Supporting Information

The Effect of Auxiliary Ligand on Mechanism and Reactivity: DFT Study on H_2 Activation by Lewis Acid-Transition Metal Complex (Tris(phosphino)borane)Fe(L)

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1. The comparison of absolute energies of different catalysts using different functionals.

Table S1. The comparison of absolute energies of different catalysts using different functionals

Catalyst	Apical Ligand	Spin State	M06L				B3LYP				B3LYP*(15% exact exchange)			
			H/(Hartree)		G/(Hartree)		H/(Hartree)		G/(Hartree)		H/(Hartree)		G/(Hartree)	
			gas	solution	gas	solution	gas	solution	gas	solution	gas	solution	gas	solution
1	N_2	singlet	**−2213.918171**	**−2214.773829**	**−2214.012574**	**−2214.868232**	−2214.011435	−2214.896796	−2214.107643	−2214.993003	**−2213.416325**	−2203.325646	**−2213.509916**	−2203.419237
		triplet	−2213.896728	−2214.758767	−2214.000212	−2214.862251	**−2214.022342**	**−2214.913627**	**−2214.125235**	**−2215.016521**	−2213.403026	**−2203.335395**	−2213.502559	**−2203.434928**
3	CN^tBu	singlet	**−2354.926184**	**−2355.828264**	**−2355.033284**	**−2355.935364**	−2355.047674	−2355.975021	−2355.159079	−2356.086425	**−2354.331236**	−2343.283275	**−2354.435483**	−2343.387522
		triplet	−2354.899597	−2355.809974	−2355.012806	−2355.923183	**−2355.054259**	**−2355.98992**	**−2355.173009**	**−2356.108669**	−2354.317254	**−2343.291387**	−2354.427574	**−2343.401707**
5	CO	singlet	**−2217.742259**	**−2218.603311**	**−2217.837571**	**−2218.698623**	**−2217.836712**	**−2218.72731**	**−2217.932209**	−2218.822807	**−2217.238821**	**−2207.145497**	**−2217.331291**	**−2207.237967**
		triplet	−2217.714052	−2218.578113	−2217.813748	−2218.677809	−2217.829959	−2218.724206	−2217.93184	**−2218.826087**	−2217.221584	−2207.13971	−2217.319187	−2207.237313

- H and G designate the thermal enthalpy and the Gibbs free energy, separately.

Several functionals that are often used when describing relative energies in transition metal complexes were examined so as to decide the most appropriate functional for our calculation. The absolute energies of catalysts **1**, **3** and **5** gained by using M06L, B3LYP and B3LYP* (15% exact exchange) functionals are listed in Table S1, where the lower energy of the two spin states are in bold type. According to these results, we choose B3LYP* (15% exact exchange) as the functional for our calculation for its better prediction of spin states.

2. The absolute energies of all optimized structures.

Table S2. The absolute energies of all optimized structures

Species	Ec	Uc	Hc	Gc	E	U	H	G	Solvation Energy	H in Solution	G in Solution
H_2	0.009707	0.012068	0.013012	−0.001813	−1.155507	−1.153147	−1.152203	−1.167028	−1.146643	−1.133631	−1.148456
N_2	0.005312	0.007673	0.008617	−0.01316	−109.505336	−109.502975	−109.502031	−109.523808	−108.900328	−108.891711	−108.913488
CN^tBu	0.12635	0.133444	0.134388	0.096435	−250.403843	−250.396749	−250.395805	−250.433758	−248.967548	−248.83316	−248.871113
CO	0.004779	0.00714	0.008084	−0.014382	−113.289198	−113.286837	−113.285893	−113.308359	−112.680747	−112.672663	−112.695129
^{s}**1**	0.471631	0.504749	0.505693	0.412102	−2213.450387	−2213.417269	−2213.416325	−2213.509916	−2203.831339	−2203.325646	−2203.419237
^{t}**1**	0.46928	0.503775	0.504719	0.405186	−2213.438465	−2213.40397	−2213.403026	−2213.502559	−2203.840114	−2203.335395	−2203.434928
^{s}**2**	0.489651	0.522922	0.523866	0.430052	−2214.625167	−2214.591896	−2214.590952	−2214.684766	−2205.017351	−2204.493485	−2204.587299
^{t}**2**	0.486443	0.519523	0.520467	0.425859	−2214.582285	−2214.549205	−2214.54826	−2214.642869	−2204.98465	−2204.464183	−2204.558791

^{s}3	0.592025	0.630523	0.631467	0.52722	−2354.370678	−2354.33218	−2354.331236	−2354.435483	−2343.914742	−2343.283275	−2343.387522
^{t}3	0.589799	0.629756	0.630701	0.520381	−2354.358155	−2354.318198	−2354.317254	−2354.427574	−2343.922088	−2343.291387	−2343.401707
^{s}4	0.610272	0.649026	0.64997	0.544854	−2355.549458	−2355.510703	−2355.509759	−2355.614875	−2345.105024	−2344.455054	−2344.56017
^{t}4	0.60751	0.64753	0.648474	0.538238	−2355.503008	−2355.462988	−2355.462044	−2355.572279	−2345.070216	−2344.421742	−2344.531978
^{s}5	0.472181	0.504913	0.505857	0.413387	−2217.272498	−2217.239765	−2217.238821	−2217.331291	−2207.651354	−2207.145497	−2207.237967
^{t}5	0.470259	0.504132	0.505076	0.407473	−2217.256401	−2217.222528	−2217.221584	−2217.319187	−2207.644786	−2207.13971	−2207.237313
^{s}6	0.490099	0.523059	0.524004	0.430935	−2218.44896	−2218.416	−2218.415055	−2218.508124	−2208.837369	−2208.313365	−2208.406434
^{t}6	0.487054	0.521328	0.522272	0.423794	−2218.398229	−2218.363955	−2218.363011	−2218.461489	−2208.796239	−2208.273967	−2208.372445
^{s}IM1−A	0.462735	0.493469	0.494414	0.406224	−2103.903701	−2103.872967	−2103.872022	−2103.960212	−2094.890969	−2094.396555	−2094.484745
^{t}IM1−A	0.461679	0.49328	0.494224	0.401914	−2103.914591	−2103.882989	−2103.882045	−2103.974355	−2094.919679	−2094.425455	−2094.517765
^{s}IM2−A	0.477997	0.509155	0.510099	0.42177	−2105.07785	−2105.046692	−2105.045748	−2105.134078	−2096.066285	−2095.556186	−2095.644515

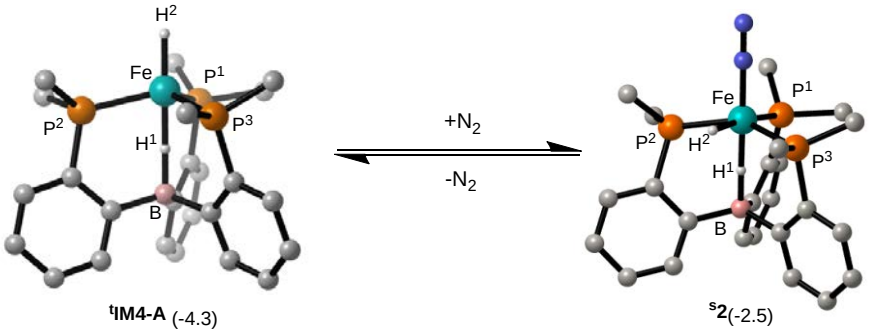
^{t}IM2−A	0.475683	0.508527	0.509471	0.415199	−2105.070914	−2105.03807	−2105.037125	−2105.131398	−2096.074992	−2095.565521	−2095.659793
^{s}TS1−A	0.47617	0.507113	0.508057	0.42006	−2105.078305	−2105.047362	−2105.046418	−2105.134415	−2096.064988	−2095.556931	−2095.644928
^{t}TS1−A	0.472942	0.505261	0.506206	0.412648	−2105.058716	−2105.026397	−2105.025453	−2105.11901	−2096.06326	−2095.557054	−2095.650612
^{s}IM3−A	0.478475	0.509441	0.510385	0.422348	−2105.078992	−2105.048027	−2105.047083	−2105.135119	−2096.068556	−2095.558171	−2095.646208
^{t}IM3−A	0.474922	0.507247	0.508191	0.415094	−2105.057299	−2105.024974	−2105.02403	−2105.117127	−2096.065302	−2095.557111	−2095.650208
^{s}TS2−A	0.477038	0.507732	0.508676	0.421002	−2105.048904	−2105.018211	−2105.017266	−2105.10494	−2096.039764	−2095.531088	−2095.618762
^{t}TS2−A	0.474958	0.506349	0.507293	0.416647	−2105.047843	−2105.016452	−2105.015508	−2105.106154	−2096.054199	−2095.546906	−2095.637552
^{s}IM4−A	0.479618	0.510967	0.511911	0.422241	−2105.073472	−2105.042123	−2105.041178	−2105.130849	−2096.075916	−2095.564005	−2095.653675
^{t}IM4−A	0.478421	0.510238	0.511183	0.418981	−2105.084486	−2105.052669	−2105.051725	−2105.143926	−2096.095703	−2095.58452	−2095.676722
^{s}TS−A	0.478177	0.509105	0.510049	0.421576	−2105.061617	−2105.030689	−2105.029745	−2105.118218	−2096.063142	−2095.553093	−2095.641566
^{s}IM5−A	0.480466	0.511431	0.512375	0.423984	−2105.068488	−2105.037523	−2105.036579	−2105.12497	−2096.073027	−2095.560652	−2095.649043

^{s}IM2'−A	0.478535	0.509836	0.51078	0.42187	−2105.05481	−2105.023509	−2105.022565	−2105.111475	−2096.05004	−2095.53926	−2095.62817
^{s}TS1'−A	0.476441	0.507509	0.508453	0.419937	−2105.055074	−2105.024006	−2105.023062	−2105.111578	−2096.050155	−2095.541702	−2095.630218
^{t}TS−1B	0.481959	0.516966	0.517910	0.417078	−2214.550654	−2214.515647	−2214.514703	−2214.615535	−2204.950907	−2204.432997	−2204.533829
^{t}TS−3B	0.602911	0.643177	0.644121	0.533322	-2355.469786	-2355.429520	-2355.428576	-2355.539375	-2345.027136	-2344.383015	-2344.493814
^{t}TS−5B[a]	0.483309	0.517515	0.518460	0.420363	-2218.384540	-2218.350333	-2218.349389	-2218.447485	-2208.7450678	-2208.226608	-2208.324705
^{s}IM1-C	0.485095	0.519461	0.520405	0.424047	-2214.544929	-2214.510563	-2214.509619	-2214.605978	-2204.929405	-2204.409	-2204.505358
^{s}IM2-C	0.486491	0.520483	0.521427	0.425683	-2214.554149	-2214.520157	-2214.519213	-2214.614957	-2204.941535	-2204.420108	-2204.515852
^{s}IM3-C	0.487612	0.521632	0.522577	0.425606	-2214.576241	-2214.542221	-2214.541277	-2214.638247	-2204.971123	-2204.448546	-2204.545517
^{t}IM1-C	0.483988	0.519531	0.520475	0.419390	-2214.556187	-2214.520644	-2214.519700	-2214.620785	-2204.949585	-2204.42911	-2204.530195
^{s}IM3-D	0.476493	0.508125	0.509069	0.418543	-2105.025397	-2104.993765	-2104.992820	-2105.083347	-2096.016726	-2095.507657	-2095.598183
^{s}TS-D	0.474818	0.506622	0.507566	0.416057	-2104.991983	-2104.960179	-2104.959235	-2105.050744	-2095.993359	-2095.485793	-2095.577302

[s]**IM4-D**	0.478383	0.510189	0.511133	0.419243	-2105.023911	-2104.992104	-2104.991160	-2105.083050	-2096.032699	-2095.521566	-2095.613456

- Ec, Uc, Hc and Gc designate zero−point correction and thermal correction to energy, enthalpy and Gibbs free energy, separately.
- E, U, H and G designate zero−point energies, thermal energies, thermal enthalpies, and thermal free energies.
- [a] The correction and free energy data (Ec, Uc, Hc, Gc, E, U, H and G) is based on the 6-311G** basis set for all the main group elements and a SDD basis set for Fe with SMD solvation model. And the solvation Energy is based on 6-31G* basis set for all the main group elements and a LanL2DZ basis set32 for Fe with SMD solvation model. This is because the single point energy refinements in benzene solvent with high basis set is not suitable for triplet transition state of (TPB)Fe(CO) with H_2, which seemly lead to singlet transition state. Indeed, several comparison are investigated and prove this adjustment is slightly change free energy data, and can not influence the comparison with other two complexes (TPB)Fe(N_2) and (TPB)Fe(CN^{t}Bu).

3. The equilibrium and Gibbs free energy between ^{t}IM4-A and ^{s}2



^{t}IM4-A (-4.3) ^{s}2(-2.5)

Figure S1. The equilibrium and Gibbs free energy between ^{t}**IM4-A** and ^{s}**2**. The Gibbs free energies relative to ^{t}**1** are provided next to each species in parentheses. All H atoms other than those originated from the dihydrogen molecule are omitted for clarity. Fe atom is depicted in cyan, B in pink, P in orange, C in gray, N in blue and O in red. Hydrogen atoms are omitted for clarity.

4. The IRC and scan curves of associative transition state in singlet state.

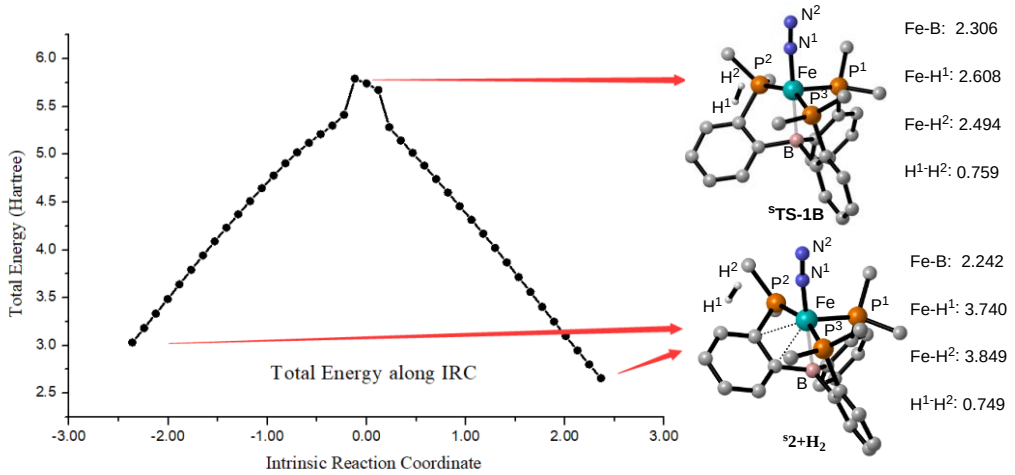


Figure S2. The IRC analysis and optimized structures of highest point and both end points.

The possible associative transition state (**^{s}TS-1B**) in singlet state ((TPB)Fe(N_2), for example) did not connect the desire reactant and product. The imaginary frequency is relatively small (-228.46 cm^{-1}), which is actually corresponding to a collision-like movement. Evidences can be obtained from the IRC analysis. The optimized structures of both end points of the IRC curve lead identically to the separate (TPB)Fe(L) complex and free H_2 molecule.

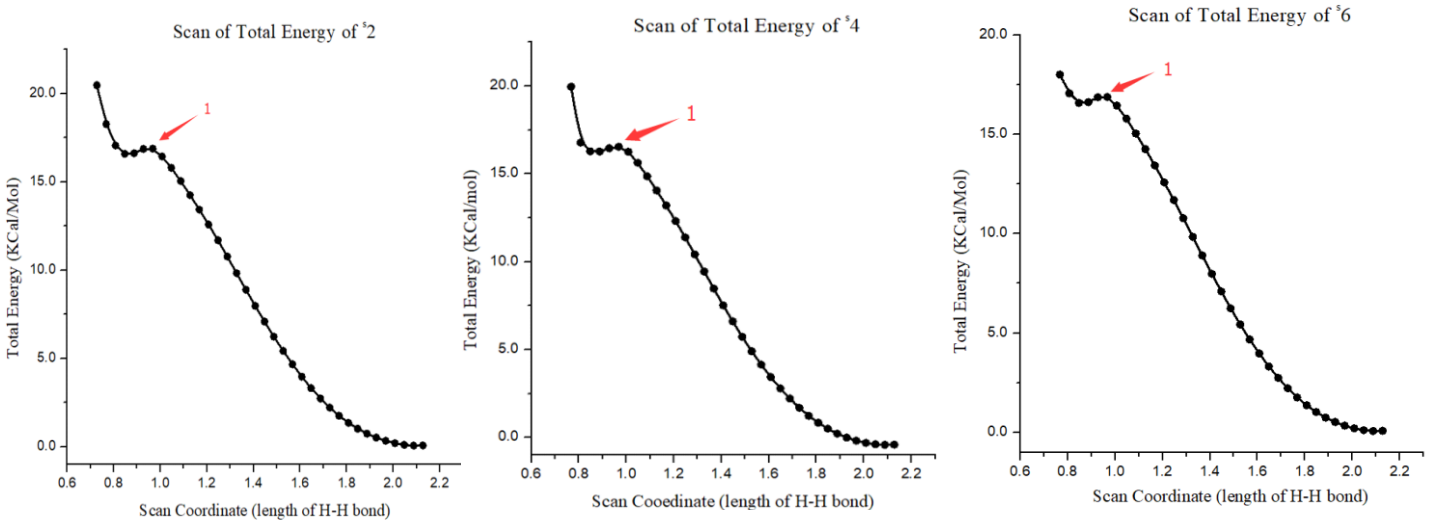


Figure S3. The curve of scanning length of H-H bond from product to reactant.

