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SUPPORTING INFORMATION

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Title: Electronic Elements Governing the Binding of Small Molecules to a [Fe]-Hydrogenase Mimic
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Hydride and Cyaninde Anion Solvation Energies. The large discrepancy between the binding free energies of predicted using the PCM and COSMO-RS models for the hydride anion prompted further investigation. We computed direct solvation energies using various density functionals coupled with large basis sets with extra diffuse functions, which better describe anionic species. The results indicate that solvation energy of the hydride anion is likely incorrect within the COSMO-RS framework, since agreements is not seen with either the standard PCM model or the SMD model of Cramer and Truhlar (A. V. Marenich, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B*, 2009, *113*, 6378-6396.). In contrast, agreement is seen between the solvation models for the cyanide ligand.

SI Table 1. Solvation energies of the hydride and cyanide anion. Values in kcal/mol.

Hydride Anion				
Basis Set	M06 PCM[a]	M06 SMD[a]	M06 COSMO-RS[b]	B3LYP-dDsC COSMO-RS[b]
cc-pVTZ	-78.89	-81.06	--	--
aug-cc-pVTZ	-68.81	-69.48	--	--
cc-pVQZ	-76.99	-78.76	--	--
aug-cc-pVQZ	-69.18	-70.14	--	--
TZP	--	--	-34.35	-34.38
aug-TZP	--	--	-32.88	-30.95
QZ3P	--	--	-34.08	-31.51
QZ3P-1D	--	--	-33.89	-30.80
Cyanide Anion				
Basis Set	M06 PCM[a]	M06 SMD[a]	M06 COSMO-RS[b]	B3LYP-dDsC COSMO-RS[b]
cc-pVTZ	-60.23	-60.96	--	--
aug-cc-pVTZ	-58.39	-58.38	--	--
cc-pVQZ	-59.62	-59.95	--	--
aug-cc-pVQZ	-58.42	-58.42	--	--
TZP	--	--	-57.50	-57.21
aug-TZP	--	--	-56.07	-55.15
QZ3P	--	--	-56.09	-55.68
QZ3P-1D	--	--	-55.90	-55.08

a) Computed using Gaussian09.
b) Computed using ADF.

SI Table 2. Electronic Energies of relevant compounds. Values in hartree.

Compound	**M06/pVDZ (Gas Phase Optimized)[a]**	**M06/pVDZ (PCM Optimized)[a]**	**M06/def2-TZVPP (Single Point in PCM)[a]**	**B3LYP-dDsC/def2-TZVPP (Single Point in PCM)[b]**	**B3LYP-dDsC/TZP (Single Point in Gas Phase)[c]**
CO	-113.16427	-113.16495	-113.30187	-113.36287	-0.66028
PPh_3	-1035.12225	-1035.12672	-1035.99275	-1036.69228	-9.18196
PMe_3	-460.77684	-460.77873	-461.03827	-461.20793	-2.72794
Pyridine	-247.90970	-247.91335	-248.18757	-248.40734	-2.96793
THF	-232.11322	-232.11594	-232.38029	-232.57819	-3.01923
H_2O	-76.32443	-76.33002	-76.43195	-76.47117	-0.62370
CH_3CN	-132.55466	-132.56122	-132.71742	-132.82257	-1.54544
CN^-	-92.70029	-92.79711	-92.91840	-92.98154	-0.71688
H_2	-1.16694	-1.16707	-1.17107	-1.17996	-0.28313
H^-	-0.48116	-0.61372	-0.62811	-0.63089	-0.07895
Fe-H (5Coord)	-2711.95586	-2711.97011	-2713.45162	-2714.41141	-11.54511
Fe-H + CO	-2825.15197	-2825.16647	-2826.77634	-2827.80011	-12.22956
Fe-H + PPh_3	-3747.11111	-3747.12704	-3749.46652	-3751.13792	-20.75637
Fe-H + PMe_3	-3172.77146	-3172.78722	-3174.52269	-3175.65777	-14.30599
Fe-H + Pyridine	-2959.88995	-2959.90806	-2961.65516	-2962.84427	-14.53408
Fe-H + THF	-2944.08362	-2944.09918	-2945.83704	-2947.00645	-14.57807
Fe-H + H_2O	-2788.30508	-2788.32300	-2789.89250	-2790.89810	-12.18415
Fe-H + CH_3CN	-2844.52434	-2844.54546	-2846.17552	-2847.24544	-13.09897
Fe-H + CN^-	-2804.74296	-2804.81304	-2806.40332	-2807.43286	-12.33927
Fe-H + H_2	-2713.12175	-2713.13644	-2714.62145	-2715.59081	-11.82606
Fe-H + H^-	-2712.58054	-2712.65083	-2714.13811	-2715.10802	-11.73721
Fe-H(SH^+) (5 Coord)	-2712.32526	-2712.38413	-2713.86808	-2714.82680	-11.47215
Fe-H(SH^+) + CO	-2825.52989	-2825.58569	-2827.19991	-2828.22125	-12.16445
Fe-H(SH^+) + PPh_3	-3747.50623	-3747.55494	-3749.89828	-3751.56946	-20.70888
Fe-H(SH^+) + PMe_3	-3173.15989	-3173.21509	-3174.95329	-3176.08684	-14.25143
Fe-H(SH^+) + Pyridine	-2960.27818	-2960.33339	-2962.08412	-2963.27225	-14.47989
Fe-H(SH^+) + THF	-2944.47484	-2944.52844	-2946.26862	-2947.43665	-14.52432
Fe-H(SH^+) + H_2O	-2788.68490	-2788.74573	-2790.31771	-2791.32191	-12.11932
Fe-H(SH^+) + CH_3CN	-2844.91801	-2844.97731	-2846.60980	-2847.67958	-13.04889
Fe-H(SH^+) + CN^-	-2805.24973	-2805.26771	-2806.85881	-2807.89038	-12.40072
Fe-H(SH^+) + H_2	-2713.50167	-2713.55888	-2715.04670	-2716.01597	-11.76426
Fe-H(SH^+) + H^-	-2713.09748	-2713.11325	-2714.60127	-2715.57346	-11.80816

a) Computed using Gaussian09.
b) Computed using Q-Chem.
c) Computed using ADF.

SI Table 3. Free Energy and Solvation Corrections of relevant Compounds. Free energy corrections in hartree. Solvation energies in kcal/mol.

Compound	**M06/pVDZ Free Energy Correction (Gas Phase)**	**M06/pVDZ Free Energy Correction (PCM)**	**COSMO-RS Solvation Energy (B3LYP-dDsC/TZP)**
CO	-0.01400	-0.01401	-0.28
PPh_3	0.22780	0.22756	-10.96
PMe_3	0.08234	0.08121	-3.35
Pyridine	0.06082	0.06085	-4.09
THF	0.08795	0.08784	-3.22
H_2O	0.00327	0.00317	-7.86
CH_3CN	0.02088	0.02087	-4.54
CN^-	-0.01411	-0.01409	-57.36
H_2	-0.00143	-0.00144	0.74
H^-	-0.01000	-0.01000	-34.25
Fe-H (5Coord)	0.25786	0.25824	-18.10
Fe-H + CO	0.26552	0.26460	-18.88
Fe-H + PPh_3	0.51326	0.51305	-25.22
Fe-H + PMe_3	0.36699	0.36597	-20.41
Fe-H + Pyridine	0.34262	0.34235	-22.62
Fe-H + THF	0.36854	0.36829	-20.28
Fe-H + H_2O	0.28267	0.28285	-21.34
Fe-H + CH_3CN	0.29887	0.29991	-24.02
Fe-H + CN^-	0.26191	0.26373	-52.49
Fe-H + H_2	0.27378	0.27313	-18.84
Fe-H + H^-	0.26157	0.25981	-53.10
Fe-H(SH^+,5 Coord)	0.26557	0.26751	-50.76
Fe-H(SH^+) + CO	0.27350	0.27540	-50.14
Fe-H(SH^+) + PPh_3	0.52461	0.52373	-50.33
Fe-H(SH^+) + PMe_3	0.37582	0.37569	-50.13
Fe-H(SH^+) + Pyridine	0.35109	0.35249	-51.30
Fe-H(SH^+) + THF	0.38033	0.37944	-49.33
Fe-H(SH^+) + H_2O	0.29172	0.29251	-59.89
Fe-H(SH^+) + CH_3CN	0.30939	0.31010	-52.29
Fe-H(SH^+) + CN^-	0.27187	0.27371	-19.59
Fe-H(SH^+) + H_2	0.28352	0.28431	-50.85
Fe-H(SH^+) + H^-	0.27227	0.27250	-19.23

