864000
H	4.265191000	-3.930429000	0.804644000
C	-3.171857000	2.043975000	1.063615000
H	-3.669149000	1.887058000	2.013987000
C	-2.928861000	3.249915000	-1.025131000
H	-3.232273000	4.029429000	-1.712820000
C	-1.869989000	2.400001000	-1.360186000
H	-1.329442000	2.485636000	-2.294213000
C	-3.581168000	3.073965000	0.199820000
H	-4.400884000	3.724558000	0.482103000
H	2.251389000	1.680181000	-2.284379000
H	4.054554000	3.303822000	-1.616525000
H	2.251337000	-1.680217000	-2.284394000
H	4.054468000	-3.303901000	-1.616551000