Exhaustive searching failed to locate the associative singlet transition states for both ^{s}**1**, ^{s}**3**, and ^{s}**5**. Further investigation by scanning, from product to reactant and from reactant to product, found there is no obvious point for transition state. Though a point with slight higher energy (point 1, Figure S3) is exist, location transition state with point 1 as initial structure actually lead to the wrong transition sate structure, exactly the same as previous sTS-1B. This is probably attributed to the strong Fe-B interaction, the rigid structure of the tetradentate ligand cage, and the steric hindrance caused by the interaction between Fe and one of the phenyl groups in singlet state complexes.

5. The energy surface profiles for the P-dissociated mechanism of hydrogen activation by complex 1.

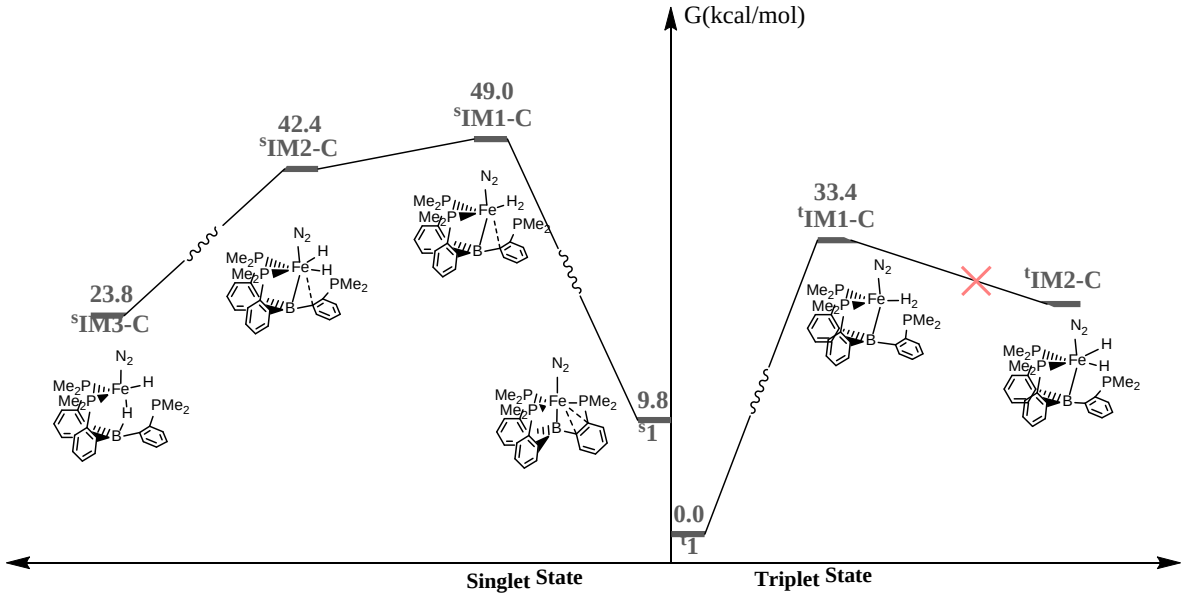


Figure S4. Potential energy surface profiles for the P-Dissociated Mechanism of hydrogen activation by catalyst 1. Solvent-corrected free energies are in kcal/mol, relative to catalyst ^{t}1.

The dissociation of one phosphine arm of the TPB ligand is another possible way to enable H_2 activation, in which the auxiliary ligand remains at the axial site. Due to the little influence of auxiliary ligand on this mechanism, the complex **1** is taken as an example to evaluate this pathway. In the Figure S2, the energy surface profile of some important intermediates for the P-Dissociated Mechanism of hydrogen activation by complex **1** is displayed. Obviously, for the singlet complex **1**, the free energies of intermediates ^{s}IM1-C and ^{s}IM2-C are over 40.0kcal/mol, which extremely higher than other two mechanisms (associative mechanism and L-dissociative mechanism). And their structures show the interaction between Fe with one of phenyl groups, which is as same as reactant ^{s}1.For triplet complex **1**, the intermediate **^{t}IM1-C** is partly distorted due to the weak dative interaction of H_2 molecule with Fe, even without the phenyl-Fe interaction. The free energy of **^{t}IM1-C** is 33.4kcal/mol (higher than other two mechanisms), and the next intermediate **^{t}IM2-C** is unable to be found for the unstable weak Fe-H interaction. The results indicate the mechanism with dissociation of phosphine arm is not suitable for H_2 activation by ferraboratrane complexes (TPB)Fe(L).

6. The energy surface profiles for the P-dissociated mechanism of H migration from $^{s/t}$IM3-A to $^{s/t}$IM4-A.

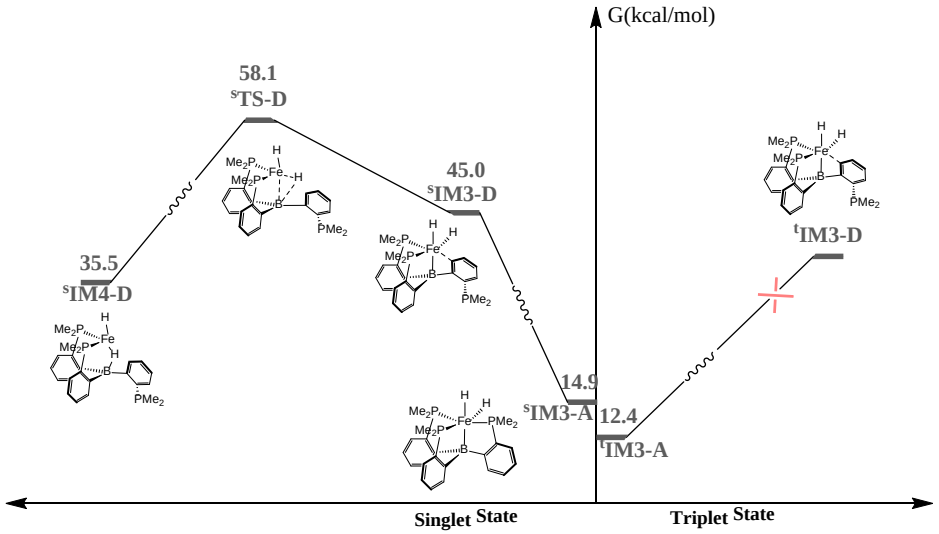


Figure S5. The energy surface profiles for the P-Dissociated Mechanism of H migration from $^{s/t}$**IM3-A** to $^{s/t}$**IM4-A**. Solvent-corrected free energies are in kcal/mol, relative to catalyst ^{t}**1**.

An alternative pathway for H migration after dissociation of one phosphine arm of the TPB ligand (Ref) is evaluated and the energy surface profiles for this possible pathway is shown in Figure S5. The results show this pathway is less favored for the following reasons. Firstly, the energy of the isomeric intermediate of singlet ^{s}**IM3-A** with dissociation of a phosphine arm, ^{s}**IM3-D,** is about 30 kcal/mol higher than ^{s}**IM3-A**, due to the strong interaction of Fe-P bond. Secondly, it should be noted that the triplet ^{t}**IM3-A** with dissociation of a phosphine arm is too unstable to be obtained. The two hydrides undergo reductive elimination to H_2 barrierlessly.

7. The Cartesian coordinates (xyz) for all optimized structures

CN^{t}Bu

C	2.394986	0.000487	0.000418
N	1.201982	0.000239	0.000612
C	−0.260822	−0.000124	−0.000046
C	−0.744047	−1.480998	−0.069099
H	−1.854039	−1.514000	−0.070516
H	−0.374644	−1.971950	−0.992992
H	−0.374501	−2.055801	0.805020
C	−0.744267	0.799948	−1.247935
H	−1.854219	0.819399	−1.274328
H	−0.373456	1.845064	−1.211993
H	−0.376538	0.329029	−2.182806
C	−0.745448	0.680610	1.316339
H	−1.855433	0.697935	1.343174
H	−0.379095	0.124700	2.203900
H	−0.374360	1.724412	1.378205

^{s}**1**

Fe	−0.302958	−0.837600	0.804133
P	−2.304613	−1.186885	−0.211604
P	1.959710	−0.934572	1.060936
P	−0.761455	1.144504	1.661075
C	−0.822604	1.800471	−0.975435
C	2.728437	0.400688	0.033941
C	−1.079629	−1.733347	−1.468535
C	2.710113	−0.760705	2.775280
H	2.448642	0.222898	3.210684
C	0.484479	2.228016	2.571456
H	0.739674	1.772391	3.551671
C	2.789848	−2.533772	0.519013
H	3.896568	−2.448884	0.571370
C	−1.340871	2.252192	0.277012
C	2.312662	2.160951	−1.586104
H	1.630118	2.729150	−2.239782
C	−2.160826	1.182329	2.925205
H	−2.395078	2.214414	3.264475
C	0.056202	−0.841196	−1.658705
B	0.237706	0.565848	−0.896504
C	−3.314857	−2.696376	0.252419
H	−3.916183	−3.076995	−0.600465
C	1.795948	1.076238	−0.819268
C	4.097604	0.763962	0.089152
H	4.793714	0.225833	0.755398
C	−3.643454	−0.129242	−1.004748
H	−4.356799	0.206707	−0.221981
C	−2.192510	3.377734	0.375374
H	−2.581709	3.710363	1.352853
C	−1.152921	−3.004505	−2.124899
H	−2.026181	−3.656009	−1.961451
C	1.101913	−1.360087	−2.513372
H	1.991479	−0.733223	−2.681299
C	4.575116	1.834942	−0.696485
H	5.636332	2.128767	−0.649116
C	1.003210	−2.587059	−3.180590
H	1.805193	−2.904869	−3.867854
C	−1.206711	2.526907	−2.137154
H	−0.836950	2.208060	−3.127205
C	3.673604	2.535668	−1.530610
H	4.035372	3.381114	−2.139691
C	−2.564996	4.073738	−0.798032
H	−3.240626	4.942425	−0.735454
C	−2.073938	3.643026	−2.052130
H	−2.370900	4.179708	−2.968884
C	−0.133784	−3.422975	−2.987490
H	−0.210336	−4.389331	−3.511805
N	−0.576534	−2.085587	2.129242
N	−0.729621	−2.811067	2.999872
H	−3.073234	0.729571	2.486036
H	−1.864794	0.576216	3.807416
H	0.058187	3.238033	2.749634
H	1.407700	2.330582	1.966914
H	2.294668	−1.556773	3.428548
H	3.816045	−0.860971	2.751504
H	2.458576	−3.359746	1.183740

H	2.490134	−2.772942	−0.520369
H	−2.647176	−3.498329	0.623579
H	−4.012300	−2.419449	1.071399
H	−4.196316	−0.726113	−1.761079
H	−3.199221	0.761050	−1.485371

^{t}1

Fe	0.008206	−0.015687	1.390953
P	−2.340127	0.392951	1.073055
P	1.544187	1.802672	1.044837
P	0.832339	−2.243862	1.017697
N	0.029832	−0.030321	3.363669
N	0.043046	−0.037948	4.500838
C	−2.626062	−0.508448	−0.523721
C	1.304295	−0.864537	−1.341737
C	0.084573	1.598338	−1.301835
C	1.751463	−1.993095	−0.574496
C	0.862259	2.521159	−0.523734
C	−1.442890	−0.687777	−1.317262
B	−0.015553	0.008614	−0.888030
C	1.032720	3.873544	−0.912604
H	1.635223	4.561518	−0.296077
C	0.412777	4.357714	−2.085190
H	0.536323	5.411551	−2.383417
C	−0.378100	3.479827	−2.860513
H	−0.876370	3.850332	−3.772293
C	−0.535547	2.129977	−2.471734
H	−1.159904	1.464659	−3.091321
C	2.037539	−0.585390	−2.533693
H	1.744870	0.283458	−3.146903
C	3.128103	−1.381582	−2.951663
H	3.668854	−1.129011	−3.879381
C	3.531099	−2.497873	−2.184501
H	4.383138	−3.119441	−2.504634
C	2.838720	−2.801265	−0.992036
H	3.163861	−3.661588	−0.383202
C	−1.598225	−1.446984	−2.515543
H	−0.713414	−1.627971	−3.148560
C	−2.846542	−1.975607	−2.915446
H	−2.922653	−2.558656	−3.848794
C	−3.997477	−1.762984	−2.123338
H	−4.972353	−2.175666	−2.430116
C	−3.883218	−1.027404	−0.923580
H	−4.777376	−0.876080	−0.295922
C	1.683831	3.236593	2.252476
H	0.675685	3.654905	2.450237
C	3.359861	1.453363	0.699683
H	3.879288	2.368799	0.343690
C	2.042265	−3.079816	2.188479
H	2.396907	−4.061768	1.808582
C	−0.371188	−3.650880	0.686333
H	−0.893941	−3.924394	1.627677
C	−2.965415	2.142952	0.784151
H	−2.918941	2.717611	1.733807
C	−3.636122	−0.256112	2.270066
H	−4.674156	−0.075784	1.917398
H	2.095298	2.855372	3.210851
H	2.346696	4.047411	1.881313
H	3.851826	1.094214	1.628783
H	3.436100	0.665604	−0.075359
H	−3.502470	0.251240	3.248697
H	−3.488547	−1.345336	2.420269
H	1.538510	−3.240644	3.164932
H	2.916669	−2.417374	2.353927
H	−1.120796	−3.316891	−0.057549
H	0.161130	−4.543626	0.293670
H	−2.319863	2.638028	0.032360
H	−4.013645	2.133528	0.415929

^{s}2

Fe	0.250561	−1.417570	−0.648931
P	−1.986614	−1.151595	−1.011505
P	2.325422	−0.598909	−1.104980
P	0.301251	−1.636619	1.645162
C	−0.650127	1.051420	1.673373
C	2.457729	1.205541	−0.579678

C	−2.291325	0.665261	−1.394304
C	3.898568	−1.398303	−0.441855
H	3.948007	−1.305932	0.660026
C	1.912446	−1.775958	2.615078
H	2.478571	−2.673659	2.287967
C	2.756444	−0.544596	−2.932345
H	3.748616	−0.076953	−3.108141
C	−0.487777	−0.143823	2.446912
C	1.543236	3.267951	0.338181
H	0.709515	3.836762	0.782352
C	−0.598971	−3.124250	2.363908
H	−0.527572	−3.175853	3.470555
C	−1.388621	1.660530	−0.885611
B	−0.160230	1.232072	0.114343
C	−2.636658	−2.092602	−2.497403
H	−3.725492	−1.948423	−2.656868
C	1.322265	1.916844	−0.060845
C	3.717608	1.852446	−0.711560
H	4.582326	1.303055	−1.118851
C	−3.348036	−1.525472	0.240260
H	−3.394377	−2.619350	0.430481
C	−0.906851	−0.195963	3.805008
H	−0.775223	−1.120804	4.390834
C	−3.412561	1.038914	−2.178311
H	−4.104638	0.272458	−2.563684
C	−1.657741	3.012482	−1.232503
H	−0.966632	3.800320	−0.890011
C	3.891359	3.196662	−0.326556
H	4.875143	3.681390	−0.434519
C	−2.768821	3.382514	−2.023444
H	−2.936156	4.442796	−2.275976
C	−1.269416	2.156760	2.327888
H	−1.452346	3.081251	1.754735
C	2.794211	3.905575	0.208678
H	2.914684	4.953459	0.529849
C	−1.500391	0.922329	4.423587
H	−1.825174	0.867347	5.475262
C	−1.684598	2.105524	3.674342
H	−2.161268	2.985284	4.137590
C	−3.656848	2.393682	−2.493820
H	−4.526187	2.668354	−3.113024
H	0.100463	0.093594	−0.383790
H	0.103807	−1.054714	−2.154643
N	0.469986	−3.175431	−1.081651
N	0.606810	−4.270106	−1.360778
H	3.873771	−2.478184	−0.701887
H	4.815844	−0.952767	−0.880484
H	2.761650	−1.580025	−3.334155
H	1.974206	0.030958	−3.465158
H	1.710427	−1.852882	3.704624
H	2.532960	−0.874425	2.437195
H	−0.142040	−4.043765	1.940291
H	−1.666960	−3.102728	2.070883
H	−2.444699	−3.174354	−2.334971
H	−2.080337	−1.773400	−3.400834
H	−4.336141	−1.184127	−0.135161
H	−3.127369	−1.003417	1.192961