Cartesian Coordinates of Relevant Structures

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Complex 1

Fe	-0.05333	-0.11244	0.04754
S	-0.16879	1.47827	1.60254
O	2.38488	1.43761	-0.88310
O	0.49963	-1.49680	-2.47211
O	-2.93178	0.07691	-0.45315
O	-1.15277	-2.47090	1.11323
N	1.88254	-0.18647	0.55887
C	-2.23854	3.20838	0.99948
C	-1.83762	2.09813	1.77088
C	-3.54415	3.68638	1.14151
C	-1.80744	-0.00201	-0.26602
C	-2.73167	1.48289	2.67008
C	2.16923	-1.09787	1.50032
C	3.46692	-1.25412	1.97750
H	3.68231	-2.00612	2.73973
C	0.98864	-1.87348	1.96412
H	0.64375	-1.46670	2.93520
H	1.20877	-2.94251	2.12873
C	2.83098	0.61012	0.05760
C	0.27145	-0.98034	-1.47262
C	4.46024	-0.42501	1.46632
H	5.48961	-0.51665	1.82370
C	-1.30698	3.85879	0.02419
H	-1.79112	4.70910	-0.47975
H	-0.96704	3.14446	-0.74639
H	-0.38951	4.22160	0.51749
C	-0.22693	-1.71127	1.03360
C	-4.02813	1.99434	2.77887
C	3.26323	2.37719	-1.45193
H	2.67497	2.96814	-2.16418
H	4.08959	1.88381	-1.99288
H	3.68003	3.05287	-0.68530
C	-2.33265	0.28414	3.47254
H	-3.11003	0.02250	4.20624
H	-1.38577	0.45705	4.01086
H	-2.17233	-0.59965	2.82851
C	4.15576	0.52433	0.49682
H	4.93049	1.17462	0.08861
C	-4.43670	3.08691	2.02295
H	-3.86145	4.54581	0.54074
H	-5.45618	3.47169	2.11937
H	-4.72803	1.51593	3.47261

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Complex 1 - CH3CN

Fe	0.06082	0.06718	0.12935
S	0.61744	-2.16304	-0.51323
O	2.44965	1.64178	-1.35261
O	-0.77314	2.83330	0.61077
O	-0.93305	-0.95961	2.68172
O	-2.67704	-0.68844	-0.05901
N	0.54965	0.53789	-1.84179
C	0.69097	-3.70766	1.79885
C	-0.02266	-3.39064	0.61892
C	0.20111	-4.69792	2.65463
C	-0.54074	-0.54817	1.69105
C	-1.19546	-4.11480	0.29970
C	-0.37200	0.11259	-2.72840
C	-0.17427	0.21005	-4.10447
H	-0.94843	-0.15496	-4.78327
C	-1.63158	-0.42056	-2.15532
H	-1.78702	-1.47084	-2.45840
H	-2.50384	0.14131	-2.53897
C	1.65885	1.13834	-2.29960
C	-0.43593	1.75064	0.43363
C	1.00433	0.76995	-4.57235
H	1.19688	0.84897	-5.64582
C	1.96414	-3.00850	2.16288
H	2.49766	-3.55373	2.95771
H	1.76817	-1.98623	2.53426
H	2.62242	-2.90295	1.28450
C	-1.65524	-0.38470	-0.62790
C	-1.64897	-5.09904	1.18417
C	3.64090	2.28738	-1.70606
H	4.11846	2.60381	-0.76880
H	3.45606	3.18380	-2.32453
H	4.32960	1.61406	-2.24738
C	-1.96630	-3.87489	-0.96190
H	-2.68634	-4.68859	-1.13913
H	-1.29592	-3.80254	-1.83361
H	-2.53820	-2.93316	-0.90276
C	1.93732	1.25503	-3.66538
H	2.85718	1.72650	-4.01244
C	-0.96788	-5.38798	2.35960
H	0.75823	-4.93081	3.56909
H	-1.34129	-6.15965	3.03940
H	-2.56116	-5.65136	0.93269
N	1.94737	0.20965	0.87101
C	2.98686	0.13207	1.36698
C	4.28626	-0.00074	1.98789
H	4.36023	-0.97717	2.49048
H	5.08296	0.06256	1.23207
H	4.44386	0.79138	2.73434

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Complex 1 - CN-

Fe	-0.50109	-0.24835	0.91623
C	1.02263	-0.35221	1.79729
O	2.02025	-0.43825	2.35711
N	-2.14938	-0.37726	-0.34322
C	-3.05573	0.58365	-0.57532
C	-2.21112	-1.52489	-1.05044
C	-3.14779	-1.70834	-2.06815
C	-4.02903	-0.67634	-2.36475
C	-3.99313	0.48866	-1.61205
C	-1.22037	-2.56092	-0.67370
C	-0.50011	-2.20166	0.64241
O	-0.00227	-3.10819	1.27605
O	-3.04411	1.59130	0.27972
C	-3.31804	2.90620	-0.13271
H	-0.40385	-2.56517	-1.42079
H	-1.65697	-3.57641	-0.64371
H	-3.15669	-2.65005	-2.62272
H	-4.76138	-0.78493	-3.17085
H	-4.70187	1.30301	-1.77884
H	-4.38233	3.16192	0.02152
H	-3.05725	3.05157	-1.19503
H	-2.66233	3.55395	0.47075
S	0.75867	-0.09810	-1.16291
C	2.48581	0.21259	-0.86974
C	3.37518	-0.85131	-0.58542
C	4.73098	-0.57484	-0.37994
C	5.22355	0.72204	-0.46770
C	4.35314	1.76027	-0.78199
C	2.98914	1.53070	-0.99056
C	2.09617	2.67746	-1.34765
C	2.89953	-2.26868	-0.51557
H	3.74970	-2.96598	-0.43835
H	2.23557	-2.45231	0.34568
H	2.30613	-2.52638	-1.40942
H	1.53098	2.46611	-2.27065
H	1.33712	2.86080	-0.56786
H	2.68283	3.59966	-1.49268
H	4.73285	2.78555	-0.86833
H	6.28705	0.92298	-0.29909
H	5.40964	-1.40483	-0.14896
C	-1.51165	-0.38606	2.35691
O	-2.17405	-0.47655	3.29421
C	-0.45804	1.73686	1.01868
N	-0.42564	2.90529	1.09806

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Complex 1 - CO

Fe	0.59790	-0.02169	0.15228
C	0.74957	-1.78613	-0.09228
O	0.81472	-2.90944	-0.27261
N	0.08986	1.98221	0.14275
C	0.88667	3.00643	0.49167
C	-1.14743	2.24700	-0.32423
C	-1.61119	3.55063	-0.48086
C	-0.77341	4.60496	-0.14779
C	0.49475	4.34056	0.35056
C	-1.99111	1.07019	-0.64074
C	-1.30022	-0.25804	-0.34215
O	-1.92339	-1.28091	-0.47960
O	2.06266	2.64270	0.99491
C	3.05745	3.59881	1.26500
H	-2.26780	1.06351	-1.71034
H	-2.94432	1.10272	-0.08100
H	-2.62020	3.71687	-0.86474
H	-1.10652	5.63952	-0.26640
H	1.16484	5.15218	0.63589
H	2.76568	4.26387	2.09609
H	3.28730	4.20496	0.37213
H	3.95486	3.03597	1.55281
S	0.83289	0.31285	-2.20529
C	0.83786	-1.23760	-3.09624
C	-0.32167	-1.65134	-3.79312
C	-0.28380	-2.84911	-4.51389
C	0.86479	-3.62875	-4.56307
C	2.00915	-3.20150	-3.90210
C	2.02113	-2.00859	-3.17373
C	3.28599	-1.59274	-2.49166
C	-1.58752	-0.84936	-3.79964
H	-2.27091	-1.21053	-4.58328
H	-2.11718	-0.93647	-2.83543
H	-1.38983	0.22009	-3.97600
H	3.48101	-0.51611	-2.61781
H	3.24443	-1.77560	-1.40296
H	4.14615	-2.16109	-2.87684
H	2.92591	-3.79912	-3.95200
H	0.87139	-4.56515	-5.12873
H	-1.18420	-3.16935	-5.04933
C	0.19971	-0.13824	1.89126
O	-0.06802	-0.19799	3.00301
C	2.44914	0.22689	0.26652
O	3.58836	0.29250	0.29355

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Complex 1 - H-
Fe -0.41720 -0.14002 0.87685
C 1.10154 -0.19294 1.74093
O 2.11003 -0.20436 2.30032
N -2.10540 -0.16335 -0.31096
C -2.98771 0.83278 -0.46834
C -2.32618 -1.34294 -0.93735
C -3.46068 -1.55021 -1.73044
C -4.35868 -0.51104 -1.90315
C -4.12769 0.70817 -1.27205
C -1.30898 -2.38198 -0.70819
C -0.51647 -2.10261 0.61086
O -0.04421 -3.06597 1.17733
O -2.71153 1.94099 0.22039
C -3.55441 3.04586 0.12384
H -0.50049 -2.26027 -1.45879
H -1.70782 -3.41070 -0.78317
H -3.60517 -2.52227 -2.20850
H -5.24685 -0.63919 -2.52999
H -4.82374 1.53898 -1.39450
H -4.57578 2.82486 0.48782
H -3.62475 3.42586 -0.91271
H -3.11931 3.83186 0.75523
S 0.78341 0.04393 -1.22606
C 2.49795 0.32471 -0.87207
C 3.40489 -0.75744 -0.78705
C 4.75364 -0.50199 -0.52119
C 5.21999 0.79537 -0.33288
C 4.32495 1.85782 -0.40964
C 2.96957 1.64424 -0.67782
C 2.02253 2.79997 -0.73147
C 2.93018 -2.16809 -0.94314
H 3.77118 -2.87931 -0.89243
H 2.20085 -2.43676 -0.15812
H 2.39988 -2.30717 -1.90057
H 1.51401 2.85342 -1.70916
H 1.21094 2.66793 0.00751
H 2.54174 3.75421 -0.54103
H 4.67797 2.88473 -0.25233
H 6.27861 0.97716 -0.11771
H 5.44762 -1.34860 -0.44965
C -1.36900 0.04858 2.32500
O -2.00675 0.24752 3.27197
H -0.34411 1.42074 0.96253

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Complex 1 - H2
Fe 0.33788 -0.01726 0.02675
S 0.55259 0.30208 -2.32756
O 2.13953 2.44676 0.80611
O -0.15299 -0.20348 2.90966
O 0.38300 -2.90810 -0.44276
O -2.33083 -0.99255 -0.21531
N 0.06725 2.01512 0.04327
C 2.16082 -1.78178 -3.21724
C 0.84878 -1.26571 -3.13156
C 2.36708 -3.00847 -3.85570
C 0.38165 -1.78532 -0.24067
C -0.23061 -1.97044 -3.70960
C -1.15718 2.40721 -0.36362
C -1.50384 3.75245 -0.45460
H -2.50787 4.02754 -0.78498
C -2.10124 1.31327 -0.70079
H -2.21431 1.24780 -1.79964
H -3.10978 1.48355 -0.28491
C 0.97915 2.94101 0.37702
C 0.05764 -0.13255 1.78538
C -0.55334 4.70904 -0.12757
H -0.79094 5.77409 -0.19582
C 3.33132 -1.05996 -2.62548
H 4.28120 -1.50523 -2.95891
H 3.32152 -1.10694 -1.52110
H 3.32414 0.00922 -2.89013
C -1.57500 -0.05683 -0.27559
C 0.02210 -3.19215 -4.33995
C 3.17611 3.32210 1.17413
H 4.02359 2.69635 1.47953
H 2.88325 3.96437 2.02291
H 3.48951 3.95765 0.32793
C -1.63421 -1.45368 -3.64610
H -2.31050 -2.08010 -4.24751
H -1.69914 -0.41646 -4.01402
H -2.01634 -1.44765 -2.61087
C 0.70760 4.31061 0.29593
H 1.46224 5.04999 0.56501
C 1.30774 -3.71561 -4.41068
H 3.38483 -3.40973 -3.91588
H 1.48495 -4.67566 -4.90448
H -0.81661 -3.74192 -4.78069
H 2.03230 0.06782 0.47003
H 2.01510 0.15569 -0.34898

45
Complex 1 - H2O
Fe 0.43493 -0.04394 0.03576
C 0.53943 -1.81095 -0.19274
O 0.59593 -2.93703 -0.36847
N 0.11763 2.02796 0.07757
C 0.92378 3.01034 0.50014
C -1.11117 2.35188 -0.37914
C -1.54470 3.67430 -0.45612
C -0.68668 4.68576 -0.05538
C 0.56983 4.35908 0.43964
C -1.98096 1.21654 -0.76601
C -1.44683 -0.12799 -0.26587
O -2.19728 -1.07026 -0.19738
O 2.09608 2.59872 1.01917
C 2.97142 3.53853 1.60366
H -1.98753 1.11884 -1.86845
H -3.02827 1.36731 -0.45005
H -2.54870 3.88644 -0.83013
H -0.99268 5.73364 -0.11405
H 1.25415 5.13784 0.77629
H 2.48095 4.07860 2.43044
H 3.34402 4.26287 0.85975
H 3.82015 2.97044 2.00402
S 0.81556 0.24645 -2.28722
C 0.87194 -1.32031 -3.15746
C -0.30636 -1.83600 -3.74253
C -0.24677 -3.05610 -4.42324
C 0.94470 -3.75922 -4.54301
C 2.10430 -3.23357 -3.98789
C 2.09266 -2.01867 -3.29638
C 3.37773 -1.51168 -2.71754
C -1.61896 -1.12111 -3.65451
H -2.35525 -1.57052 -4.33803
H -2.04107 -1.17575 -2.63633
H -1.51141 -0.05393 -3.91042
H 3.56009 -0.45950 -2.99283
H 3.38339 -1.56229 -1.61449
H 4.22979 -2.11132 -3.07197
H 3.05167 -3.77451 -4.08754
H 0.97145 -4.71394 -5.07636
H -1.16454 -3.45512 -4.86870
C 0.22338 -0.15205 1.80104
O 0.08202 -0.21431 2.93770
O 2.60848 0.10908 0.09599
H 2.73606 0.98710 0.48543
H 2.63265 0.25895 -0.87179