ᵗ2

Fe	0.361860	−1.695105	−0.550636
P	−1.950366	−1.307642	−1.015434
P	2.209566	−0.364705	−1.342144
P	0.507311	−1.458262	1.863174
C	−0.804146	1.085916	1.703522
C	2.301526	1.376334	−0.638458
C	−2.259391	0.475653	−1.510312
C	3.931613	−1.086389	−1.089728
H	4.161844	−1.148985	−0.006786
C	2.240305	−1.143240	2.527005
H	2.907394	−1.988783	2.254314
C	2.229767	−0.051628	−3.193012
H	3.078993	0.602582	−3.484014
C	−0.483358	−0.028527	2.553868
C	1.330143	3.302614	0.488664
H	0.486879	3.782919	1.013297
C	0.008042	−2.951729	2.893511

H	0.228126	−2.830619	3.974757
C	−1.450991	1.524801	−0.945078
B	−0.275791	1.184162	0.148453
C	−2.710150	−2.353448	−2.375099
H	−3.806773	−2.211523	−2.472843
C	1.155256	1.978128	−0.011266
C	3.521439	2.098600	−0.770648
H	4.393374	1.637633	−1.262804
C	−3.193911	−1.588262	0.372928
H	−3.180178	−2.657406	0.676607
C	−0.915518	−0.061720	3.909248
H	−0.661722	−0.915286	4.558301
C	−3.296341	0.772700	−2.435127
H	−3.913121	−0.032634	−2.864498
C	−1.735786	2.849847	−1.380673
H	−1.114487	3.676265	−0.995895
C	3.644727	3.413577	−0.279508
H	4.597263	3.957470	−0.387968
C	−2.764441	3.145598	−2.301574
H	−2.946060	4.188682	−2.610788
C	−1.599547	2.117059	2.283370
H	−1.903086	2.967172	1.648787
C	2.539184	4.016459	0.359750
H	2.622622	5.040356	0.761142
C	−1.680931	0.991671	4.449889
H	−2.010477	0.952097	5.500881
C	−2.030128	2.084468	3.626205
H	−2.642728	2.907753	4.030385
C	−3.554564	2.102966	−2.829687
H	−4.359513	2.317552	−3.551457
H	0.023751	0.020848	−0.144104
H	0.204807	−1.746302	−2.107732
N	0.809091	−3.640297	−0.805691
N	1.052801	−4.731046	−0.977540
H	3.939437	−2.114844	−1.509223
H	4.727377	−0.497528	−1.592150
H	2.300152	−1.020674	−3.729909
H	1.277036	0.438343	−3.478115
H	2.227311	−1.028968	3.631791
H	2.636774	−0.211407	2.075765
H	0.568939	−3.833670	2.518368
H	−1.076175	−3.150421	2.767081
H	−2.512699	−3.420033	−2.137123
H	−2.217157	−2.119353	−3.340060
H	−4.220201	−1.316173	0.046264
H	−2.914806	−0.963320	1.243906

^{s}3

Fe	−0.560989	−0.066274	0.087831
P	0.222037	−0.985272	−1.758055
P	−0.616271	−1.941477	1.330655
P	−0.283019	2.138150	−0.329034
C	2.375866	1.393653	−0.198888
C	0.098814	−0.677320	2.456454
C	1.810577	−1.889811	−1.371031
C	−2.212647	−2.531905	2.117479
H	−2.902538	−1.675710	2.247819
C	−0.903525	3.312138	1.003154
H	−2.009239	3.231617	1.066594
C	0.381172	−3.537884	1.425220
H	0.322172	−3.959215	2.451589
C	1.528321	2.508189	−0.505461
C	1.570640	1.261149	2.722546
H	2.344201	1.939741	2.330809
C	−1.081127	2.933791	−1.834903
H	−0.878148	4.025169	−1.878341
C	2.423481	−1.330561	−0.207800
B	1.719002	0.009475	0.387504
C	−0.868893	−2.307457	−2.549807
H	−0.371482	−2.808984	−3.408134
C	1.143248	0.161939	1.882031
C	−0.409964	−0.440833	3.775931
H	−1.197133	−1.094942	4.183436
C	0.674173	−0.021964	−3.316937
H	−0.243178	0.389996	−3.788685
C	2.053233	3.752435	−0.935792

H	1.378691	4.596251	−1.161957
C	2.376695	−2.988568	−2.060006
H	1.890274	−3.405721	−2.958365
C	3.630972	−1.931606	0.245612
H	4.133658	−1.535095	1.144950
C	0.094347	0.598992	4.562414
H	−0.279891	0.753488	5.587652
C	4.194195	−3.043989	−0.425299
H	5.122188	−3.503749	−0.045449
C	3.774501	1.589449	−0.390792
H	4.465545	0.753232	−0.191946
C	1.097163	1.457192	4.024500
H	1.508852	2.272857	4.642399
C	3.446290	3.914694	−1.097645
H	3.857291	4.877693	−1.442329
C	4.304433	2.823364	−0.829791
H	5.393411	2.936537	−0.964670
C	3.572948	−3.571480	−1.580708
H	4.014024	−4.437373	−2.101323
N	−3.575806	0.252724	−0.090159
C	−2.370045	0.096583	−0.044045
C	−4.872149	0.180689	−0.771518
C	−5.707551	1.430315	−0.355030
H	−5.197000	2.365249	−0.668803
H	−6.710453	1.400432	−0.832232
H	−5.840674	1.460420	0.746573
C	−5.595846	−1.122672	−0.310161
H	−5.007659	−2.019609	−0.597182
H	−5.726204	−1.127381	0.792217
H	−6.598964	−1.193546	−0.783076
C	−4.656018	0.163611	−2.316593
H	−4.056900	−0.721310	−2.617439
H	−5.634023	0.121874	−2.843110
H	−4.119313	1.077439	−2.647602
H	−2.178837	2.777869	−1.779104
H	−0.703724	2.461866	−2.762863
H	−0.625025	4.364791	0.780115
H	−0.471624	3.017099	1.979551
H	1.353398	0.813706	−3.054711
H	1.184790	−0.683251	−4.048949
H	−1.804786	−1.831173	−2.910501
H	−1.138033	−3.069857	−1.790555
H	−0.038198	−4.278760	0.710978
H	1.437701	−3.350612	1.161324
H	−2.691941	−3.265677	1.434507
H	−2.040906	−3.032487	3.094525

ᵗ3

Fe	0.938510	0.004444	0.026230
P	0.308912	1.966955	−1.112226
P	0.257719	0.004069	2.283403
P	0.314586	−1.967189	−1.105335
C	−2.096993	−0.695769	−1.444873
C	−1.362906	−0.876465	2.480738
C	−1.323060	2.598971	−0.498393
C	1.400161	−0.833402	3.529963
H	1.541211	−1.897059	3.246166
C	0.069328	−3.531548	−0.083136
H	1.024282	−3.802983	0.416034
C	0.006985	1.664847	3.138163
H	−0.354540	1.526269	4.179655
C	−1.285367	−1.728449	−2.012091
C	−3.367966	−1.614727	1.324776
H	−3.993431	−1.665185	0.417632
C	1.500622	−2.624095	−2.418273
H	1.145836	−3.565124	−2.891277
C	−2.133728	1.572465	0.081154
B	−1.683772	−0.000549	−0.019549
C	1.466460	3.450826	−0.974553
H	1.107300	4.335673	−1.542995
C	−2.144481	−0.882940	1.282368
C	−1.795540	−1.530294	3.661051
H	−1.176786	−1.509565	4.573788
C	0.119314	1.875256	−2.984963
H	1.095724	1.613787	−3.446605
C	−1.675642	−2.433947	−3.177258

H	−1.034727	−3.229196	−3.593718
C	−1.738896	3.953112	−0.532037
H	−1.097430	4.726671	−0.986549
C	−3.370485	1.987498	0.657541
H	−4.019658	1.233922	1.134217
C	−3.018934	−2.236409	3.670678
H	−3.351570	−2.757623	4.583304
C	−3.785850	3.338895	0.642037
H	−4.746171	3.623625	1.104352
C	−3.304995	−0.384469	−2.135798
H	−3.951731	0.419654	−1.746595
C	−3.800050	−2.281714	2.494024
H	−4.750097	−2.842486	2.486909
C	−2.884551	−2.105960	−3.830536
H	−3.184063	−2.642765	−4.745669
C	−3.693943	−1.072000	−3.308479
H	−4.632597	−0.798484	−3.819541
C	−2.974867	4.327464	0.040556
H	−3.294501	5.382465	0.029556
N	4.051779	0.005617	0.032751
C	2.853510	0.005724	0.037603
C	5.506979	0.005777	0.013387
C	5.980311	−0.403480	−1.416854
H	5.605317	0.315093	−2.174887
H	7.090170	−0.413010	−1.457953
H	5.608665	−1.416167	−1.677635
C	6.014393	−1.022407	1.072807
H	5.661114	−0.746432	2.088110
H	5.646023	−2.042482	0.837370
H	7.124914	−1.040240	1.078038
C	6.003628	1.443482	0.364469
H	5.647886	1.746030	1.371322
H	7.113916	1.470363	0.359159
H	5.629587	2.179874	−0.376804
H	2.484307	−2.817562	−1.940148
H	1.643250	−1.856899	−3.207574
H	−0.259972	−4.379052	−0.721778
H	−0.698010	−3.340523	0.692699
H	−0.616772	1.085637	−3.234141
H	−0.230084	2.845079	−3.399573
H	2.463490	3.158647	−1.367102
H	1.582682	3.732001	0.092856
H	0.966638	2.224539	3.158116
H	−0.739241	2.253742	2.569205
H	2.389944	−0.330809	3.494981
H	1.015396	−0.786524	4.571536

^{s}4

Fe	0.865403	0.009238	−0.133082
P	0.367825	−2.145338	−0.649338
P	0.572275	2.176476	−0.730072
P	0.399854	0.033070	2.094788
C	−2.306680	−0.399334	1.303274
C	−1.260979	2.617267	−0.813566
C	−1.286163	−2.170915	−1.554638
C	1.340160	3.620306	0.212583
H	0.930269	3.678248	1.239179
C	0.560338	1.593621	3.144512
H	1.596837	1.987763	3.083627
C	1.180195	2.605696	−2.457230
H	0.944015	3.656122	−2.731026
C	−1.386757	−0.432433	2.401925
C	−3.627644	2.077134	−0.618625
H	−4.435631	1.360722	−0.395531
C	1.400441	−1.134840	3.181645
H	1.132460	−1.060311	4.256554
C	−2.234315	−1.113737	−1.335249
B	−1.920139	0.060052	−0.229366
C	1.573834	−2.969477	−1.829039
H	1.304548	−4.020590	−2.062924
C	−2.274930	1.627465	−0.575169
C	−1.619573	3.960180	−1.115706
H	−0.836980	4.712902	−1.307573
C	0.132359	−3.552076	0.591594
H	1.099988	−3.787308	1.084909
C	−1.820023	−0.805333	3.704277

H	−1.102802	−0.823078	4.541771
C	−1.587327	−3.238981	−2.438256
H	−0.860030	−4.051473	−2.599985
C	−3.453081	−1.180290	−2.064375
H	−4.190503	−0.368911	−1.948540
C	−2.969211	4.361108	−1.173809
H	−3.227600	5.406530	−1.408682
C	−3.746028	−2.237819	−2.954449
H	−4.700796	−2.245033	−3.506436
C	−3.651180	−0.783174	1.585655
H	−4.381534	−0.813260	0.759475
C	−3.979647	3.409999	−0.914798
H	−5.041186	3.707760	−0.939007
C	−3.160917	−1.162429	3.948848
H	−3.482253	−1.454201	4.962041
C	−4.080201	−1.154620	2.876246
H	−5.130161	−1.446578	3.045179
C	−2.813017	−3.278738	−3.138561
H	−3.027570	−4.109855	−3.830115
H	−0.668066	0.116492	−0.368881
H	0.992660	−0.093416	−1.683002
C	2.678626	−0.053289	−0.034647
N	3.878372	−0.093352	0.039301
C	5.307991	−0.078556	−0.241721
C	6.022268	0.740455	0.877872
H	5.841130	0.283977	1.873426
H	7.117500	0.762415	0.694306
H	5.647730	1.785382	0.898210
C	5.825130	−1.551328	−0.247192
H	5.640086	−2.035411	0.734503
H	5.311396	−2.142932	−1.033667
H	6.917285	−1.571017	−0.449203
C	5.537826	0.585311	−1.635755
H	5.157721	1.628409	−1.638467
H	6.622658	0.605717	−1.874707
H	5.010591	0.018055	−2.430638
H	1.174820	4.594386	−0.293895
H	2.434456	3.441070	0.283556
H	2.279656	2.453700	−2.501189
H	0.705514	1.916645	−3.183060
H	2.578529	−2.958653	−1.356052
H	1.623680	−2.378757	−2.765175
H	−0.244102	−4.466774	0.086053
H	−0.600748	−3.245388	1.364955
H	0.313655	1.387695	4.208049
H	−0.139507	2.366401	2.767740
H	1.262040	−2.181341	2.846943
H	2.473569	−0.873251	3.064593

ᵗ4

Fe	1.152953	−0.049442	−0.157301
P	0.224584	−2.214095	−0.795378
P	0.278577	1.949699	−1.318017
P	0.433803	0.232912	2.127354
C	−2.253857	−0.515041	1.502925
C	−1.426864	2.542007	−0.801107
C	−1.463649	−2.088820	−1.610958
C	1.341311	3.504049	−1.383924
H	1.402955	3.965102	−0.376187
C	0.345918	2.039738	2.645479
H	1.344128	2.511123	2.520891
C	0.023121	1.624148	−3.151940
H	−0.433738	2.500248	−3.659933
C	−1.265885	−0.428013	2.544271
C	−3.643376	2.100708	0.109234
H	−4.373645	1.410624	0.565217
C	1.573846	−0.460347	3.452471
H	1.294664	−0.146852	4.480147
C	−2.369521	−1.044152	−1.205816
B	−1.955939	0.016726	−0.025234
C	1.264838	−3.239363	−1.978029
H	0.864530	−4.261092	−2.147646
C	−2.362446	1.592941	−0.255408
C	−1.792109	3.906579	−0.969880
H	−1.074196	4.630404	−1.387829
C	−0.070415	−3.481544	0.570890

H	0.896169	−3.725908	1.062649
C	−1.561482	−0.851546	3.869648
H	−0.801786	−0.779503	4.664400
C	−1.833620	−3.016888	−2.621520
H	−1.139566	−3.814539	−2.930400
C	−3.622495	−0.989227	−1.880273
H	−4.326093	−0.180414	−1.618846
C	−3.076925	4.364068	−0.609893
H	−3.343953	5.424868	−0.747533
C	−3.989334	−1.912771	−2.883412
H	−4.971538	−1.830119	−3.378817
C	−3.513418	−1.072999	1.868564
H	−4.282182	−1.193728	1.086142
C	−4.007740	3.452497	−0.066320
H	−5.013439	3.797225	0.227950
C	−2.829269	−1.377656	4.193996
H	−3.044545	−1.703713	5.224754
C	−3.808136	−1.493675	3.182845
H	−4.798764	−1.917773	3.418541
C	−3.092349	−2.936449	−3.255310
H	−3.362556	−3.663351	−4.038934
H	−0.715522	0.029657	−0.106625
H	1.636942	−0.245230	−1.629294
C	3.061012	−0.011912	0.000300
N	4.254970	0.012862	0.066372
C	5.706138	0.014015	−0.078453
C	6.296221	1.070304	0.906427
H	6.027037	0.823677	1.954629
H	7.403330	1.086780	0.821637
H	5.910024	2.084324	0.672896
C	6.229111	−1.413782	0.273713
H	5.954812	−1.687128	1.313850
H	5.798691	−2.170086	−0.415025
H	7.335476	−1.441355	0.181841
C	6.054216	0.380337	−1.554751
H	5.663280	1.386936	−1.810903
H	7.156440	0.384084	−1.692108
H	5.612050	−0.357097	−2.256120
H	0.972320	4.262425	−2.106463
H	2.364418	3.198444	−1.689448
H	0.999366	1.380790	−3.621193
H	−0.647101	0.747803	−3.261461
H	2.282271	−3.326581	−1.541420
H	1.352140	−2.709681	−2.948389
H	−0.519470	−4.413133	0.164784
H	−0.755826	−3.050114	1.326842
H	0.021245	2.136986	3.703468
H	−0.381758	2.563979	1.994206
H	1.578779	−1.568754	3.400712
H	2.601257	−0.098472	3.238413