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Complex 1 - PMe3

Fe	-0.33275	0.17691	-1.28601
C	-0.11532	1.86989	-1.75653
O	-0.00754	2.96743	-2.06457
N	-1.01883	-1.75836	-0.81663
C	-0.33689	-2.77713	-0.27314
C	-2.32911	-1.93223	-1.08443
C	-3.01941	-3.07773	-0.68770
C	-2.32662	-4.08301	-0.03431
C	-0.95667	-3.95051	0.16359
C	-2.97925	-0.87112	-1.88785
C	-2.00684	0.23182	-2.30129
O	-2.35693	1.01276	-3.15395
O	0.98898	-2.59205	-0.21431
C	1.79641	-3.58902	0.36057
H	-3.80226	-0.38956	-1.32932
H	-3.44569	-1.30115	-2.79386
H	-4.08800	-3.15529	-0.90202
H	-2.83950	-4.98842	0.30132
H	-0.38384	-4.75281	0.62866
H	1.74560	-4.53229	-0.21030
H	1.51709	-3.78469	1.41156
H	2.82870	-3.21413	0.33623
S	-1.35426	1.17732	0.66219
C	-3.11101	0.91980	0.73547
C	-3.61706	-0.15969	1.49672
C	-4.99783	-0.38163	1.52423
C	-5.87292	0.45892	0.84366
C	-5.37104	1.55560	0.14974
C	-3.99729	1.81255	0.08864
C	-3.50246	3.01106	-0.65859
C	-2.71167	-1.04641	2.29650
H	-3.26878	-1.88781	2.73893
H	-1.88085	-1.44596	1.69258
H	-2.23187	-0.48292	3.11598
H	-2.72650	3.54352	-0.08583
H	-3.04156	2.73038	-1.62047
H	-4.32881	3.70473	-0.87688
H	-6.05820	2.24006	-0.35976
H	-6.95067	0.27206	0.87233
H	-5.38846	-1.22668	2.10291
C	0.56666	-0.49298	-2.65405
O	1.17941	-0.94575	-3.51509
P	1.54684	0.28178	0.11907
C	3.13976	-0.33536	-0.55967
C	1.46760	-0.38228	1.83211
C	2.03216	2.01231	0.50366
H	2.88149	2.03638	1.20682
H	2.31791	2.53910	-0.42029
H	1.17424	2.54106	0.94977
H	2.46828	-0.38437	2.29682
H	0.79772	0.27616	2.40621
H	1.03842	-1.39284	1.86491
H	3.95579	-0.26470	0.17924
H	3.04390	-1.37010	-0.91768
H	3.40174	0.28908	-1.42970

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Complex 1 - PPh3

Fe	-0.41810	0.11572	-1.19408
C	-0.28774	1.84068	-1.61130
O	-0.23908	2.94068	-1.91816
N	-0.94091	-1.89368	-0.81178
C	-0.16549	-2.87015	-0.31876
C	-2.23055	-2.16733	-1.08885
C	-2.80784	-3.39972	-0.78675
C	-2.02336	-4.37435	-0.19004
C	-0.67763	-4.12043	0.04457
C	-2.99657	-1.09637	-1.76937
C	-2.14714	0.12525	-2.09551
O	-2.59857	0.96288	-2.83720
O	1.12649	-2.55325	-0.21315
C	2.03132	-3.50925	0.28906
H	-3.83515	-0.74562	-1.13930
H	-3.45911	-1.47183	-2.70065
H	-3.86252	-3.56698	-1.01776
H	-2.44862	-5.34459	0.08084
H	-0.03536	-4.88434	0.48284
H	2.01375	-4.43406	-0.31245
H	1.81085	-3.74906	1.34502
H	3.03043	-3.05842	0.22651
S	-1.47982	0.81278	0.84129
C	-3.25965	0.85101	0.77863
C	-3.96977	-0.18245	1.43842
C	-5.36581	-0.19379	1.37744
C	-6.06264	0.80548	0.70396
C	-5.36097	1.85328	0.12067
C	-3.96255	1.90924	0.15990
C	-3.26315	3.08682	-0.44176
C	-3.26102	-1.24985	2.21749
H	-3.98092	-1.95498	2.66241
H	-2.55356	-1.82272	1.59447
H	-2.65454	-0.81359	3.02986
H	-2.37524	3.36780	0.14747
H	-2.91283	2.86847	-1.46395
H	-3.94144	3.95171	-0.50539
H	-5.90491	2.66518	-0.37468
H	-7.15551	0.78019	0.65735
H	-5.91279	-1.00042	1.87874
C	0.28092	-0.42512	-2.72579
O	0.64518	-0.79089	-3.75440
P	1.61808	0.36065	0.17648
C	3.21424	-0.42070	-0.34752
C	1.57248	-0.01633	1.98583
C	2.09511	2.14575	0.18843
C	3.43640	-0.66275	-1.70781
C	4.62862	-1.23238	-2.14898
C	5.62266	-1.57265	-1.23422
C	5.41696	-1.33106	0.12189
C	4.22375	-0.75975	0.56209
C	0.72670	-1.01656	2.47871
C	2.38191	0.68146	2.89236
C	1.30088	3.05530	0.90349
C	1.55233	4.42048	0.82671
C	2.58995	4.90157	0.02906
C	3.38147	4.00665	-0.68352
C	3.13952	2.63547	-0.60231
C	0.71235	-1.33174	3.83534
C	1.53435	-0.64317	4.72396
C	2.36710	0.36768	4.24957
H	3.77678	1.94784	-1.16742
H	0.45744	2.69192	1.50210
H	0.92207	5.11671	1.38747
H	2.77945	5.97676	-0.03758
H	4.19916	4.37390	-1.31056
H	3.03365	1.48585	2.53461
H	3.00727	0.92360	4.94072
H	1.51712	-0.88564	5.79051
H	0.03573	-2.10996	4.20128
H	0.04160	-1.53104	1.80277
H	4.08094	-0.59051	1.63314
H	6.19155	-1.58971	0.84999
H	6.55776	-2.02371	-1.57852
H	4.77711	-1.41268	-3.21745
H	2.67220	-0.40447	-2.44436