^{s}5

Fe	−0.299300	−0.876514	0.773116
P	−2.263905	−1.260830	−0.248080
P	1.948686	−0.929015	1.038088
P	−0.816709	1.081336	1.654998
C	−0.856389	1.826131	−0.953278
C	2.708457	0.455666	0.064287
C	−1.006752	−1.725181	−1.505397
C	2.677345	−0.791590	2.763495
H	2.395372	0.174790	3.223856
C	0.391604	2.156014	2.623104
H	0.649899	1.664031	3.584606
C	2.813361	−2.492858	0.455068
H	3.917871	−2.384773	0.511810
C	−1.402114	2.226971	0.304430
C	2.285101	2.273604	−1.490621
H	1.601595	2.856728	−2.130046
C	−2.237159	1.040982	2.892029
H	−2.517305	2.056226	3.246855
C	0.093266	−0.784221	−1.675606
B	0.232381	0.618529	−0.897932
C	−3.244853	−2.804650	0.152305
H	−3.838172	−3.165194	−0.715062
C	1.777478	1.150799	−0.774904
C	4.070612	0.837651	0.150350

H	4.767127	0.284626	0.803681
C	−3.614216	−0.203354	−1.023720
H	−4.332909	0.112653	−0.237483
C	−2.280724	3.329370	0.423410
H	−2.692020	3.622407	1.404416
C	−1.028064	−2.982971	−2.193013
H	−1.873440	−3.673205	−2.043551
C	1.158361	−1.241090	−2.542669
H	2.022572	−0.575977	−2.694343
C	4.540905	1.946624	−0.585873
H	5.596629	2.254507	−0.512499
C	1.105345	−2.450895	−3.243805
H	1.915902	−2.717481	−3.942509
C	−1.238298	2.578367	−2.098870
H	−0.846646	2.298634	−3.092258
C	3.639181	2.667010	−1.402309
H	3.994716	3.542154	−1.971708
C	−2.651028	4.052522	−0.734149
H	−3.346960	4.903735	−0.656035
C	−2.131960	3.671646	−1.992998
H	−2.427740	4.229259	−2.897491
C	0.002546	−3.336272	−3.069115
H	−0.037629	−4.290580	−3.618961
H	−3.122623	0.562637	2.425942
H	−1.933245	0.426641	3.765405
H	−0.061835	3.146240	2.841095
H	1.316899	2.308122	2.031999
H	2.265968	−1.612744	3.387174
H	3.784942	−0.872734	2.748039
H	2.496481	−3.341002	1.097890
H	2.520010	−2.711470	−0.590400
H	−2.558461	−3.602417	0.497079
H	−3.947590	−2.570864	0.980258
H	−4.159853	−0.792637	−1.791231
H	−3.177934	0.699558	−1.488100
C	−0.516710	−2.078283	2.062710
O	−0.638072	−2.804931	2.989497

5

Fe	−0.235095	−0.614276	−1.371948
P	−2.239374	0.540826	−1.154777
P	1.959509	0.021512	−1.608094
P	−0.320406	−2.323422	0.162711
C	−0.660203	−0.259950	1.979498
C	2.739283	0.396998	0.042461
C	−1.637403	2.120233	−0.359128
C	3.142239	−1.188705	−2.424773
H	3.178353	−2.123159	−1.828985
C	1.228288	−3.310636	0.596809
H	1.575815	−3.858438	−0.305348
C	2.301357	1.577924	−2.615261
H	3.382895	1.833282	−2.617765
C	−0.878620	−1.663046	1.815393
C	2.377497	0.760475	2.424582
H	1.702044	0.857916	3.290695
C	−1.512402	−3.741720	−0.176738
H	−1.481775	−4.533147	0.602683
C	−0.431880	2.009595	0.419242
B	0.210038	0.603154	0.918650
C	−3.063238	1.094239	−2.751428
H	−3.922349	1.778201	−2.582637
C	1.820467	0.560082	1.127271
C	4.139461	0.468898	0.250445
H	4.835084	0.338749	−0.595213
C	−3.747701	0.034777	−0.150460
H	−4.227224	−0.845242	−0.629892
C	−1.536175	−2.420460	2.815475
H	−1.702360	−3.501444	2.676303
C	−2.233336	3.380990	−0.601712
H	−3.154947	3.452744	−1.202035
C	0.148540	3.227902	0.884502
H	1.085713	3.186054	1.462567
C	4.660361	0.690882	1.544024
H	5.750126	0.738239	1.701579
C	−0.448838	4.485304	0.639141
H	0.028370	5.403090	1.020731

C	−1.158269	0.349248	3.167495
H	−1.033395	1.435911	3.311954
C	3.773082	0.830744	2.633539
H	4.168816	0.985860	3.650919
C	−2.003318	−1.795099	3.993722
H	−2.521969	−2.386859	4.765534
C	−1.818699	−0.405559	4.164241
H	−2.197406	0.094165	5.071262
C	−1.648882	4.565445	−0.097518
H	−2.120518	5.541773	−0.294947
H	−2.545917	−3.344817	−0.250926
H	−1.247235	−4.195161	−1.154765
H	1.037981	−4.041225	1.412340
H	2.027258	−2.610982	0.916460
H	2.748000	−1.435295	−3.432531
H	4.170375	−0.781525	−2.530204
H	1.960052	1.424474	−3.660994
H	1.730793	2.422243	−2.177478
H	−2.315983	1.596210	−3.399308
H	−3.428422	0.190335	−3.282651
H	−4.486295	0.862911	−0.090974
H	−3.428283	−0.245671	0.872074
C	−0.414165	−1.702584	−2.788158
O	−0.540741	−2.407922	−3.729329

s6

Fe	0.267969	−1.431978	−0.605577
P	−1.965714	−1.208324	−0.974858
P	2.318675	−0.591977	−1.089153
P	0.318818	−1.587161	1.678266
C	−0.647964	1.097796	1.653688
C	2.432775	1.229589	−0.620534
C	−2.310680	0.594613	−1.394902
C	3.902960	−1.354226	−0.413211
H	3.955477	−1.236109	0.685761
C	1.938800	−1.707659	2.633856
H	2.506438	−2.603836	2.305977
C	2.735701	−0.587533	−2.919716
H	3.719525	−0.110218	−3.114513
C	−0.465609	−0.076504	2.454475
C	1.493430	3.311137	0.223789
H	0.653530	3.885034	0.649122
C	−0.573309	−3.057370	2.439602
H	−0.506008	−3.071398	3.547527
C	−1.427182	1.620487	−0.914564
B	−0.180775	1.241556	0.083483
C	−2.599535	−2.192504	−2.438826
H	−3.689525	−2.065611	−2.604230
C	1.289203	1.943623	−0.125039
C	3.684514	1.886442	−0.778143
H	4.555554	1.333818	−1.167194
C	−3.313617	−1.584339	0.289063
H	−3.338373	−2.675114	0.498524
C	−0.861191	−0.096234	3.820557
H	−0.713117	−1.004434	4.427913
C	−3.446349	0.925765	−2.177461
H	−4.123325	0.135957	−2.541752
C	−1.731319	2.958414	−1.286736
H	−1.056844	3.769421	−0.965973
C	3.841516	3.245800	−0.442149
H	4.818896	3.738728	−0.569183
C	−2.856296	3.286189	−2.076438
H	−3.050013	4.336807	−2.349550
C	−1.264121	2.215415	2.290060
H	−1.462033	3.124279	1.697216
C	2.735881	3.959576	0.068615
H	2.843311	5.019897	0.351197
C	−1.451681	1.033836	4.420230
H	−1.758109	1.004010	5.478391
C	−1.657076	2.195908	3.643908
H	−2.132220	3.084088	4.092408
C	−3.724535	2.267481	−2.519165
H	−4.604380	2.508726	−3.137400
H	0.088592	0.092028	−0.377817
H	0.117405	−1.129363	−2.119602
H	3.891299	−2.439438	−0.649537

H	4.811191	−0.904352	−0.865786
H	2.753482	−1.634445	−3.289453
H	1.942563	−0.038821	−3.464607
H	1.745471	−1.779476	3.725241
H	2.552006	−0.803272	2.446299
H	−0.105888	−3.984744	2.046327
H	−1.640037	−3.055068	2.142483
H	−2.392260	−3.266870	−2.249751
H	−2.044899	−1.887263	−3.348099
H	−4.308071	−1.268165	−0.091318
H	−3.101524	−1.039945	1.231074
C	0.517236	−3.132182	−1.001330
O	0.685321	−4.262551	−1.285459

^{t}6

Fe	0.304611	1.795653	−0.459133
P	2.340481	0.487829	−0.931603
P	−1.875466	1.108136	−1.450283
P	0.002938	1.528039	1.918228
C	0.333753	−1.300046	1.686734
C	−2.658218	−0.404841	−0.667375
C	1.933625	−1.255860	−1.490014
C	−3.258599	2.371856	−1.612265
H	−3.646916	2.639787	−0.607921
C	−1.775368	1.812785	2.455182
H	−2.089752	2.840927	2.176626
C	−1.662043	0.567966	−3.236468
H	−2.614962	0.182386	−3.657124
C	0.419084	−0.170358	2.571545
C	−2.484768	−2.505283	0.552926
H	−1.883384	−3.252167	1.098367
C	0.923078	2.742504	3.013943
H	0.628993	2.670264	4.081632
C	0.761882	−1.912411	−0.969000
B	−0.198314	−1.170954	0.134359
C	3.470495	1.191383	−2.254236
H	4.418409	0.624487	−2.365463
C	−1.822525	−1.374836	−0.008550
C	−4.066015	−0.594763	−0.751680
H	−4.701698	0.150434	−1.255836
C	3.572199	0.222672	0.469541
H	3.955212	1.206824	0.815376
C	0.832439	−0.327018	3.923642
H	0.892741	0.543231	4.596602
C	2.777523	−1.911649	−2.426260
H	3.672878	−1.407115	−2.822472
C	0.496109	−3.223500	−1.456125
H	−0.411133	−3.742844	−1.103449
C	−4.678104	−1.737143	−0.196130
H	−5.769837	−1.869653	−0.270541
C	1.335367	−3.874480	−2.386844
H	1.088343	−4.890852	−2.736825
C	0.716534	−2.560378	2.231470
H	0.706336	−3.443624	1.570373
C	−3.879263	−2.698061	0.460596
H	−4.344440	−3.592403	0.907960
C	1.179512	−1.596936	4.428717
H	1.499807	−1.705172	5.477632
C	1.126798	−2.718495	3.572192
H	1.412173	−3.715067	3.948568
C	2.486036	−3.218515	−2.872757
H	3.149317	−3.712827	−3.601224
H	−0.039049	0.031590	−0.155271
H	0.539350	1.943050	−1.993766
H	−2.829021	3.286141	−2.073235
H	−4.101520	2.022139	−2.244892
H	−1.303388	1.427386	−3.840864
H	−0.896213	−0.232872	−3.272739
H	−1.880432	1.680759	3.553092
H	−2.430458	1.082209	1.939712
H	0.699731	3.768274	2.653689
H	2.016025	2.574001	2.926456
H	3.714778	2.237069	−1.971496
H	2.937001	1.213940	−3.226126
H	4.426201	−0.402528	0.131887
H	3.066585	−0.283753	1.314793

C	0.583964	3.588050	−0.718671
O	0.773716	4.719729	−0.961708

^{s}IM1−A

Fe	0.184661	0.592494	1.101874
P	0.891532	−1.447611	1.521026
P	2.135682	1.547337	0.451456
P	−2.062598	0.432002	1.373098
C	−1.616060	−0.859438	−1.035903
C	0.899281	2.323843	−0.669841
C	1.612490	−1.960748	−0.127903
C	2.853412	2.931641	1.502399
H	2.046890	3.432163	2.076143
C	−3.083751	2.014488	1.283595
H	−2.888326	2.633381	2.186022
C	3.662856	1.034825	−0.518303
H	4.136487	1.920815	−0.992468
C	−2.635147	−0.599811	−0.060091
C	−1.181530	2.048776	−1.930380
H	−1.971433	1.406923	−2.351736
C	−2.848615	−0.349269	2.896306
H	−3.956139	−0.389246	2.818724
C	1.084182	−1.202571	−1.222513
B	−0.131067	−0.171141	−0.877281
C	2.284763	−1.744565	2.764037
H	2.650754	−2.793934	2.753604
C	−0.104185	1.411370	−1.207889
C	0.807005	3.738367	−0.869450
H	1.577434	4.403128	−0.445870
C	−0.216256	−2.908194	1.971379
H	−0.571938	−2.808259	3.019409
C	−3.941506	−1.138232	−0.178903
H	−4.707978	−0.923739	0.585882
C	2.606791	−2.950384	−0.318222
H	2.999935	−3.527630	0.535986
C	1.620283	−1.473211	−2.513347
H	1.249171	−0.902682	−3.382747
C	−0.239011	4.290728	−1.619901
H	−0.284684	5.377780	−1.795900
C	2.625055	−2.451023	−2.709664
H	3.026831	−2.633311	−3.720796
C	−1.980199	−1.714330	−2.117228
H	−1.222552	−1.964702	−2.878835
C	−1.239027	3.430756	−2.155671
H	−2.060753	3.855845	−2.756554
C	−4.268780	−1.966114	−1.274300
H	−5.282528	−2.388925	−1.367645
C	−3.278641	−2.256721	−2.241115
H	−3.521621	−2.912381	−3.094390
C	3.116385	−3.196716	−1.614113
H	3.897473	−3.959777	−1.765813
H	−2.580426	0.253557	3.790225
H	−2.460769	−1.376949	3.037435
H	−4.171173	1.791265	1.231851
H	−2.787179	2.593329	0.386354
H	3.391551	3.689946	0.894010
H	3.574265	2.491616	2.223905
H	4.392788	0.560389	0.172160
H	3.383338	0.300182	−1.296511
H	3.132889	−1.064421	2.543088
H	1.911124	−1.514122	3.784617
H	0.335913	−3.867128	1.872348
H	−1.093180	−2.928981	1.293599

^{t}IM1−A

Fe	0.002129	−0.000206	−1.404833
P	−0.299221	2.351918	−1.288243
P	2.191480	−0.914822	−1.288337
P	−1.890130	−1.431621	−1.291248
C	−1.599140	−0.031029	1.131688
C	1.912492	−1.840224	0.308106
C	0.644452	2.574275	0.306944
C	2.924968	−2.182611	−2.473610
H	2.202117	−3.010379	−2.624317
C	−1.729870	−3.279771	−0.962675
H	−1.436920	−3.799686	−1.900010

C	3.705881	0.157463	−0.962349
H	4.560425	−0.452056	−0.597225
C	−2.551809	−0.725620	0.304176
C	0.522351	−2.152288	2.285097
H	−0.318960	−1.841154	2.926876
C	−3.352501	−1.429070	−2.479255
H	−4.204067	−2.043978	−2.116701
C	0.774253	1.399628	1.130696
B	0.000250	−0.000091	0.790861
C	0.424623	3.619335	−2.478688
H	0.307043	4.664990	−2.121730
C	0.826641	−1.370300	1.130003
C	2.654345	−2.996892	0.658080
H	3.480354	−3.344372	0.015656
C	−1.987293	3.119323	−0.958466
H	−2.588561	3.106703	−1.892916
C	−3.923842	−0.791741	0.657560
H	−4.640869	−1.327328	0.013488
C	1.276417	3.794202	0.658946
H	1.169480	4.683536	0.016091
C	1.595308	1.526899	2.291702
H	1.738236	0.644152	2.937389
C	2.337878	−3.728090	1.823631
H	2.920021	−4.625697	2.089123
C	2.222621	2.742477	2.644419
H	2.840656	2.798665	3.556320
C	−2.120670	0.615720	2.292772
H	−1.428393	1.182164	2.938095
C	1.261705	−3.304270	2.634676
H	0.996804	−3.874285	3.541070
C	−4.394868	−0.161965	1.830118
H	−5.462755	−0.218079	2.097523
C	−3.487201	0.550601	2.644890
H	−3.845743	1.057864	3.556347
C	2.059144	3.885615	1.830772
H	2.543975	4.838383	2.099540
H	−3.015943	−1.840250	−3.454580
H	−3.697249	−0.387139	−2.639943
H	−2.686728	−3.707865	−0.593682
H	−0.940807	−3.444445	−0.202662
H	3.889918	−2.602002	−2.115485
H	3.099997	−1.689634	−3.453304
H	4.003233	0.674939	−1.899721
H	3.449930	0.919896	−0.200277
H	1.501777	3.406579	−2.636726
H	−0.096861	3.522872	−3.454582
H	−1.894539	4.167080	−0.599412
H	−2.509411	2.514215	−0.190885

^{s}IM2−A

Fe	0.202861	0.739295	1.104322
P	2.171852	1.533987	0.358217
P	−2.049376	0.569312	1.301949
P	0.862155	−1.326124	1.536429
C	1.059248	−1.345251	−1.172743
C	−2.647229	−0.577343	−0.029494
C	0.924635	2.215906	−0.808558
C	−2.825830	−0.068546	2.892325
H	−2.450471	−1.085018	3.119947
C	−0.279858	−2.717686	2.101510
H	−0.630506	−2.525267	3.137642
C	−3.060970	2.141330	1.077733
H	−4.149040	1.919935	1.029563
C	1.598092	−2.017691	−0.033470
C	−2.007989	−1.883950	−1.975913
H	−1.252808	−2.220347	−2.705808
C	2.225741	−1.540110	2.823609
H	2.576192	−2.592563	2.896031
C	−0.091949	1.276754	−1.264222
B	−0.134442	−0.282581	−0.861345
C	2.990005	2.996378	1.203220
H	3.557121	3.636445	0.493442
C	−1.629645	−0.950204	−0.967952
C	−3.969065	−1.081049	−0.119151
H	−4.735146	−0.776458	0.614739
C	3.644260	0.844460	−0.590417

H	4.371303	0.406725	0.126895
C	2.570936	−3.037518	−0.156085
H	2.976195	−3.544664	0.736035
C	0.862981	3.607182	−1.151609
H	1.647011	4.292946	−0.792859
C	−1.166538	1.865166	−2.034740
H	−1.971112	1.201612	−2.388273
C	−4.310659	−1.993893	−1.140500
H	−5.334938	−2.395754	−1.206705
C	−1.190619	3.214667	−2.403528
H	−2.000181	3.594606	−3.049024
C	1.547412	−1.736289	−2.450532
H	1.163671	−1.237606	−3.357614
C	−3.320916	−2.397934	−2.065725
H	−3.575279	−3.119496	−2.860325
C	3.044549	−3.398746	−1.438848
H	3.813412	−4.181621	−1.544682
C	2.533945	−2.743567	−2.582928
H	2.908906	−3.018388	−3.583227
C	−0.166411	4.100167	−1.958192
H	−0.186052	5.163703	−2.247149
H	0.395408	1.137513	2.677073
H	0.178688	1.927233	2.264577
H	0.257483	−3.689743	2.083099
H	−1.157119	−2.780012	1.427388
H	1.834816	−1.226434	3.814483
H	3.087081	−0.889324	2.569160
H	3.315782	0.052667	−1.288257
H	4.146664	1.657133	−1.157406
H	2.221869	3.604041	1.721324
H	3.700976	2.608889	1.963884
H	−2.747728	2.647437	0.143351
H	−2.867006	2.824534	1.931777
H	−3.934553	−0.099603	2.828284
H	−2.537017	0.607076	3.725338

^{t}IM2−A

Fe	0.008786	0.000745	−1.514381
P	−2.078468	−1.141981	−1.271081
P	0.036713	2.353775	−1.251515
P	2.070077	−1.179026	−1.240948
C	0.630718	−1.469417	1.123643
C	0.970309	2.466915	0.352802
C	−2.642780	−0.384282	0.330055
C	0.915121	3.529230	−2.429310
H	1.954524	3.178918	−2.595141
C	3.675087	−0.261843	−0.885831
H	4.039769	0.224419	−1.815811
C	−1.565589	3.295298	−0.955072
H	−1.364535	4.325421	−0.589890
C	1.667215	−2.077765	0.335960
C	1.716153	1.281603	2.340410
H	1.737296	0.376215	2.970204
C	2.686694	−2.502356	−2.428294
H	3.586985	−3.033190	−2.050644
C	−1.588671	0.167569	1.135583
B	−0.006431	−0.008598	0.720970
C	−3.532179	−0.971483	−2.454462
H	−4.448862	−1.480802	−2.086713
C	0.934421	1.270373	1.146897
C	1.713880	3.606015	0.752332
H	1.728273	4.513649	0.125935
C	−2.108526	−2.998183	−0.956894
H	−1.870715	−3.541021	−1.896660
C	2.277613	−3.298265	0.720908
H	3.071871	−3.747594	0.101498
C	−4.003135	−0.299073	0.720240
H	−4.795863	−0.728446	0.084938
C	−1.992030	0.831470	2.332548
H	−1.219085	1.289409	2.972433
C	2.461367	3.583363	1.949982
H	3.045106	4.466854	2.256073
C	−3.347052	0.924715	2.723311
H	−3.615155	1.447423	3.657026
C	0.228360	−2.180785	2.293494
H	−0.579741	−1.762133	2.916454

C	2.464415	2.411943	2.740351
H	3.055037	2.378883	3.671496
C	1.861432	−3.963430	1.894777
H	2.331647	−4.916154	2.188366
C	0.827922	−3.401522	2.677522
H	0.486664	−3.918359	3.590393
C	−4.359856	0.354202	1.920201
H	−5.418564	0.426588	2.218389
H	0.143630	−0.402924	−3.366222
H	−0.156923	0.343446	−3.382335
H	4.455389	−0.957488	−0.508812
H	3.484152	0.519174	−0.123805
H	2.943279	−2.020550	−3.395507
H	1.879128	−3.240813	−2.610107
H	−1.342412	−3.246601	−0.195888
H	−3.105819	−3.324428	−0.590981
H	−3.753712	0.103140	−2.617788
H	−3.249240	−1.420948	−3.429968
H	−2.166825	2.750934	−0.200521
H	−2.143746	3.351036	−1.902131
H	0.938413	4.575153	−2.054589
H	0.383572	3.517150	−3.404396

^{s}TS1−A

Fe	0.205703	0.759895	1.109783
P	2.185550	1.525544	0.394913
P	−2.037560	0.641560	1.292585
P	0.835765	−1.322481	1.529712
C	1.033872	−1.399606	−1.161377
C	−2.660153	−0.521863	−0.016038
C	0.981580	2.167559	−0.843990
C	−2.845466	0.072487	2.891155
H	−2.528397	−0.959414	3.137729
C	−0.341237	−2.664535	2.135522
H	−0.699078	−2.417870	3.157467
C	−2.994809	2.236298	1.014823
H	−4.088961	2.050041	0.956647
C	1.563072	−2.067562	−0.016186
C	−2.047643	−1.895921	−1.926118
H	−1.298749	−2.270013	−2.644003
C	2.191518	−1.519590	2.823849
H	2.513745	−2.577781	2.932753
C	−0.052312	1.238629	−1.276025
B	−0.139557	−0.316322	−0.852815
C	2.998725	3.012519	1.193576
H	3.603624	3.608433	0.476593
C	−1.650195	−0.945304	−0.941975
C	−3.992889	−0.996570	−0.097748
H	−4.752987	−0.655215	0.625961
C	3.663296	0.773576	−0.496501
H	4.374949	0.360234	0.250275
C	2.519587	−3.103598	−0.127929
H	2.919279	−3.606462	0.769065
C	0.956467	3.543363	−1.244507
H	1.748196	4.226601	−0.898819
C	−1.100073	1.816823	−2.087386
H	−1.916236	1.158527	−2.423109
C	−4.354178	−1.927399	−1.096147
H	−5.387766	−2.305917	−1.154687
C	−1.084102	3.148838	−2.517501
H	−1.873498	3.519628	−3.192300
C	1.512209	−1.809063	−2.436475
H	1.135943	−1.313102	−3.348051
C	−3.372751	−2.379826	−2.007223
H	−3.642245	−3.115883	−2.783210
C	2.984214	−3.484977	−1.408235
H	3.740462	−4.280781	−1.507916
C	2.482605	−2.833230	−2.558507
H	2.852668	−3.123830	−3.556081
C	−0.045898	4.025358	−2.091922
H	−0.032388	5.075456	−2.426901
H	0.373139	1.003327	2.633200
H	0.137198	2.007389	2.079057
H	1.809093	−1.157229	3.800722
H	3.068534	−0.901326	2.544231
H	0.175130	−3.647547	2.165574

H	−1.212092	−2.735947	1.454140
H	−2.786170	2.932816	1.854061
H	−2.650906	2.707528	0.073512
H	−3.954157	0.102425	2.826174
H	−2.517203	0.746431	3.710269
H	4.185949	1.550380	−1.094569
H	3.332996	−0.045604	−1.161393
H	2.218496	3.650671	1.652638
H	3.671981	2.650599	1.999730

^{t}TS1−A

Fe	0.137446	0.065641	−1.786921
P	2.280955	−0.735421	−1.106374
P	−1.963071	−0.962245	−1.421812
P	−0.048250	2.260892	−1.091535
C	0.706796	1.167238	1.321479
C	−2.669458	−0.584628	0.242966
C	1.877232	−1.904609	0.277510
C	−3.282671	−0.492299	−2.669849
H	−3.476530	0.597624	−2.610261
C	−1.742344	3.065918	−0.944489
H	−2.201707	3.139794	−1.952872
C	−2.000967	−2.838764	−1.540624
H	−3.024562	−3.232478	−1.361790
C	0.688931	2.405949	0.609330
C	−2.119157	0.221388	2.466027
H	−1.388756	0.592057	3.204262
C	0.857190	3.559034	−2.107670
H	0.762078	4.580380	−1.680438
C	0.687816	−1.566360	1.003794
B	−0.081585	−0.146566	0.753153
C	3.157297	−1.774750	−2.402475
H	4.095452	−2.232439	−2.021398
C	−1.670311	−0.144144	1.163374
C	−4.035941	−0.682387	0.604507
H	−4.786813	−1.024347	−0.127889
C	3.712138	0.318281	−0.487700
H	4.079950	0.959986	−1.316773
C	1.248522	3.585544	1.158217
H	1.225625	4.532575	0.593606
C	2.624367	−3.070638	0.571104
H	3.535454	−3.310042	−0.001935
C	0.277194	−2.484378	2.014254
H	−0.640179	−2.273482	2.587905
C	−4.445530	−0.320659	1.906310
H	−5.508702	−0.380708	2.190569
C	1.012754	−3.656948	2.303796
H	0.660323	−4.344980	3.090393
C	1.343272	1.163921	2.596494
H	1.399629	0.221304	3.166975
C	−3.481294	0.135177	2.833928
H	−3.794523	0.432854	3.848620
C	1.864445	3.552943	2.429721
H	2.312273	4.467357	2.851765
C	1.916989	2.335217	3.143864
H	2.410967	2.296354	4.129199
C	2.193274	−3.952264	1.587699
H	2.767375	−4.867009	1.807431
H	−0.209342	0.693837	−3.237014
H	0.252721	−0.636687	−3.212011
H	0.434300	3.556920	−3.133551
H	1.932521	3.294003	−2.175039
H	−1.666364	4.082414	−0.502688
H	−2.390041	2.437812	−0.300705
H	−1.656455	−3.150663	−2.548791
H	−1.311522	−3.261415	−0.782239
H	−4.233083	−1.043831	−2.505158
H	−2.901081	−0.721850	−3.686138
H	4.546080	−0.323286	−0.130880
H	3.366410	0.965746	0.340869
H	2.471540	−2.571213	−2.754679
H	3.403514	−1.125527	−3.268744

^{s}IM3−A

Fe	−0.220785	0.763725	−1.135488
P	−2.262247	1.416158	−0.507344

P	2.007322	0.839243	−1.282667
P	−0.727193	−1.378480	−1.519771
C	−0.909083	−1.505951	1.146967
C	2.712944	−0.300139	0.010889
C	−1.220508	2.028450	0.897878
C	2.868367	0.373128	−2.884249
H	2.625971	−0.671485	−3.160891
C	0.561353	−2.588530	−2.167493
H	0.892097	−2.271063	−3.178815
C	2.838112	2.491095	−0.947829
H	3.943878	2.389600	−0.899616
C	−1.392116	−2.210184	0.005290
C	2.194692	−1.764994	1.884117
H	1.470460	−2.216943	2.582092
C	−2.070347	−1.634715	−2.811902
H	−2.322400	−2.710012	−2.935080
C	−0.087030	1.198652	1.269023
B	0.175368	−0.340230	0.821286
C	−3.119786	2.910932	−1.236289
H	−3.832910	3.387211	−0.529243
C	1.733252	−0.828648	0.914691
C	4.078261	−0.667659	0.100754
H	4.815372	−0.250463	−0.606585
C	−3.738577	0.502457	0.223634
H	−4.389852	0.130662	−0.596674
C	−2.271176	−3.312190	0.121425
H	−2.638553	−3.843197	−0.773065
C	−1.366327	3.347139	1.424218
H	−2.222921	3.966507	1.115201
C	0.868261	1.808826	2.158879
H	1.753890	1.224362	2.451702
C	4.504231	−1.586964	1.084581
H	5.564856	−1.880397	1.148035
C	0.682937	3.082506	2.717452
H	1.412581	3.477648	3.443306
C	−1.351051	−1.940277	2.425915
H	−1.010101	−1.414169	3.334287
C	3.554675	−2.138210	1.974092
H	3.875154	−2.866336	2.737911
C	−2.699841	−3.722405	1.405271
H	−3.395581	−4.570831	1.510880
C	−2.243608	−3.031990	2.552459
H	−2.589923	−3.345192	3.551581
C	−0.445639	3.860044	2.349254
H	−0.597302	4.861666	2.784054
H	−0.315506	0.713329	−2.657563
H	−0.139245	2.208986	−1.706730
H	−1.717025	−1.229515	−3.782001
H	−2.982790	−1.079346	−2.515525
H	0.140195	−3.614205	−2.231910
H	1.436354	−2.597370	−1.487424
H	2.567410	3.197058	−1.760391
H	2.463332	2.901731	0.010368
H	3.971496	0.481520	−2.809175
H	2.493123	1.043540	−3.685263
H	−4.335356	1.183337	0.867457
H	−3.394238	−0.361927	0.821755
H	−2.353816	3.642088	−1.560003
H	−3.685283	2.581459	−2.133849

^{t}IM3−A

Fe	−0.212905	0.061628	−1.838366
P	−2.224796	1.002244	−0.971236
P	1.985715	0.821776	−1.425446
P	−0.305826	−2.141197	−1.190313
C	−0.765839	−1.167168	1.345298
C	2.729651	0.263439	0.174412
C	−1.604958	2.071866	0.417070
C	3.170788	0.274253	−2.770202
H	3.246995	−0.831679	−2.767392
C	1.273763	−3.159468	−1.220065
H	1.674864	−3.178710	−2.255043
C	2.230062	2.684307	−1.435106
H	3.297823	2.950752	−1.282162
C	−0.950823	−2.335701	0.546623
C	2.207896	−0.620595	2.377044

H	1.479393	−0.954345	3.134246
C	−1.441861	−3.230057	−2.218133
H	−1.463882	−4.281831	−1.860783
C	−0.445485	1.568232	1.095997
B	0.144089	0.075510	0.819723
C	−3.069007	2.167822	−2.174045
H	−3.942235	2.689467	−1.726926
C	1.738619	−0.123159	1.126917
C	4.114598	0.182568	0.459906
H	4.860041	0.483240	−0.295407
C	−3.720082	0.095683	−0.273473
H	−4.191408	−0.506629	−1.079475
C	−1.627167	−3.473739	1.049967
H	−1.766155	−4.367705	0.419873
C	−2.174151	3.323565	0.754867
H	−3.062385	3.696259	0.218876
C	0.119367	2.403704	2.104175
H	1.020484	2.061475	2.638658
C	4.547728	−0.308516	1.711287
H	5.624283	−0.388978	1.933115
C	−0.442483	3.657231	2.438844
H	0.024967	4.276061	3.222755
C	−1.313592	−1.181127	2.660279
H	−1.211848	−0.286226	3.297486
C	3.588593	−0.712408	2.667001
H	3.918294	−1.110289	3.641188
C	−2.152937	−3.463760	2.361881
H	−2.691386	−4.344185	2.748719
C	−2.000480	−2.310651	3.163282
H	−2.423905	−2.288056	4.181246
C	−1.594985	4.120089	1.768353
H	−2.034036	5.098822	2.021073
H	0.004342	−0.736368	−3.225045
H	−0.255615	1.106438	−3.020794
H	−1.085003	−3.208412	−3.267802
H	−2.471674	−2.817449	−2.193452
H	1.085334	−4.200049	−0.880018
H	2.023881	−2.690904	−0.552167
H	1.879461	3.090466	−2.406204
H	1.623244	3.130809	−0.621704
H	4.183308	0.712756	−2.640001
H	2.754776	0.591150	−3.748214
H	−4.466432	0.819561	0.118080
H	−3.404139	−0.581954	0.542360
H	−2.330580	2.909691	−2.537147
H	−3.415420	1.576134	−3.047198