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Complex 1 - Pyridine

Fe	0.02135	-0.09690	-0.14495
S	-0.21631	1.32890	1.74985
O	3.04467	0.41245	-1.12577
O	0.39991	-2.07977	-2.25993
O	-2.79222	0.37634	-0.77813
O	-1.60275	-1.98103	1.23481
N	1.92495	-0.51545	0.58896
C	-2.51506	2.84633	1.32493
C	-1.92039	1.78593	2.04827
C	-3.84244	3.19431	1.59080
C	-1.69113	0.19063	-0.53335
C	-2.65641	1.12929	3.06157
C	1.90103	-1.24167	1.72465
C	3.06009	-1.50937	2.45089
H	2.99187	-2.09251	3.37209
C	0.57929	-1.79037	2.11736
H	0.25713	-1.38700	3.09340
H	0.63465	-2.88842	2.23976
C	3.11067	-0.13643	0.08677
C	0.25328	-1.29448	-1.43329
C	4.27178	-1.02869	1.97809
H	5.19675	-1.20749	2.53324
C	-1.76411	3.61748	0.28418
H	-2.33440	4.50355	-0.03458
H	-1.56219	3.01259	-0.61808
H	-0.78221	3.94696	0.66174
C	-0.52426	-1.45066	1.11354
C	-3.98091	1.51359	3.29479
C	4.19873	0.93272	-1.72902
H	3.88249	1.36301	-2.68902
H	4.95082	0.14724	-1.92198
H	4.65614	1.72911	-1.11439
C	-2.06660	0.04135	3.90561
H	-2.70943	-0.16823	4.77433
H	-1.06357	0.31589	4.27098
H	-1.96763	-0.89662	3.33299
C	4.31267	-0.34309	0.77026
H	5.26035	0.00313	0.35628
C	-4.58036	2.52967	2.56216
H	-4.29863	4.01125	1.02071
H	-5.61916	2.81247	2.75688
H	-4.54799	0.99682	4.07685
N	0.60757	1.60961	-1.34535
C	1.26864	2.64547	-0.81979
C	1.64661	3.75578	-1.56695
C	1.31591	3.80228	-2.91773
C	0.63113	2.72404	-3.46928
C	0.30528	1.65067	-2.64627
H	-0.23122	0.78717	-3.05673
H	0.34306	2.70771	-4.52287
H	1.58472	4.66683	-3.53146
H	2.18042	4.57784	-1.08362
H	1.46286	2.58901	0.25856

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Complex 1 - THF

Fe	-0.93401	-0.64817	-0.27355
S	1.10425	-0.92889	0.92399
O	-1.55329	2.03076	1.34937
O	-3.48977	-0.27618	-1.64638
O	-1.13261	-3.56389	-0.01866
O	-0.06182	-1.81240	-2.68221
N	-0.46269	1.36633	-0.50125
C	2.90460	-1.79801	-1.01633
C	2.48090	-0.73105	-0.18888
C	3.94397	-1.57145	-1.92564
C	-1.06371	-2.42914	-0.13663
C	3.18804	0.49496	-0.20049
C	0.29526	1.61502	-1.58470
C	0.81351	2.88213	-1.84893
H	1.43675	3.03104	-2.73396
C	0.53035	0.46305	-2.49009
H	1.61293	0.27276	-2.61508
H	0.14288	0.67135	-3.50481
C	-0.75638	2.37160	0.33433
C	-2.49226	-0.42344	-1.09484
C	0.52509	3.91532	-0.97136
H	0.91740	4.92094	-1.14575
C	2.28955	-3.15944	-0.93300
H	2.95375	-3.91393	-1.38209
H	1.32848	-3.20511	-1.47104
H	2.08347	-3.43611	0.11316
C	-0.11427	-0.82579	-1.98846
C	4.21942	0.67707	-1.12725
C	-1.90729	2.99850	2.30086
H	-2.55856	2.49966	3.03179
H	-2.46458	3.83741	1.84726
H	-1.02196	3.39562	2.82849
C	2.89370	1.58147	0.78805
H	3.45673	2.49842	0.55077
H	3.17145	1.26539	1.80883
H	1.82132	1.82235	0.84081
C	-0.27458	3.66932	0.13873
H	-0.51927	4.47218	0.83459
C	4.58400	-0.33947	-2.00455
H	4.25963	-2.39325	-2.57780
H	5.38932	-0.18167	-2.72837
H	4.75276	1.63460	-1.14559
O	-1.88503	-0.65109	1.76403
C	-3.29647	-0.51722	1.88811
C	-1.26956	-0.75993	3.04505
C	-2.39053	-1.19087	3.96638
C	-3.57355	-0.43493	3.38027
H	-3.62715	0.37782	1.33190
H	-3.77954	-1.39990	1.42423
H	-3.55622	0.61631	3.72028
H	-4.55427	-0.85091	3.65504
H	-2.19296	-0.95850	5.02343
H	-2.55100	-2.27999	3.88460
H	-0.84376	0.22306	3.33213
H	-0.43493	-1.47494	2.97514

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Complex 1 - SH+

Fe	-0.02373	-0.17597	0.19133
S	-0.31344	1.18574	2.08982
O	2.10301	1.71658	-0.52527
O	0.52450	-1.75138	-2.22037
O	-2.94501	-0.16041	-0.29008
O	-1.09540	-2.27283	1.64391
N	1.90834	-0.16601	0.63255
C	-2.02956	3.07843	0.95825
C	-1.87998	2.05408	1.90961
C	-3.29635	3.65418	0.83807
C	-1.82245	-0.17432	-0.11451
C	-2.93867	1.56951	2.69475
C	2.35540	-1.19957	1.36748
C	3.69999	-1.30312	1.69885
H	4.05566	-2.14434	2.29750
C	1.29242	-2.17381	1.74721
H	1.24596	-2.34441	2.83791
H	1.48541	-3.16946	1.30425
C	2.73770	0.78373	0.18630
C	0.29477	-1.14858	-1.28141
C	4.57074	-0.31553	1.24171
H	5.63520	-0.37224	1.48383
C	-0.90437	3.54095	0.08627
H	-1.25688	4.27661	-0.65006
H	-0.43971	2.70547	-0.47065
H	-0.09638	4.02718	0.66462
C	-0.09649	-1.73265	1.27538
C	-4.18612	2.17611	2.52358
C	2.85075	2.76102	-1.12834
H	2.13348	3.38439	-1.67514
H	3.59180	2.35675	-1.83675
H	3.35968	3.37547	-0.36738
C	-2.76753	0.42382	3.64317
H	-3.69958	0.22557	4.18991
H	-1.97764	0.61945	4.38740
H	-2.49682	-0.50864	3.11488
C	4.10191	0.74643	0.47366
H	4.78089	1.51912	0.11018
C	-4.36335	3.20968	1.61192
H	-3.44397	4.46012	0.11280
H	-5.34786	3.66965	1.49501
H	-5.03100	1.81900	3.11984
H	0.52372	2.20248	1.75965

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Complex 1 - SH+ - CH3CN

Fe	-0.17114	-0.05463	0.02488
S	0.01807	-1.27920	2.09947
O	-2.05466	2.36393	0.98317
O	-0.11315	1.67610	-2.33743
O	-0.08223	-2.54456	-1.54581
O	2.48874	-0.90514	-0.47017
N	0.08339	1.67482	1.15829
C	-0.64948	-3.94726	1.54363
C	0.36986	-3.03562	1.88780
C	-0.29386	-5.28916	1.39722
C	-0.12426	-1.57999	-0.94572
C	1.70223	-3.43957	2.09574
C	1.36495	1.89173	1.53452
C	1.73562	2.97787	2.31750
H	2.78362	3.10683	2.59679
C	2.36639	0.91683	1.03248
H	2.82234	0.34799	1.86531
H	3.21297	1.42778	0.53878
C	-0.84879	2.58843	1.49219
C	-0.13318	0.98093	-1.43460
C	0.75739	3.88003	2.71421
H	1.01320	4.74090	3.33718
C	-2.07777	-3.54810	1.33382
H	-2.69981	-4.43456	1.14655
H	-2.19343	-2.87608	0.46627
H	-2.51123	-3.03562	2.21271
C	1.77308	-0.10191	0.06973
C	1.99949	-4.79566	1.92298
C	-3.09353	3.29249	1.19846
H	-3.96702	2.91708	0.65015
H	-2.83279	4.28923	0.80473
H	-3.35030	3.37652	2.26819
C	2.79975	-2.49714	2.48186
H	3.65013	-3.05002	2.90498
H	2.47249	-1.76269	3.23619
H	3.17937	-1.94897	1.60158
C	-0.55076	3.69610	2.29256
H	-1.32743	4.40981	2.56820
C	1.01827	-5.71203	1.57500
H	-1.07074	-6.01392	1.13573
H	1.27394	-6.76713	1.44932
H	3.03018	-5.12858	2.07755
N	-2.19136	-0.19196	0.16535
C	-3.33167	-0.37690	0.14764
C	-4.75419	-0.62881	0.11990
H	-4.95235	-1.69266	0.32097
H	-5.27105	-0.02451	0.87954
H	-5.16377	-0.37935	-0.87010
H	-1.28422	-1.39501	2.45745

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Complex 1 - SH+ - CN-

Fe	0.27380	0.00655	0.11242
C	0.32256	-1.77069	-0.02444
O	0.32948	-2.90628	-0.14403
N	-0.04147	2.05170	0.12017
C	0.81073	2.99177	0.57173
C	-1.21177	2.43673	-0.43547
C	-1.51059	3.77661	-0.66129
C	-0.57735	4.74053	-0.29457
C	0.59575	4.35602	0.33643
C	-2.15342	1.33355	-0.75642
C	-1.68463	-0.00089	-0.14920
O	-2.50334	-0.87147	0.02969
O	1.81651	2.52765	1.28334
C	3.00842	3.25963	1.43819
H	-2.19930	1.16524	-1.85002
H	-3.18777	1.56721	-0.44544
H	-2.46459	4.04575	-1.12032
H	-0.77650	5.80075	-0.47409
H	1.31923	5.09329	0.68847
H	2.90545	4.03966	2.21235
H	3.31591	3.72070	0.48451
H	3.77576	2.53215	1.73389
S	0.55416	0.20392	-2.31666
C	0.80417	-1.40555	-3.08954
C	-0.35670	-2.11398	-3.44839
C	-0.20198	-3.39085	-3.99406
C	1.05831	-3.93987	-4.18691
C	2.18919	-3.20346	-3.85770
C	2.09731	-1.92119	-3.30657
C	3.35292	-1.16139	-3.01068
C	-1.73071	-1.55471	-3.25252
H	-2.47112	-2.13467	-3.82200
H	-2.04474	-1.58464	-2.19464
H	-1.79785	-0.50639	-3.59188
H	3.40099	-0.21820	-3.58488
H	3.46402	-0.90222	-1.94315
H	4.23438	-1.75147	-3.29888
H	3.18474	-3.62451	-4.02982
H	1.16180	-4.94353	-4.60823
H	-1.09836	-3.95546	-4.26955
C	0.09636	-0.03480	1.87514
O	-0.00038	-0.02973	3.01426
C	2.24489	0.14132	0.18377
N	3.40757	0.23299	0.09320
H	1.85812	0.56939	-2.28185

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Complex 1 - SH+ - CO
Fe 0.02124 -0.02032 -0.06535
C 1.83021 -0.10464 -0.13352
O 2.96405 -0.10605 -0.16849
N -1.97019 0.50279 0.04814
C -2.96927 -0.27133 0.51466
C -2.25301 1.76309 -0.35941
C -3.54485 2.27002 -0.33995
C -4.57680 1.45459 0.11116
C -4.29498 0.16942 0.54849
C -1.09353 2.57034 -0.82277
C 0.22857 1.93083 -0.44068
O 1.24021 2.57010 -0.36877
O -2.58260 -1.46501 0.95034
C -3.53161 -2.42358 1.38375
H -1.13637 3.61656 -0.47129
H -1.08601 2.62945 -1.93073
H -3.72864 3.29215 -0.67758
H -5.60562 1.82283 0.13250
H -5.08767 -0.47874 0.92356
H -4.25656 -2.65365 0.58630
H -4.06280 -2.07886 2.28586
H -2.96223 -3.33032 1.62354
S 0.02810 0.63929 2.22764
C 1.62761 1.18361 2.84189
C 1.82338 2.57253 2.95377
C 3.06971 3.00431 3.42166
C 4.06434 2.10170 3.76661
C 3.83315 0.73334 3.66441
C 2.61378 0.23967 3.20108
C 2.39518 -1.24052 3.13608
C 0.79251 3.59860 2.59611
H 0.87604 4.47286 3.25829
H 0.94418 3.95547 1.56330
H -0.23928 3.22075 2.67399
H 1.59213 -1.57628 3.81782
H 2.13521 -1.59542 2.12396
H 3.30370 -1.77990 3.43737
H 4.61377 0.02340 3.95330
H 5.02931 2.46478 4.12935
H 3.24765 4.07971 3.51813
C -0.14981 -0.24669 -1.84371
O -0.29909 -0.36757 -2.96525
C -0.14452 -1.83630 0.40106
O -0.10693 -2.93359 0.69526
H -0.02116 -0.54430 2.89065

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Complex 1 - SH+ - H-

Fe	0.14674	-0.02081	-0.04166
C	0.20233	-1.78026	-0.11273
O	0.25152	-2.92423	-0.19073
N	-0.04656	2.04741	-0.06151
C	0.91301	2.93801	0.24649
C	-1.30421	2.48974	-0.29392
C	-1.63928	3.83915	-0.19349
C	-0.64865	4.75215	0.13603
C	0.64861	4.30864	0.35491
C	-2.29406	1.45040	-0.65993
C	-1.81968	0.03125	-0.26323
O	-2.66576	-0.83683	-0.21950
O	2.12169	2.41733	0.43493
C	3.18439	3.24147	0.83496
H	-2.38504	1.40647	-1.76459
H	-3.30750	1.67013	-0.27964
H	-2.66999	4.15037	-0.37729
H	-0.88013	5.81753	0.22185
H	1.44060	5.01346	0.60935
H	2.97420	3.73885	1.79803
H	3.41749	4.00978	0.07606
H	4.05749	2.58879	0.95819
S	0.42933	0.20698	-2.38108
C	0.78787	-1.40415	-3.08930
C	-0.31509	-2.12963	-3.57115
C	-0.08106	-3.41584	-4.06430
C	1.19673	-3.96093	-4.07190
C	2.26775	-3.22515	-3.57894
C	2.08952	-1.93632	-3.06824
C	3.25607	-1.18488	-2.50730
C	-1.70636	-1.57984	-3.52392
H	-2.39992	-2.21877	-4.08927
H	-2.08574	-1.52356	-2.48697
H	-1.75969	-0.56286	-3.94906
H	3.52706	-0.31293	-3.13077
H	3.03908	-0.81403	-1.48851
H	4.14637	-1.82766	-2.45385
H	3.27334	-3.65799	-3.57138
H	1.35886	-4.97132	-4.45737
H	-0.92950	-3.99612	-4.44075
C	0.25888	-0.00327	1.70705
O	0.40299	0.05032	2.84707
H	1.70607	-0.00330	0.09622
H	1.69177	0.69356	-2.43974