^{s}TS2−A

Fe	0.190367	−0.654673	−1.485189
P	−2.007918	−0.105402	−1.638888
P	2.364444	−0.142318	−1.448135
P	−0.012310	−2.304647	−0.005974
C	−0.723256	−0.329903	1.757087
C	2.661132	0.829500	0.111158
C	−2.124412	1.513388	−0.726323
C	3.782339	−1.387879	−1.491401
H	3.758401	−2.046191	−0.602584
C	1.529194	−3.204416	0.589773
H	2.047012	−3.682482	−0.266819
C	2.949587	0.983907	−2.837649
H	4.016573	1.268767	−2.716284
C	−0.772030	−1.742722	1.590279
C	1.829769	1.680318	2.231291
H	1.015304	1.819963	2.960484
C	−1.043015	−3.798326	−0.505624
H	−1.134036	−4.536837	0.318718
C	−1.033039	1.798708	0.159075
B	0.000770	0.635361	0.657146
C	−2.493060	0.306606	−3.408575
H	−3.511076	0.746183	−3.470085
C	1.546520	1.041697	0.984529
C	3.962896	1.280432	0.457939
H	4.807501	1.110993	−0.230878
C	−3.537704	−1.051741	−1.077158
H	−3.680389	−1.953578	−1.709953
C	−1.366192	−2.586709	2.564428

H	−1.394494	−3.679208	2.417173
C	−3.140436	2.465513	−0.972290
H	−3.973554	2.228572	−1.655999
C	−0.993179	3.101145	0.731551
H	−0.153161	3.375050	1.390360
C	4.197873	1.940758	1.680319
H	5.210859	2.289749	1.938503
C	−2.000810	4.060545	0.474113
H	−1.932827	5.061634	0.931841
C	−1.330642	0.207024	2.930865
H	−1.362601	1.299967	3.074957
C	3.121887	2.130502	2.575129
H	3.290591	2.624189	3.546598
C	−1.935336	−2.029656	3.728390
H	−2.401129	−2.681769	4.485056
C	−1.919620	−0.626570	3.905508
H	−2.380657	−0.180865	4.802605
C	−3.087576	3.742087	−0.366509
H	−3.877301	4.484104	−0.567245
H	0.443778	−2.059136	−2.084387
H	0.247163	0.863523	−1.954994
H	−0.552830	−4.286009	−1.373309
H	−2.056572	−3.477805	−0.815983
H	1.255169	−3.984982	1.331219
H	2.215999	−2.482394	1.075085
H	2.828816	0.456904	−3.808707
H	2.319717	1.894565	−2.853496
H	4.771259	−0.884306	−1.534924
H	3.665911	−2.017925	−2.398790
H	−4.444627	−0.414894	−1.154279
H	−3.412530	−1.369016	−0.022008
H	−1.757839	1.021581	−3.828222
H	−2.470390	−0.623410	−4.014948

^{t}TS2−A

Fe	−0.190228	0.672433	−1.541953
P	2.120303	0.317789	−1.571836
P	−2.232172	−0.221220	−1.547097
P	−0.490020	2.394416	0.009531
C	0.548841	0.461281	1.700188
C	−2.507351	−1.214235	0.005214
C	2.401520	−1.240027	−0.585769
C	−3.779155	0.833272	−1.719957
H	−3.896837	1.503124	−0.847341
C	−2.133832	3.136852	0.550936
H	−2.659422	3.573104	−0.323870
C	−2.522746	−1.432376	−2.950542
H	−3.523560	−1.908953	−2.873312
C	0.281515	1.860962	1.605900
C	−1.640667	−1.995112	2.136811
H	−0.835536	−2.051169	2.887706
C	0.410896	3.976065	−0.469848
H	0.325215	4.765535	0.307434
C	1.329516	−1.675169	0.262989
B	0.074665	−0.680292	0.607232
C	2.708051	−0.099537	−3.305405
H	3.763981	−0.443831	−3.320384
C	−1.399521	−1.312127	0.905910
C	−3.760989	−1.808733	0.308301
H	−4.599755	−1.724880	−0.403080
C	3.466318	1.497670	−0.996314
H	3.464347	2.407895	−1.632689
C	0.625796	2.757391	2.651228
H	0.408809	3.834468	2.551508
C	3.578716	−2.011320	−0.740809
H	4.396168	−1.658393	−1.392494
C	1.483937	−2.945682	0.885234
H	0.668827	−3.338274	1.514500
C	−3.952942	−2.503682	1.519383
H	−4.928298	−2.962526	1.749038
C	2.650130	−3.727685	0.715316
H	2.728040	−4.709635	1.211144
C	1.218958	0.021231	2.883563
H	1.489947	−1.042395	2.985025
C	−2.885271	−2.586419	2.440693
H	−3.025133	−3.107334	3.402465

C	1.262036	2.285108	3.816927
H	1.534961	2.983651	4.624489
C	1.562779	0.908358	3.925624
H	2.077401	0.525934	4.822854
C	3.711131	−3.256198	−0.085807
H	4.624852	−3.857696	−0.218314
H	−0.832783	1.402958	−2.878329
H	−0.095644	−0.886789	−1.523121
H	−0.026899	4.353606	−1.417569
H	1.483137	3.758333	−0.645916
H	−1.973874	3.932991	1.308994
H	−2.770170	2.346551	0.997982
H	−2.447841	−0.887689	−3.914462
H	−1.739574	−2.215808	−2.924006
H	−4.689727	0.203851	−1.813493
H	−3.669421	1.453223	−2.633167
H	4.467827	1.020556	−1.053492
H	3.269176	1.792045	0.054241
H	2.056462	−0.892776	−3.723435
H	2.610245	0.804408	−3.941863

^{s}IM4−A

Fe	0.081684	−1.118776	−1.363282
P	−2.151719	−0.548600	−1.412997
P	2.208375	−0.349467	−1.556850
P	0.172627	−2.360398	0.436022
C	−0.369291	0.030874	1.875831
C	2.574072	1.008745	−0.298371
C	−2.321102	1.226699	−0.779318
C	3.809955	−1.314794	−1.745508
H	4.091416	−1.781170	−0.780112
C	1.825454	−3.126144	0.900964
H	2.188591	−3.758438	0.064251
C	2.183390	0.595821	−3.192007
H	3.091445	1.226889	−3.298703
C	−0.300032	−1.398669	1.965331
C	1.903230	2.546663	1.466912
H	1.146370	2.938995	2.166032
C	−0.914941	−3.888739	0.442025
H	−0.775999	−4.502999	1.356861
C	−1.282270	1.817789	0.025129
B	−0.003376	0.911515	0.528806
C	−2.761930	−0.456018	−3.191048
H	−3.778234	−0.018737	−3.281431
C	1.528200	1.521407	0.550559
C	3.892906	1.535196	−0.220536
H	4.687428	1.142158	−0.875490
C	−3.592496	−1.431892	−0.588760
H	−3.695829	−2.451128	−1.016513
C	−0.588987	−2.072666	3.184405
H	−0.526413	−3.172710	3.237233
C	−3.481562	1.971238	−1.120494
H	−4.280198	1.510519	−1.725680
C	−1.467557	3.174998	0.411099
H	−0.679086	3.674336	0.997723
C	4.216591	2.563340	0.687802
H	5.244342	2.958563	0.734044
C	−2.615681	3.916757	0.056561
H	−2.712028	4.968369	0.374350
C	−0.768225	0.720631	3.058903
H	−0.873188	1.818330	3.026895
C	3.211759	3.068056	1.540243
H	3.448574	3.862918	2.266913
C	−0.962557	−1.354016	4.337007
H	−1.187537	−1.886226	5.275539
C	−1.057356	0.054067	4.267045
H	−1.363385	0.631985	5.155017
C	−3.636698	3.310676	−0.705218
H	−4.540299	3.876099	−0.985348
H	0.107690	0.176462	−0.478317
H	0.106275	−2.376211	−2.305642
H	1.734121	−3.746865	1.817887
H	2.563177	−2.320754	1.092412
H	3.624805	−2.122084	−2.484082
H	4.653931	−0.688481	−2.103205
H	2.129864	−0.122557	−4.036641

H	1.293621	1.259360	−3.228736
H	−2.767646	−1.484835	−3.606683
H	−2.057123	0.155056	−3.793034
H	−3.399070	−1.514182	0.500131
H	−4.540554	−0.874170	−0.741700
H	−1.980007	−3.596681	0.362118
H	−0.650436	−4.494359	−0.448749

^{t}IM4−A

Fe	0.007843	−0.000271	−1.898787
P	1.911488	−1.294392	−1.369674
P	−2.070878	−0.997986	−1.388996
P	0.182559	2.296332	−1.375570
C	0.550096	1.500750	1.364558
C	−2.553930	−0.759999	0.406982
C	1.933167	−1.827048	0.428237
C	−3.545375	−0.367761	−2.368907
H	−3.668470	0.720184	−2.190811
C	−1.337297	3.369221	−1.653253
H	−1.616960	3.338200	−2.727349
C	−2.234371	−2.853794	−1.652338
H	−3.236919	−3.222192	−1.346649
C	0.612388	2.586492	0.426347
C	−2.060912	−0.051742	2.680229
H	−1.369946	0.372941	3.427015
C	1.481598	3.255393	−2.336387
H	1.517855	4.331343	−2.064680
C	1.015110	−1.238841	1.363174
B	−0.006124	−0.002908	0.981862
C	2.125450	−2.887103	−2.343625
H	3.048496	−3.441018	−2.072026
C	−1.589548	−0.270360	1.351903
C	−3.886818	−1.049789	0.808887
H	−4.614762	−1.435780	0.075941
C	3.597547	−0.496406	−1.617437
H	3.727113	−0.233454	−2.688440
C	1.020308	3.884645	0.839340
H	1.053675	4.712386	0.111382
C	2.850482	−2.832192	0.841298
H	3.557990	−3.268035	0.116318
C	1.049078	−1.754963	2.692390
H	0.326906	−1.370253	3.431255
C	−4.306791	−0.845376	2.138276
H	−5.344249	−1.071074	2.433865
C	1.953043	−2.758244	3.099155
H	1.937957	−3.124041	4.139371
C	0.963606	1.793113	2.698034
H	0.981566	0.978278	3.440567
C	−3.385401	−0.331398	3.076285
H	−3.700430	−0.143332	4.116220
C	1.395212	4.139654	2.173410
H	1.712318	5.150318	2.477733
C	1.376003	3.079014	3.104957
H	1.687418	3.252718	4.148469
C	2.871265	−3.296310	2.171556
H	3.585477	−4.078600	2.475752
H	−0.001397	0.000136	−0.282705
H	0.014550	0.002064	−3.478684
H	−1.156827	4.423226	−1.351983
H	−2.179886	2.966234	−1.054655
H	−3.331805	−0.520537	−3.447293
H	−4.493168	−0.885370	−2.110430
H	−2.068972	−3.089690	−2.724709
H	−1.463377	−3.376491	−1.049893
H	2.162833	−2.628113	−3.422261
H	1.247608	−3.543718	−2.174604
H	3.653594	0.432599	−1.013717
H	4.419513	−1.175293	−1.304791
H	2.478866	2.804497	−2.156177
H	1.249136	3.162410	−3.417716

^{s}TS−A

Fe	−0.017796	0.494955	−1.705844
P	2.195267	−0.027801	−1.460971
P	−2.144017	−0.264397	−1.660388
P	−0.150600	2.343903	−0.401969

C	0.472583	0.660393	1.798370
C	−2.582783	−0.899952	0.065505
C	2.187372	−1.562400	−0.355505
C	−3.659307	0.690265	−2.241021
H	−3.854028	1.553482	−1.574624
C	−1.811590	3.188822	−0.138964
H	−2.226728	3.513536	−1.116455
C	−2.319020	−1.823437	−2.695139
H	−3.298083	−2.318625	−2.519268
C	0.420763	2.020413	1.348068
C	−1.999075	−1.551685	2.342229
H	−1.261753	−1.639683	3.157902
C	0.865824	3.800611	−1.013882
H	0.710820	4.713153	−0.400268
C	1.149003	−1.741960	0.627010
B	−0.004012	−0.604766	0.865290
C	3.126075	−0.543138	−3.005438
H	4.179270	−0.835205	−2.808340
C	−1.572252	−1.045003	1.079926
C	−3.927936	−1.276042	0.334234
H	−4.698553	−1.172111	−0.447058
C	3.504287	1.052202	−0.636642
H	3.750783	1.909629	−1.299135
C	0.797944	3.088940	2.205770
H	0.751783	4.131426	1.848887
C	3.208352	−2.537272	−0.504173
H	3.999634	−2.403802	−1.258822
C	1.194810	−2.929899	1.407486
H	0.394714	−3.113746	2.143753
C	−4.309153	−1.785808	1.592065
H	−5.357913	−2.067205	1.780684
C	2.214175	−3.895837	1.257115
H	2.208985	−4.805184	1.880791
C	0.945208	0.440142	3.123790
H	1.039060	−0.595503	3.492486
C	−3.334776	−1.921203	2.603725
H	−3.615864	−2.307318	3.597539
C	1.245109	2.834775	3.518665
H	1.541093	3.669376	4.174641
C	1.322844	1.500031	3.975113
H	1.686498	1.285233	4.993648
C	3.229867	−3.698224	0.299205
H	4.028806	−4.445749	0.166110
H	−0.089722	−0.121393	−0.301083
H	0.068343	0.033647	−3.281944
H	−1.710610	4.073676	0.525175
H	−2.514347	2.470565	0.330074
H	0.561451	4.020533	−2.059063
H	1.942648	3.541098	−1.011673
H	3.119955	1.440603	0.327421
H	4.429393	0.467061	−0.448741
H	2.586046	−1.378027	−3.494377
H	3.117126	0.320370	−3.702683
H	−1.501711	−2.524187	−2.429674
H	−2.211219	−1.557082	−3.766558
H	−4.570529	0.057908	−2.289207
H	−3.442287	1.074525	−3.259792

^{s}IM5−A

Fe	−0.105693	0.696501	−1.610308
P	2.103061	0.152680	−1.554929
P	−2.257948	−0.045899	−1.591543
P	−0.174615	2.442438	−0.117198
C	0.518953	0.433641	1.782249
C	−2.567571	−1.002731	0.010409
C	2.221237	−1.468543	−0.599232
C	−3.773024	1.070878	−1.751382
H	−3.813129	1.794916	−0.914791
C	−1.768535	3.319474	0.388894
H	−2.237212	3.806051	−0.493007
C	−2.686244	−1.311763	−2.913461
H	−3.709741	−1.722620	−2.780556
C	0.454020	1.844037	1.538172
C	−1.871802	−1.947288	2.148023
H	−1.101925	−2.113996	2.919757
C	0.869362	3.962773	−0.512913

H	0.778261	4.759136	0.255679
C	1.217751	−1.801692	0.375104
B	0.028164	−0.730651	0.731310
C	2.893841	−0.205314	−3.222065
H	3.960742	−0.501240	−3.139585
C	−1.514197	−1.248062	0.958212
C	−3.882827	−1.483901	0.259309
H	−4.686517	−1.305681	−0.473879
C	3.493525	1.159918	−0.764654
H	3.656186	2.095477	−1.342432
C	0.858940	2.775607	2.533443
H	0.801162	3.858747	2.334809
C	3.303428	−2.350959	−0.847623
H	4.074040	−2.092555	−1.591901
C	1.348802	−3.052481	1.037353
H	0.577109	−3.355613	1.764252
C	−4.192930	−2.193144	1.436980
H	−5.218742	−2.556808	1.610569
C	2.423347	−3.933690	0.781398
H	2.484523	−4.897401	1.313945
C	1.033241	0.027979	3.049449
H	1.142037	−1.049282	3.259901
C	−3.178065	−2.418903	2.391471
H	−3.404833	−2.957983	3.326269
C	1.344279	2.337955	3.781808
H	1.658465	3.070469	4.543004
C	1.434888	0.951491	4.036268
H	1.827865	0.590539	5.001249
C	3.411174	−3.580180	−0.160259
H	4.254488	−4.257957	−0.370650
H	−0.136344	−0.272330	−0.440426
H	0.026787	−0.512412	−2.607684
H	−1.568399	4.091117	1.162677
H	−2.479100	2.578453	0.807991
H	0.528667	4.379160	−1.485534
H	1.935594	3.678160	−0.611334
H	3.218287	1.424191	0.276049
H	4.441700	0.581378	−0.747765
H	2.319976	−1.004430	−3.731016
H	2.833702	0.715041	−3.841904
H	−1.945272	−2.133835	−2.868346
H	−2.610132	−0.831905	−3.912428
H	−4.723826	0.498112	−1.776386
H	−3.684253	1.640422	−2.701734

^{s}IM2'−A

Fe	−0.119606	0.445969	−1.502343
P	2.191805	0.229207	−1.361237
P	−2.309365	−0.170819	−1.528959
P	−0.319930	2.327651	−0.250462
C	0.611707	0.507557	1.581352
C	−2.638892	−0.918738	0.136574
C	2.321709	−1.420151	−0.502801
C	−3.797137	0.927193	−1.906077
H	−3.869689	1.760401	−1.181725
C	−1.953755	3.120850	0.253763
H	−2.473755	3.546202	−0.630409
C	−2.712253	−1.580012	−2.719392
H	−3.746157	−1.953471	−2.561111
C	0.448338	1.910810	1.374650
C	−1.724156	−1.680141	2.248704
H	−0.878025	−1.808007	2.943794
C	0.564394	3.871563	−0.875575
H	0.510049	4.704511	−0.142858
C	1.158100	−1.772262	0.266027
B	0.024117	−0.611375	0.502950
C	3.088845	−0.020634	−3.002383
H	4.150246	−0.315909	−2.860259
C	−1.485740	−1.096065	0.966472
C	−3.936583	−1.318343	0.556395
H	−4.807396	−1.173255	−0.105585
C	3.450260	1.339088	−0.504028
H	3.588527	2.274885	−1.087594
C	0.883328	2.873751	2.322062
H	0.741211	3.952090	2.134337
C	3.405510	−2.314441	−0.669985