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Complex 1 - SH+ - H2

Fe	0.03471	-0.33411	-0.30264
S	2.41629	-0.18125	-0.22001
O	0.44793	2.74153	0.23114
O	-2.86592	-0.43011	-0.73782
O	0.11724	-2.97245	1.01652
O	0.65720	-2.39000	-2.16603
N	0.17015	1.32926	-1.50036
C	3.06633	-0.44320	2.49688
C	3.04626	-1.05091	1.22732
C	3.54096	-1.21223	3.56301
C	0.07106	-1.94758	0.53065
C	3.49513	-2.36382	0.99766
C	0.08337	1.06852	-2.82656
C	0.13731	2.07904	-3.77702
H	0.06788	1.82723	-4.83729
C	-0.07058	-0.36559	-3.18496
H	0.51324	-0.64921	-4.07717
H	-1.12956	-0.58408	-3.43256
C	0.32700	2.60248	-1.09111
C	-1.74303	-0.40637	-0.55069
C	0.27679	3.39344	-3.34717
H	0.31589	4.21147	-4.07095
C	2.65575	0.97835	2.73410
H	2.65878	1.21051	3.80818
H	1.64553	1.19889	2.35130
H	3.35264	1.69090	2.25474
C	0.27366	-1.26612	-2.00843
C	3.94943	-3.08591	2.10463
C	0.55520	4.03616	0.80205
H	0.61211	3.89293	1.88765
H	-0.32952	4.64846	0.56441
H	1.46789	4.54855	0.45641
C	3.50532	-2.97996	-0.36690
H	3.93631	-3.98998	-0.33367
H	4.11005	-2.38464	-1.07221
H	2.49792	-3.07126	-0.80848
C	0.37531	3.66921	-1.99013
H	0.49730	4.69400	-1.63838
C	3.96944	-2.52116	3.37380
H	3.57388	-0.76472	4.56106
H	4.33064	-3.10400	4.22489
H	4.29984	-4.11133	1.95417
H	-0.13676	0.88256	0.94943
H	-0.08489	0.17105	1.35712
H	2.51805	1.07782	0.27354

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Complex 1 - SH+ - H2O

Fe	0.03919	0.08344	0.04242
C	1.84648	0.10519	0.10528
O	2.98146	0.13390	0.16033
N	-2.04227	0.29463	0.00356
C	-2.99855	-0.64743	-0.06707
C	-2.41975	1.59548	-0.01673
C	-3.75577	1.97799	-0.04837
C	-4.73464	0.99536	-0.06906
C	-4.35851	-0.34099	-0.08764
C	-1.32550	2.60011	-0.03327
C	0.05179	1.98316	-0.23940
O	1.00835	2.68501	-0.43219
O	-2.54650	-1.91420	-0.13779
C	-3.46703	-2.98065	-0.33466
H	-1.28377	3.14871	0.92808
H	-1.49852	3.37649	-0.79973
H	-4.00945	3.04022	-0.06403
H	-5.79406	1.26298	-0.08609
H	-5.11263	-1.12693	-0.12576
H	-4.04032	-2.83559	-1.26358
H	-4.15279	-3.07861	0.52186
H	-2.87035	-3.89627	-0.42267
S	-0.08376	0.59781	2.40120
C	1.53982	0.93977	3.10894
C	1.89099	2.29556	3.23970
C	3.16543	2.58401	3.73865
C	4.04253	1.57302	4.10427
C	3.65466	0.24270	3.99322
C	2.39868	-0.10869	3.49476
C	2.01519	-1.55443	3.42408
C	0.97163	3.42087	2.87705
H	1.30306	4.35557	3.35086
H	0.96362	3.60197	1.78834
H	-0.06388	3.23315	3.20734
H	1.19167	-1.79500	4.12150
H	1.68448	-1.86335	2.41950
H	2.86223	-2.19439	3.70746
H	4.33894	-0.55371	4.30093
H	5.03377	1.82212	4.49133
H	3.46085	3.63206	3.84544
C	0.01028	-0.18732	-1.72362
O	-0.04444	-0.36172	-2.84954
O	-0.03664	-1.96672	0.65761
H	0.58999	-2.56589	0.23245
H	-0.93112	-2.25761	0.39535
H	-0.22157	-0.67334	2.85239

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Complex 1 - SH+ - PMe3
Fe -0.33106 0.17814 -1.24867
C -0.01371 1.83697 -1.81352
O 0.14014 2.91641 -2.15115
N -1.02390 -1.73973 -0.78138
C -0.33916 -2.75533 -0.21989
C -2.31670 -1.95181 -1.12414
C -2.99102 -3.12107 -0.78687
C -2.30369 -4.12013 -0.11346
C -0.95332 -3.95083 0.16194
C -2.96133 -0.89592 -1.94172
C -2.03575 0.27628 -2.22925
O -2.42026 1.17065 -2.93745
O 0.96970 -2.53882 -0.08667
C 1.78049 -3.52600 0.52282
H -3.87894 -0.50228 -1.46755
H -3.29537 -1.31476 -2.90990
H -4.03962 -3.23404 -1.07211
H -2.80517 -5.04842 0.17214
H -0.38248 -4.74657 0.64031
H 1.78110 -4.46044 -0.06173
H 1.45172 -3.73372 1.55569
H 2.80043 -3.12079 0.54958
S -1.42183 1.12985 0.70927
C -3.20812 0.93273 0.75712
C -3.67487 -0.18326 1.47512
C -5.05159 -0.42152 1.47249
C -5.92339 0.43619 0.81015
C -5.43426 1.56217 0.15638
C -4.06495 1.84457 0.11155
C -3.58260 3.08481 -0.57490
C -2.75511 -1.07032 2.25886
H -3.29707 -1.93645 2.66524
H -1.91417 -1.45749 1.65857
H -2.31195 -0.52571 3.11092
H -3.04204 3.75345 0.11980
H -2.92368 2.86625 -1.43143
H -4.43103 3.66321 -0.96544
H -6.12687 2.25110 -0.33631
H -6.99825 0.23756 0.82067
H -5.44011 -1.28723 2.01818
C 0.50919 -0.55614 -2.63208
O 1.07425 -1.07400 -3.47908
P 1.63646 0.27692 0.09022
C 3.14695 -0.43634 -0.65808
C 1.57154 -0.31222 1.83163
C 2.21284 1.99799 0.37745
H 3.10426 2.00175 1.02617
H 2.47282 2.48367 -0.57596
H 1.42832 2.59799 0.86706
H 2.58918 -0.48485 2.21985
H 1.10007 0.47105 2.44573
H 0.97853 -1.23085 1.94170
H 3.99315 -0.41229 0.04813
H 2.97831 -1.46244 -1.01116
H 3.41228 0.17710 -1.53465
H -1.41266 2.45362 0.41355

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Complex 1 - SH+ - PPh3

Fe	-0.03400	-0.09271	-0.07727
C	1.73591	0.03599	-0.32934
O	2.86663	0.14299	-0.42988
N	-2.05379	0.07398	0.40038
C	-3.08714	-0.53646	-0.21188
C	-2.31713	0.94419	1.40282
C	-3.59491	1.10318	1.92682
C	-4.63714	0.36964	1.37510
C	-4.39373	-0.45017	0.28174
C	-1.17293	1.76848	1.86514
C	0.10505	1.48030	1.09111
O	1.08148	2.15626	1.28405
O	-2.76387	-1.19966	-1.31606
C	-3.78704	-1.82713	-2.06854
H	-0.96190	1.62571	2.94102
H	-1.40685	2.84420	1.75694
H	-3.75470	1.80622	2.74766
H	-5.65157	0.45744	1.77282
H	-5.20874	-0.99224	-0.19769
H	-4.56869	-1.10402	-2.35247
H	-4.23353	-2.66505	-1.50541
H	-3.30925	-2.21222	-2.97740
S	0.41123	-1.49849	1.88289
C	0.21848	-0.68400	3.47443
C	-1.01372	-0.89314	4.12229
C	-1.23561	-0.21664	5.32414
C	-0.25712	0.60623	5.87235
C	0.97215	0.74565	5.23851
C	1.24704	0.10376	4.02599
C	2.59737	0.25339	3.39703
C	-2.05610	-1.82414	3.58005
H	-2.93234	-1.85593	4.24324
H	-2.41522	-1.52606	2.57997
H	-1.66614	-2.85267	3.48659
H	3.09814	-0.72221	3.25860
H	2.55250	0.76145	2.41994
H	3.25609	0.85390	4.03925
H	1.75140	1.36726	5.68954
H	-0.44597	1.12683	6.81480
H	-2.18870	-0.35826	5.84337
C	-0.42022	0.99961	-1.42523
O	-0.73869	1.73081	-2.24315
P	0.03566	-2.20826	-1.35907
C	-0.34060	-2.06179	-3.15350
C	-0.85570	-3.71268	-0.78493
C	1.77480	-2.83524	-1.35440
C	0.16821	-0.95720	-3.85017
C	-0.06608	-0.80173	-5.21345
C	-0.82141	-1.74741	-5.90299
C	-1.33020	-2.85082	-5.22320
C	-1.08947	-3.01115	-3.85926
C	-1.83871	-3.64094	0.20680
C	-0.51631	-4.97028	-1.30658
C	2.24632	-3.49083	-0.20564
C	3.58522	-3.85265	-0.09377
C	4.47507	-3.57194	-1.12992
C	4.01159	-2.94628	-2.28259
C	2.67071	-2.58059	-2.39709
C	-2.48947	-4.79061	0.65040
C	-2.16124	-6.03035	0.10783
C	-1.17066	-6.11802	-0.86925
H	2.33170	-2.09546	-3.31695
H	1.55512	-3.74923	0.60531
H	3.93407	-4.37039	0.80431
H	5.52737	-3.85472	-1.04246
H	4.69769	-2.74022	-3.10850
H	0.27563	-5.05615	-2.05878
H	-0.89840	-7.08999	-1.28937
H	-2.67016	-6.93374	0.45470
H	-3.25142	-4.71600	1.43211
H	-2.09051	-2.67870	0.65863
H	-1.49713	-3.88768	-3.34671
H	-1.91768	-3.60184	-5.75882
H	-1.01073	-1.62524	-6.97270
H	0.34302	0.06615	-5.73733
H	0.77500	-0.20665	-3.33239
H	1.76670	-1.52782	1.87608

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Complex 1 - SH+ - Pyridine

Fe	0.11352	0.08375	-0.00847
S	2.55940	-0.04921	0.01223
O	-0.82790	3.14210	-0.00506
O	-2.78660	0.15637	-0.37281
O	0.01324	-2.40762	1.54743
O	0.21584	-2.18124	-1.73284
N	0.18326	1.66164	-1.36319
C	3.18483	-1.76401	2.13472
C	3.15138	-1.59290	0.73546
C	3.62358	-2.99670	2.62110
C	0.05412	-1.43857	0.95154
C	3.56551	-2.59587	-0.15990
C	0.61781	1.29925	-2.59231
C	0.77828	2.22092	-3.61994
H	1.14002	1.88457	-4.59403
C	0.84689	-0.15508	-2.78947
H	1.92595	-0.38490	-2.87994
H	0.39445	-0.51090	-3.73233
C	-0.23457	2.92927	-1.17446
C	-1.65649	0.10666	-0.22532
C	0.45071	3.54994	-3.38223
H	0.57515	4.30161	-4.16599
C	2.79407	-0.69333	3.10659
H	2.91585	-1.04772	4.13947
H	1.74298	-0.37824	2.98945
H	3.42016	0.21310	3.00899
C	0.32283	-0.98829	-1.62125
C	3.98410	-3.81330	0.38780
C	-1.27400	4.43410	0.34548
H	-1.69191	4.35376	1.35753
H	-2.06169	4.78921	-0.33972
H	-0.44106	5.15858	0.35672
C	3.58213	-2.41842	-1.64649
H	4.21990	-3.17972	-2.11710
H	3.97385	-1.43041	-1.94037
H	2.57290	-2.53717	-2.07691
C	-0.07963	3.91544	-2.15294
H	-0.39633	4.94224	-1.96756
C	4.00769	-4.01795	1.75960
H	3.66096	-3.15181	3.70357
H	4.33980	-4.97742	2.16407
H	4.30606	-4.60879	-0.29084
N	0.15596	1.28123	1.75704
C	1.00794	2.30314	1.91398
C	1.07536	3.06985	3.06901
C	0.20567	2.77763	4.11716
C	-0.70024	1.73559	3.95403
C	-0.68907	1.01757	2.76293
H	-1.39050	0.18779	2.62229
H	-1.41068	1.46856	4.73918
H	0.23230	3.35623	5.04424
H	1.80044	3.88378	3.14067
H	1.66435	2.53597	1.06691
H	2.90127	0.75798	1.04612

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Complex 1 - SH+ - THF

Fe	-0.92026	-0.71746	-0.23671
S	1.14188	-0.90637	1.00766
O	-1.11910	1.90939	1.59819
O	-3.36225	-0.29255	-1.79384
O	-1.25584	-3.63414	-0.03055
O	0.21642	-1.94543	-2.48799
N	-0.44562	1.28831	-0.46227
C	3.01826	-1.78946	-0.87882
C	2.55516	-0.71459	-0.09450
C	4.05699	-1.51844	-1.77551
C	-1.15368	-2.50545	-0.14012
C	3.15135	0.56055	-0.12157
C	0.11299	1.57407	-1.66085
C	0.43927	2.87224	-2.03543
H	0.89247	3.05168	-3.01292
C	0.37145	0.41576	-2.55541
H	1.43661	0.36387	-2.85110
H	-0.19047	0.51215	-3.50432
C	-0.66509	2.29294	0.40742
C	-2.42132	-0.47459	-1.17458
C	0.16383	3.90962	-1.15473
H	0.38862	4.94444	-1.42573
C	2.48931	-3.18467	-0.76326
H	3.07826	-3.87024	-1.38787
H	1.44395	-3.26532	-1.10214
H	2.55647	-3.56749	0.27140
C	-0.02377	-0.90872	-1.92678
C	4.17497	0.77476	-1.04865
C	-1.26735	2.87171	2.62169
H	-1.56402	2.32567	3.52610
H	-2.04937	3.60987	2.37581
H	-0.31642	3.39501	2.82030
C	2.79223	1.64744	0.84662
H	3.23668	2.60606	0.54201
H	3.17784	1.40918	1.85328
H	1.70838	1.80162	0.95814
C	-0.39239	3.62590	0.08445
H	-0.60176	4.42723	0.79312
C	4.61367	-0.24920	-1.88061
H	4.43371	-2.33373	-2.40020
H	5.41731	-0.06438	-2.59821
H	4.64790	1.76078	-1.09457
O	-1.98693	-0.67205	1.67244
C	-3.35011	-0.23417	1.75583
C	-1.48883	-1.03206	2.96204
C	-2.72177	-1.17557	3.82894
C	-3.64023	-0.11566	3.23782
H	-3.45047	0.71764	1.20715
H	-3.99476	-0.98821	1.26477
H	-3.35984	0.88648	3.60628
H	-4.70267	-0.26741	3.47585
H	-2.51086	-1.03499	4.89871
H	-3.16138	-2.17956	3.70367
H	-0.80839	-0.23570	3.32341
H	-0.90662	-1.96643	2.87103
H	1.28044	-2.23889	1.22381