H	4.290955	−2.021599	−1.259355
C	1.130566	−3.090789	0.804465
H	0.246764	−3.417536	1.377105
C	−4.125564	−1.904328	1.823532
H	−5.132216	−2.212777	2.149948
C	2.204643	−3.993843	0.627706
H	2.146248	−5.007118	1.060249
C	1.280163	0.124090	2.783367
H	1.472148	−0.945745	2.970831
C	−3.008392	−2.082233	2.672084
H	−3.142823	−2.530492	3.671026
C	1.520781	2.454758	3.508229
H	1.867849	3.197057	4.245354
C	1.723880	1.072120	3.730666
H	2.238436	0.734585	4.646216
C	3.353118	−3.605878	−0.097266
H	4.193711	−4.306114	−0.231466
H	−0.020977	−1.156170	−1.768520
H	0.130087	−0.816837	−2.568067
H	−3.674361	1.354779	−2.924403
H	−4.746794	0.351761	−1.882571
H	−2.610854	−1.230556	−3.769446
H	−2.003120	−2.416850	−2.556429
H	−1.774040	3.934178	0.988449
H	−2.603895	2.356746	0.725713
H	0.086060	4.206207	−1.821055
H	1.628358	3.644683	−1.084397
H	3.063397	0.928403	−3.579597
H	2.573111	−0.803667	−3.594596
H	4.429449	0.819631	−0.432853
H	3.101796	1.597557	0.514083

^{s}TS1'−A

Fe	−0.166845	0.528881	−1.474575
P	2.138520	0.332090	−1.422934
P	−2.341815	−0.132801	−1.523360
P	−0.376342	2.348487	−0.116031
C	0.605883	0.433887	1.600432
C	−2.604542	−1.019412	0.089897
C	2.362684	−1.330297	−0.606312
C	−3.867429	0.948328	−1.767126
H	−3.950601	1.704781	−0.964036
C	−2.013267	3.089670	0.453254
H	−2.557206	3.545382	−0.401024
C	−2.724444	−1.447338	−2.818775
H	−3.737918	−1.877668	−2.670886
C	0.412934	1.842276	1.473010
C	−1.652587	−1.880942	2.147760
H	−0.799320	−2.020505	2.831549
C	0.482387	3.939499	−0.653219
H	0.426755	4.726897	0.128241
C	1.248589	−1.756964	0.194708
B	0.053977	−0.657198	0.471493
C	2.968656	0.159457	−3.104939
H	4.045571	−0.098643	−3.019493
C	−1.439654	−1.214967	0.901908
C	−3.885135	−1.485639	0.493278
H	−4.765292	−1.325850	−0.152607
C	3.399609	1.447854	−0.575123
H	3.493473	2.405487	−1.131533
C	0.825643	2.758711	2.475458
H	0.660563	3.842414	2.347374
C	3.492425	−2.157864	−0.811318
H	4.341039	−1.811100	−1.425564
C	1.314558	−3.075304	0.726349
H	0.467834	−3.459277	1.319152
C	−4.047784	−2.154405	1.722510
H	−5.042390	−2.513379	2.033719
C	2.434971	−3.911867	0.512173
H	2.449832	−4.928877	0.939367
C	1.277348	−0.001437	2.783234
H	1.493128	−1.075203	2.911403
C	−2.920594	−2.347327	2.553523
H	−3.033972	−2.857229	3.525033
C	1.467817	2.288295	3.639005
H	1.797617	2.995565	4.417293

C	1.697344	0.899970	3.784859
H	2.215114	0.521261	4.682212
C	3.534341	−3.452624	−0.245686
H	4.410160	−4.101136	−0.410848
H	−0.088780	−0.999418	−1.486429
H	0.067622	−0.685683	−2.488282
H	−3.777039	1.475727	−2.741105
H	−4.798668	0.343565	−1.784932
H	−2.664525	−1.001231	−3.834624
H	−1.973482	−2.259755	−2.749345
H	−1.834927	3.871404	1.221788
H	−2.641389	2.292752	0.900088
H	−0.011032	4.324128	−1.571660
H	1.546365	3.739642	−0.887321
H	2.881694	1.121837	−3.653670
H	2.449697	−0.625207	−3.691155
H	4.394522	0.954504	−0.552112
H	3.079693	1.663899	0.462588

^{t}TS−1B

Fe	−0.226975	0.580069	−1.694860
P	2.443394	0.195532	−1.430869
P	−2.649555	−0.380601	−1.477581
P	−0.487859	2.463155	−0.282557
C	0.667939	0.645470	1.451652
C	−2.632877	−1.062682	0.268462
C	2.426951	−1.419717	−0.475727
C	−4.347203	0.425602	−1.658880
H	−4.452143	1.258664	−0.934706
C	−2.187669	3.037340	0.279665
H	−2.776158	3.393801	−0.592063
C	−2.919339	−1.923467	−2.526647
H	−3.786824	−2.516271	−2.165515
C	0.400860	2.038661	1.278525
C	−1.502590	−1.555363	2.361954
H	−0.599384	−1.547423	2.992869
C	0.259897	4.082631	−0.870176
H	0.185993	4.889643	−0.110870
C	1.254860	−1.720187	0.304331
B	0.076666	−0.576409	0.486270
C	3.327518	−0.237049	−3.037940
H	4.347085	−0.650225	−2.884632
C	−1.405051	−1.077620	1.016905
C	−3.845988	−1.537613	0.842819
H	−4.776413	−1.528252	0.251883
C	3.784052	1.207767	−0.570309
H	3.971370	2.139449	−1.146610
C	0.828924	3.013246	2.217473
H	0.603716	4.080466	2.053080
C	3.499011	−2.341909	−0.563549
H	4.396126	−2.099439	−1.157562
C	1.213452	−2.996379	0.931864
H	0.320887	−3.277535	1.513423
C	−3.890558	−2.021686	2.163895
H	−4.839377	−2.383981	2.592095
C	2.280291	−3.919444	0.833689
H	2.206338	−4.898269	1.336771
C	1.435346	0.298851	2.606998
H	1.712444	−0.755494	2.767808
C	−2.705069	−2.021356	2.930509
H	−2.717921	−2.379109	3.973585
C	1.562365	2.628316	3.357812
H	1.903060	3.384830	4.083119
C	1.871447	1.261599	3.542979
H	2.463647	0.945297	4.417941
C	3.435339	−3.590527	0.094647
H	4.274156	−4.301340	0.016856
H	−0.056817	−0.965726	−1.216641
H	0.009169	−1.008427	−2.211001
H	−4.418556	0.846517	−2.684709
H	−5.191855	−0.280983	−1.514263
H	−3.094119	−1.628774	−3.583605
H	−2.009398	−2.555823	−2.486773
H	−2.102429	3.860325	1.020909
H	−2.720229	2.186410	0.750476
H	−0.269081	4.411672	−1.789449

H	1.327308	3.919404	−1.123656
H	3.410187	0.683966	−3.654037
H	2.718261	−0.974899	−3.599048
H	4.735352	0.639036	−0.489817
H	3.441789	1.481537	0.447408
N	−0.334978	2.140908	−4.325815
N	−0.297697	1.575909	−3.342263

^{t}TS−3B

P	0.243042	−2.503437	−0.472695
P	0.336135	2.592735	−0.932886
P	0.563808	0.365108	2.055368
C	−1.910790	−0.611815	1.313293
C	−1.515681	2.706632	−0.684870
C	−1.355694	−2.366666	−1.444337
C	0.999380	4.246731	−0.299996
H	0.794163	4.348305	0.784967
C	0.446262	2.073840	2.834273
H	1.411541	2.610186	2.715151
C	0.525467	2.880437	−2.787828
H	−0.012532	3.794472	−3.119403
C	−1.060793	−0.425526	2.447467
C	−3.646147	1.685941	−0.125648
H	−4.246639	0.809146	0.165251
C	1.803317	−0.455395	3.206764
H	1.541979	−0.339451	4.280161
C	−2.090746	−1.134529	−1.322475
B	−1.613675	−0.007630	−0.211283
C	1.381320	−3.471891	−1.624291
H	0.967475	−4.453765	−1.938953
C	−2.245500	1.512152	−0.360534
C	−2.173648	3.963892	−0.795427
H	−1.596658	4.866665	−1.054908
C	−0.130963	−3.842286	0.807865
H	0.802353	−4.101378	1.353616
C	−1.429607	−0.860289	3.747094
H	−0.750406	−0.699875	4.601580
C	−1.797024	−3.397812	−2.309229
H	−1.231306	−4.341784	−2.384865
C	−3.239457	−0.993282	−2.150629
H	−3.815199	−0.054703	−2.109921
C	−3.558925	4.084824	−0.575438
H	−4.053420	5.066220	−0.662590
C	−3.669287	−2.017620	−3.026071
H	−4.565488	−1.864427	−3.650967
C	−3.136832	−1.303982	1.561699
H	−3.810521	−1.517166	0.715796
C	−4.297359	2.931704	−0.230180
H	−5.380919	3.003936	−0.037085
C	−2.658167	−1.520018	3.955226
H	−2.941023	−1.867261	4.962385
C	−3.508668	−1.747624	2.849511
H	−4.463306	−2.281971	2.990583
C	−2.956958	−3.232598	−3.099273
H	−3.288725	−4.039342	−3.773386
H	−0.271516	0.044962	−1.417634
H	0.577389	−0.081539	−1.914578
H	2.101233	4.250481	−0.444838
H	0.577081	5.129408	−0.826315
H	1.603290	2.980571	−3.039312
H	0.120898	2.004904	−3.334816
H	0.198473	2.004635	3.915035
H	−0.350389	2.649168	2.320172
H	2.802217	−0.002955	3.031496
H	1.864308	−1.535953	2.963156
H	2.343570	−3.649344	−1.096921
H	1.586953	−2.859447	−2.525988
H	−0.536486	−4.763278	0.335935
H	−0.871091	−3.455928	1.536402
C	2.794373	0.059930	−0.226078
Fe	0.882141	0.137196	−0.261888
N	3.989527	0.004758	−0.213962
C	5.433197	−0.105372	−0.368860
C	5.798901	0.249748	−1.844188
C	6.113180	0.890644	0.621229
C	5.847006	−1.573897	−0.038924

H	5.296015	−0.443813	−2.549421
H	5.484239	1.285978	−2.086937
H	6.897117	0.170334	−1.990686
H	5.835179	0.653815	1.669477
H	7.217553	0.823419	0.525881
H	5.803700	1.933941	0.402451
H	6.946519	−1.688550	−0.145404
H	5.563746	−1.837252	1.001387
H	5.348936	−2.284920	−0.730372

^{t}TS−5B

P	−2.381574	−0.939231	−0.958339
P	2.629637	−0.323650	−1.261504
P	0.499575	−1.915843	1.385746
C	−0.718660	0.558258	1.635031
C	2.568319	1.292009	−0.318699
C	−2.461509	0.919888	−1.188602
C	4.334511	−1.039926	−0.890667
H	4.434742	−1.249565	0.193274
C	2.199866	−1.974324	2.182366
H	2.810996	−2.775584	1.716405
C	2.897037	0.230554	−3.041701
H	3.755563	0.930591	−3.125632
C	−0.428089	−0.643358	2.351390
C	1.369845	2.940440	1.002438
H	0.450493	3.296979	1.493893
C	−0.205108	−3.571823	1.919953
H	−0.119219	−3.741200	3.014235
C	−1.333158	1.688677	−0.733995
B	−0.133397	0.952498	0.129664
C	−3.222213	−1.633593	−2.492197
H	−4.261765	−1.267726	−2.630676
C	1.320160	1.727221	0.245713
C	3.756449	2.058030	−0.152599
H	4.702375	1.711551	−0.600277
C	−3.700049	−1.293730	0.343604
H	−3.817345	−2.392598	0.461371
C	−0.863561	−0.850971	3.686584
H	−0.621709	−1.790600	4.211179
C	−3.555229	1.543539	−1.837891
H	−4.417397	0.945241	−2.176967
C	−1.354676	3.083402	−1.013507
H	−0.495588	3.703392	−0.711190
C	3.754311	3.259168	0.581516
H	4.683385	3.839678	0.702331
C	−2.442523	3.702518	−1.671923
H	−2.417587	4.787272	−1.870005
C	−1.514225	1.520710	2.331235
H	−1.810285	2.446160	1.811339
C	2.547476	3.696877	1.169314
H	2.524664	4.625210	1.764093
C	−1.626123	0.132987	4.347454
H	−1.972336	−0.031197	5.380678
C	−1.957464	1.320428	3.656367
H	−2.573174	2.090785	4.149951
C	−3.555110	2.936263	−2.076300
H	−4.408784	3.411167	−2.586699
H	0.054865	0.205971	−1.456840
H	0.026453	−0.347769	−2.277068
H	4.428885	−2.000430	−1.440726
H	5.167495	−0.375206	−1.203639
H	3.084380	−0.657686	−3.681882
H	1.981544	0.737347	−3.408175
H	2.113721	−2.169139	3.272406
H	2.704886	−0.999071	2.032616
H	0.341422	−4.379008	1.388612
H	−1.273574	−3.626513	1.627623
H	−3.245507	−2.741092	−2.407734
H	−2.620770	−1.368568	−3.385576
H	−4.680707	−0.857916	0.055320
H	−3.385319	−0.862013	1.314148
C	0.412295	−3.021213	−1.621838
O	0.511317	−4.102221	−2.070426
Fe	0.264679	−1.340559	−0.910696

^{s}IM1−C

C	1.523037	2.136573	−2.044386
C	0.999892	1.570405	−0.847094
C	1.565603	2.012415	0.380602
C	2.571546	3.004266	0.434309
C	3.054752	3.567464	−0.767271
C	2.539154	3.119904	−2.005490
B	−0.200652	0.480208	−0.768129
P	0.867156	1.052830	1.792603
C	−0.204208	2.332108	2.679048
C	0.188106	−1.093570	−1.111911
C	−0.810257	−1.815869	−1.866549
C	−0.578742	−3.038592	−2.514872
C	0.697967	−3.632185	−2.424049
C	1.709029	−2.973695	−1.700964
C	1.499634	−1.727383	−1.047125
P	3.005286	−0.977815	−0.158669
C	4.208201	−0.860800	−1.623678
C	−1.661373	1.016676	−1.261309
C	−1.819270	2.019989	−2.262330
C	−3.090636	2.416134	−2.732951
C	−4.261985	1.820502	−2.215390
C	−4.145438	0.842304	−1.204496
C	−2.867974	0.463608	−0.724893
P	−2.596760	−0.699775	0.695334
C	−3.638234	−2.221595	0.300635
C	−3.676547	0.055309	2.041759
C	2.258731	0.902205	3.051779
C	3.743433	−2.501428	0.696891
H	2.700234	−3.449281	−1.654063
H	2.995431	3.326307	1.399892
H	3.840859	4.339516	−0.740421
H	2.933858	3.537562	−2.946606
H	1.153663	1.791468	−3.024861
H	−0.929583	2.510704	−2.683019
H	−3.167169	3.195797	−3.508953
H	−5.255332	2.127916	−2.580603
H	−5.057802	0.393363	−0.776320
H	2.665295	1.893722	3.346224
H	−0.665813	1.885071	3.584130
H	−3.277923	1.052068	2.318232
H	−1.797602	−1.355858	−1.995544
H	0.910598	−4.592720	−2.922028
H	−1.384094	−3.518819	−3.093912
H	−4.676223	−1.958927	0.002063
H	4.704418	−2.187557	1.159635
H	5.211781	−0.585803	−1.232875
H	0.399864	3.212800	2.985447
H	−1.010330	2.668664	1.996096
H	1.864873	0.398275	3.959634
H	3.068552	0.283924	2.619136
H	−3.665366	−0.589868	2.944444
H	−4.725664	0.168731	1.697612
H	−3.678116	−2.862565	1.206973
H	−3.158662	−2.804352	−0.510546
H	3.872358	−0.048528	−2.300697
H	4.299346	−1.802852	−2.206968
H	3.949014	−3.366982	0.031204
H	3.062948	−2.828350	1.510561
Fe	−0.363269	−0.807585	1.190132
N	−0.810456	−0.878814	2.961788
N	−1.068900	−0.953244	4.069215
H	−0.181214	−2.446260	1.274109
H	0.639782	−2.083675	1.501631

[s]IM2−C

C	1.637818	2.487645	−1.589400
C	0.992958	1.719276	−0.580311
C	1.270216	2.047984	0.776756
C	2.139833	3.107721	1.122105
C	2.763557	3.860911	0.102959
C	2.517464	3.542093	−1.251745
B	−0.089691	0.556172	−0.860523
P	0.441798	0.879076	1.948033
C	−0.793293	1.983632	2.848815
C	0.357421	−0.932653	−1.285018
C	−0.598444	−1.662971	−2.085872

C	−0.297004	−2.842252	−2.783448
C	1.006961	−3.370451	−2.691876
C	1.975756	−2.707022	−1.914005
C	1.695181	−1.510538	−1.204041
P	3.132950	−0.721225	−0.231642
C	4.332038	−0.403727	−1.672165
C	−1.565081	1.097005	−1.289444
C	−1.699843	2.155813	−2.235755
C	−2.960941	2.602237	−2.685150
C	−4.143793	2.010907	−2.188210
C	−4.047718	0.977870	−1.232792
C	−2.779496	0.531595	−0.782532
P	−2.559317	−0.770600	0.525174
C	−3.565617	−2.241505	−0.073847
C	−3.694800	−0.193402	1.913387
C	1.697084	0.598136	3.313251
C	3.969481	−2.254112	0.504893
H	2.983986	−3.143831	−1.864839
H	2.349522	3.341248	2.179176
H	3.446030	4.686061	0.363259
H	3.016003	4.116444	−2.049944
H	1.474811	2.249233	−2.654338
H	−0.797586	2.647206	−2.630346
H	−3.021259	3.419863	−3.422155
H	−5.130885	2.361462	−2.530641
H	−4.969455	0.527819	−0.826961
H	1.987610	1.546361	3.813197
H	−1.306970	1.400859	3.642432
H	−3.371149	0.796474	2.288954
H	−1.603608	−1.238916	−2.206699
H	1.275621	−4.294240	−3.231105
H	−1.066254	−3.339743	−3.395317
H	−4.593970	−1.951415	−0.378313
H	4.870727	−1.905782	1.054867
H	5.313110	−0.100371	−1.246525
H	−0.287849	2.856158	3.314558
H	−1.550802	2.353081	2.128081
H	1.264737	−0.088633	4.070248
H	2.591665	0.119931	2.869324
H	−3.642505	−0.921373	2.750388
H	−4.749477	−0.120815	1.573680
H	−3.626960	−2.979966	0.753204
H	−3.047329	−2.727776	−0.923068
H	3.953615	0.441244	−2.284253
H	4.489474	−1.284290	−2.332119
H	4.292750	−3.020708	−0.231937
H	3.274127	−2.720504	1.232246
Fe	−0.333959	−1.108135	1.007185
N	−0.724732	−1.729523	2.666380
N	−0.952374	−2.158577	3.694327
H	−0.532180	−2.591675	0.614334
H	1.095697	−1.619965	1.308657

^{s}IM3−C

Fe	−1.105375	−0.780849	−1.454966
P	−2.335317	1.146540	−1.097904
P	3.058006	−1.025374	−0.993149
P	−1.386353	−2.084111	0.304799
C	0.814855	−0.712522	1.476494
C	2.907977	0.849847	−0.730843
C	−1.980258	1.811926	0.594687
C	4.788361	−1.334052	−0.277650
H	4.741719	−1.242514	0.827637
C	−1.466241	−3.906885	−0.109903
H	−2.282632	−4.075128	−0.842509
C	3.489342	−1.082363	−2.840157
H	4.334805	−0.423963	−3.135683
C	0.010948	−1.894938	1.518388
C	1.738929	2.850714	0.037986
H	0.878052	3.331121	0.527799
C	−2.941007	−1.861750	1.339664
H	−2.938514	−2.549176	2.212113
C	−0.717233	1.476791	1.183771
B	0.478304	0.557184	0.495391
C	−1.757264	2.515759	−2.254829
H	−2.265858	3.475487	−2.022261

C	1.757665	1.427171	−0.080690
C	3.951113	1.692037	−1.200698
H	4.831567	1.248206	−1.693846
C	−4.195258	1.216761	−1.325387
H	−4.438812	0.815779	−2.331682
C	0.258720	−2.919991	2.468551
H	−0.363500	−3.829634	2.486437
C	−2.933542	2.612666	1.283110
H	−3.901146	2.853037	0.814469
C	−0.481457	1.998306	2.491631
H	0.470448	1.758742	2.992677
C	3.901383	3.094549	−1.059051
H	4.727923	3.720489	−1.434638
C	−1.421276	2.794330	3.178157
H	−1.190644	3.166380	4.190075
C	1.866472	−0.621091	2.433142
H	2.516955	0.269523	2.420189
C	2.781276	3.677247	−0.434091
H	2.715567	4.771357	−0.311160
C	1.309542	−2.795682	3.401682
H	1.497796	−3.598689	4.132379
C	2.117266	−1.638398	3.379377
H	2.946788	−1.529696	4.097802
C	−2.659323	3.105838	2.573745
H	−3.404643	3.721770	3.102368
H	0.051564	−0.010252	−0.628810
H	0.010751	−1.826614	−1.705753
H	−1.661233	−4.532208	0.785776
H	−0.507226	−4.207843	−0.575478
H	5.088214	−2.376829	−0.519353
H	5.570651	−0.643089	−0.660291
H	3.747502	−2.130379	−3.106315
H	2.592080	−0.796694	−3.428881
H	−1.967467	2.239873	−3.310633
H	−0.663181	2.651364	−2.130437
H	−4.693917	0.577688	−0.568050
H	−4.597443	2.248809	−1.251902
H	−2.990600	−0.816401	1.704931
H	−3.836536	−2.069602	0.715685
N	−2.210953	−1.680064	−2.589900
N	−2.869302	−2.229678	−3.337125

^{t}IM1−C

C	−0.522654	−0.269371	2.790943
C	−0.491679	0.278022	1.471789
C	−0.932609	1.643330	1.337844
C	−1.439211	2.364425	2.444742
C	−1.499590	1.770036	3.724599
C	−1.023662	0.452607	3.896221
B	−0.015057	−0.633306	0.217079
P	−0.614844	2.439729	−0.314198
C	−0.309948	4.250412	0.097792
C	−0.954003	−0.935228	−1.079741
C	−0.243282	−1.340027	−2.257945
C	−0.865584	−1.630762	−3.486543
C	−2.270250	−1.567537	−3.574626
C	−3.017629	−1.249110	−2.420977
C	−2.402834	−0.943224	−1.173362
P	−3.506527	−0.549467	0.318225
C	−3.439843	−2.188724	1.269997
C	0.959435	−1.903819	0.555854
C	0.423126	−3.153796	0.989771
C	1.252271	−4.252562	1.300655
C	2.657068	−4.146073	1.173461
C	3.217189	−2.934331	0.722826
C	2.375125	−1.833557	0.415746
P	2.967378	−0.200066	−0.214906
C	4.330817	−0.619635	−1.442848
C	3.988486	0.479752	1.214568
C	−2.242837	2.622077	−1.237055
C	−5.254978	−0.754411	−0.382349
H	−4.113536	−1.253345	−2.505799
H	−1.779893	3.405121	2.320820
H	−1.893180	2.340039	4.581794
H	−1.037791	−0.014014	4.895231
H	−0.155969	−1.296020	2.950250

H	−0.668734	−3.277306	1.069400
H	0.801514	−5.202146	1.633902
H	3.305661	−5.005074	1.409977
H	4.310789	−2.852605	0.603353
H	−3.042853	2.991463	−0.561675
H	−0.014832	4.780949	−0.832009
H	3.312229	0.715675	2.061620
H	0.853714	−1.421143	−2.197169
H	−2.788016	−1.792182	−4.521643
H	−0.258444	−1.914763	−4.362032
H	5.124785	−1.253440	−0.993568
H	−5.955206	−0.637087	0.472471
H	−4.251588	−2.181939	2.029539
H	−1.213214	4.746575	0.511705
H	0.520542	4.339676	0.826367
H	−2.091260	3.355265	−2.058606
H	−2.547848	1.654798	−1.676868
H	4.502835	1.412708	0.902839
H	4.746104	−0.258589	1.552846
H	4.790076	0.324347	−1.804608
H	3.893880	−1.152118	−2.312738
H	−2.477550	−2.269898	1.812181
H	−3.570082	−3.073841	0.610640
H	−5.448766	−1.740382	−0.858339
H	−5.483710	0.050967	−1.111409
Fe	1.290971	1.242128	−0.872036
N	2.506101	2.745731	−0.831989
N	3.186563	3.654506	−0.931281
H	1.755573	0.960552	−2.704371
H	1.088512	1.403391	−2.758664

^{s}IM3-D

Fe	−1.367190	0.304371	−1.347441
P	−3.093348	−0.179735	−0.084296
P	3.433642	0.480123	1.280405
P	−0.380455	−1.713433	−1.373535
C	0.322096	−0.995541	1.120238
C	2.734308	0.965367	−0.406882
C	−2.448988	1.254736	0.893772
C	5.035944	1.492448	1.343250
H	4.796305	2.576207	1.319028
C	1.092786	−1.964760	−2.510617
H	0.775880	−1.769472	−3.556267
C	4.186275	−1.216968	0.897929
H	4.835018	−1.199174	−0.005078
C	0.201238	−2.180645	0.329425
C	0.841730	1.564050	−1.833575
H	−0.252168	1.780811	−1.995878
C	−1.471653	−3.138238	−1.925082
H	−0.920250	−4.102643	−1.910032
C	−1.022196	1.475694	0.767050
B	0.106187	0.395790	0.309166
C	−4.849065	0.231295	−0.573235
H	−5.529336	0.308631	0.302011
C	1.310446	1.029900	−0.589576
C	3.594983	1.366664	−1.467785
H	4.687411	1.318821	−1.333409
C	−3.366986	−1.618963	1.095291
H	−3.823983	−2.473021	0.551023
C	0.411776	−3.470434	0.874079
H	0.316822	−4.372134	0.245733
C	−3.294914	2.243649	1.464234
H	−4.381035	2.069655	1.526481
C	−0.540895	2.759475	1.189087
H	0.529815	2.983826	1.065734
C	3.094196	1.836388	−2.700901
H	3.789623	2.136901	−3.501643
C	−1.373514	3.708882	1.808689
H	−0.950122	4.659309	2.172094
C	0.621374	−1.156761	2.500455
H	0.720321	−0.269242	3.144931
C	1.698384	1.941721	−2.886907
H	1.281202	2.326541	−3.831527
C	0.711767	−3.600410	2.249550
H	0.858174	−4.599289	2.692079
C	0.801764	−2.443768	3.059493

H	1.016751	−2.546944	4.136036
C	−2.757054	3.447190	1.955945
H	−3.414787	4.189875	2.436422
H	−1.745182	−0.228459	−2.729047
H	−2.311680	1.352740	−2.020560
H	−1.821089	−2.935274	−2.957917
H	−2.358036	−3.222265	−1.265459
H	1.481317	−3.002466	−2.430824
H	1.896397	−1.250141	−2.246139
H	4.792698	−1.548853	1.768245
H	3.373169	−1.955677	0.746052
H	5.761127	1.267627	0.531406
H	5.530164	1.275971	2.314750
H	−4.051870	−1.318619	1.916605
H	−2.399302	−1.943900	1.523806
H	−4.844190	1.181169	−1.142131
H	−5.223552	−0.573232	−1.241058

^{s}TS-D

Fe	−2.057814	−0.875432	−1.780732
P	−2.961467	0.223976	−0.105405
P	3.542478	0.290543	1.136848
P	−0.624723	−2.317178	−0.888665
C	0.210912	−0.504864	1.146783
C	2.944651	0.725715	−0.606843
C	−2.134732	1.799671	0.497373
C	5.352213	0.849244	1.102009
H	5.408645	1.942221	0.917035
C	0.941163	−2.496491	−1.923236
H	0.654847	−2.827889	−2.944983
C	3.829725	−1.577483	0.987454
H	4.414512	−1.842945	0.080010
C	−0.059175	−1.879339	0.834398
C	1.203911	1.517899	−2.152061
H	0.145070	1.724877	−2.364397
C	−1.138247	−4.119900	−0.777966
H	−0.315232	−4.790104	−0.448576
C	−0.709230	1.934522	0.395596
B	0.314875	0.737543	0.125086
C	−4.605688	0.820552	−0.799479
H	−5.249584	1.285397	−0.023558
C	1.546289	0.986499	−0.867683
C	3.893912	0.947555	−1.640194
H	4.960724	0.752920	−1.454513
C	−3.516082	−0.628412	1.474287
H	−4.146048	−1.498634	1.196598
C	−0.069590	−2.857240	1.865805
H	−0.288350	−3.908435	1.628624
C	−2.916094	2.889639	0.951189
H	−4.011255	2.796991	1.022156
C	−0.137142	3.196877	0.726741
H	0.952364	3.330027	0.627831
C	3.514679	1.425283	−2.913204
H	4.278986	1.576289	−3.693523
C	−0.923034	4.276843	1.189035
H	−0.445924	5.237343	1.442916
C	0.411988	−0.175408	2.521444
H	0.590294	0.875440	2.796987
C	2.161012	1.724295	−3.166182
H	1.847043	2.121395	−4.145109
C	0.175882	−2.503240	3.210043
H	0.164853	−3.278029	3.993553
C	0.405394	−1.151895	3.539836
H	0.572269	−0.853367	4.587320
C	−2.317301	4.120408	1.309346
H	−2.945671	4.954214	1.662234
H	−1.645344	0.585730	−2.427911
H	−3.069648	−2.088713	−1.609479
H	1.629672	−3.248339	−1.481855
H	1.457070	−1.521348	−2.002182
H	5.774804	0.653859	2.110960
H	5.988004	0.323985	0.356725
H	4.382224	−1.927168	1.886246
H	2.854410	−2.103498	0.959225
H	−5.135033	−0.059579	−1.219073
H	−4.420506	1.549977	−1.612870

H	−2.634693	−0.990173	2.039314
H	−4.099639	0.063203	2.118842
H	−2.009139	−4.223293	−0.100672
H	−1.467753	−4.423323	−1.792896

^{s}IM4-D

Fe	−2.090514	−0.485520	−1.606643
P	−2.801895	1.128088	−0.233254
P	3.611002	0.312074	1.010954
P	−1.770800	−2.237354	−0.316084
C	0.038143	−0.594889	1.121805
C	3.071896	−0.123163	−0.748535
C	−1.411036	2.336014	0.087690
C	5.327063	1.072816	0.743464
H	5.235675	1.993998	0.130371
C	−0.759410	−3.515617	−1.253856
H	−1.333940	−3.885600	−2.129617
C	4.141657	−1.392806	1.646562
H	4.820666	−1.918040	0.939912
C	−0.782164	−1.775412	1.182982
C	1.451379	−0.350257	−2.542261
H	0.412764	−0.290251	−2.916653
C	−3.237095	−3.234042	0.276533
H	−2.938889	−4.182634	0.770440
C	−0.050295	1.881725	−0.026171
B	0.324769	0.290616	−0.259848
C	−4.169712	2.133680	−1.029955
H	−4.527512	2.960657	−0.381554
C	1.690533	−0.057031	−1.160496
C	4.080901	−0.496196	−1.681991
H	5.128635	−0.564325	−1.349864
C	−3.543381	0.727633	1.440456
H	−4.445167	0.094603	1.303807
C	−0.953859	−2.503796	2.393593
H	−1.580216	−3.409996	2.413609
C	−1.711742	3.690166	0.395077
H	−2.758808	4.023107	0.484762
C	0.958258	2.871021	0.141507
H	2.012238	2.572572	0.034307
C	3.793480	−0.783758	−3.029938
H	4.601314	−1.066495	−3.724832
C	0.661279	4.219470	0.437885
H	1.480306	4.947979	0.557990
C	0.582180	−0.161431	2.367927
H	1.165572	0.769423	2.390636
C	2.457050	−0.696880	−3.466686
H	2.194194	−0.900702	−4.518349
C	−0.346326	−2.069072	3.588104
H	−0.483387	−2.639780	4.520862
C	0.406725	−0.875335	3.573093
H	0.854866	−0.491834	4.504753
C	−0.679909	4.634176	0.578074
H	−0.923998	5.683103	0.811931
H	−0.549733	−0.102152	−1.133658
H	−3.509324	−0.896399	−2.160234
H	−0.507276	−4.373822	−0.595380
H	0.179659	−3.044356	−1.608949
H	5.721243	1.366240	1.740321
H	6.070392	0.399519	0.264780
H	4.659853	−1.274428	2.622912
H	3.239750	−2.017520	1.811324
H	−5.012611	1.446946	−1.248166
H	−3.809555	2.558279	−1.989753
H	−2.801529	0.179099	2.052922
H	−3.829351	1.662766	1.966882
H	−3.841607	−2.629296	0.982228
H	−3.862998	−3.464462	−0.609185