Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Supporting information for

$[Cp'FeI]_2$ as Convenient Entry into Iron-modified Pincer Complexes: Bimetallic η^6, κ^1-POCOP-Pincer Iron Iridium Compounds

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*1. Variable Temperature ^{1}H NMR Behavior of Complexes **2**.*

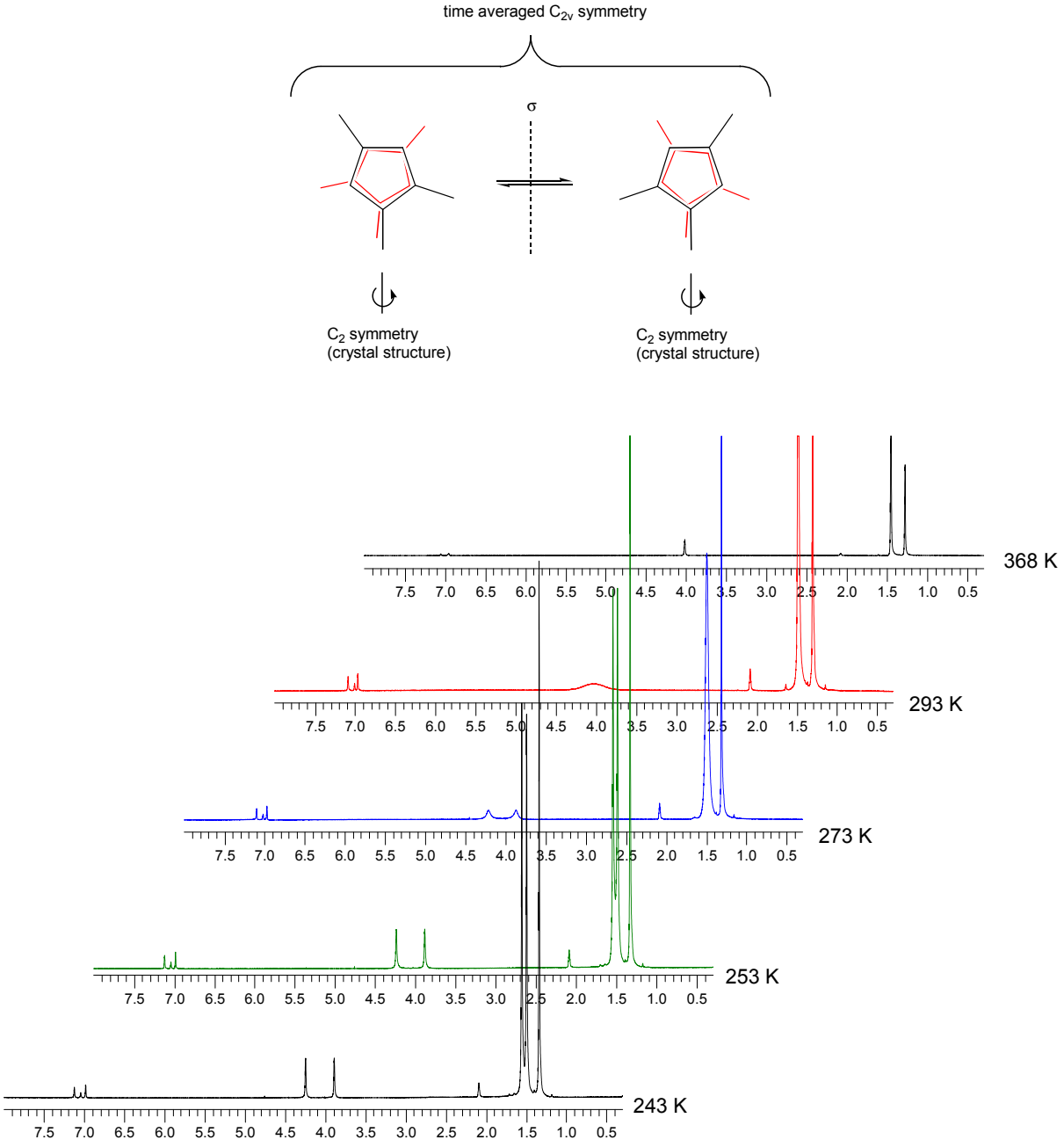

Figure S1. Stacked plot of ^{1}H NMR spectra of Cp'$_2$Fe (**2**) in toluene-d_8 from 243 K to 368 K.

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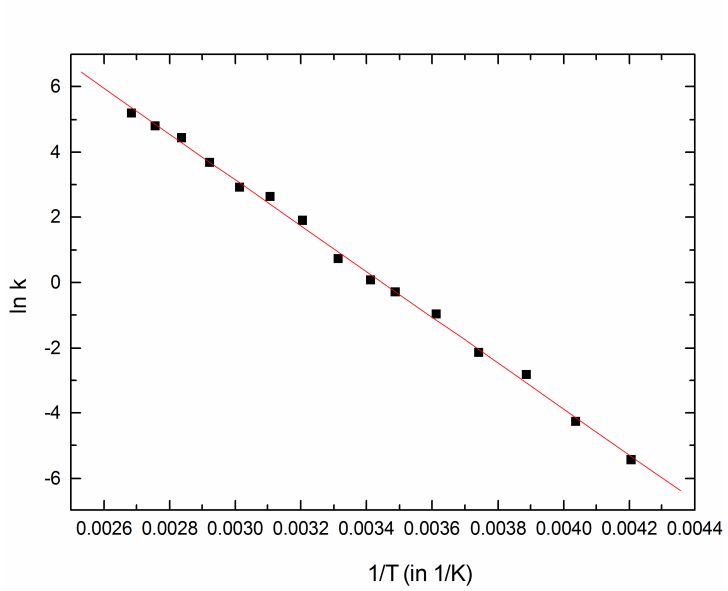

Figure S2. Arrhenius plot derived from line shape analysis of variable temperature ^{1}H NMR data of Cp'$_2$Fe (**2**) in toluene-d_8 (R^2= 0.9985): $\Delta H^{\ddagger}$= 14.2±1.0 kcal/mol and $\Delta S^{\ddagger}$= 1.0±0.5 cal/(mol K).

*2. Variable Temperature ^{1}H NMR Behavior of Complexes **1-I** in Various Solvents*

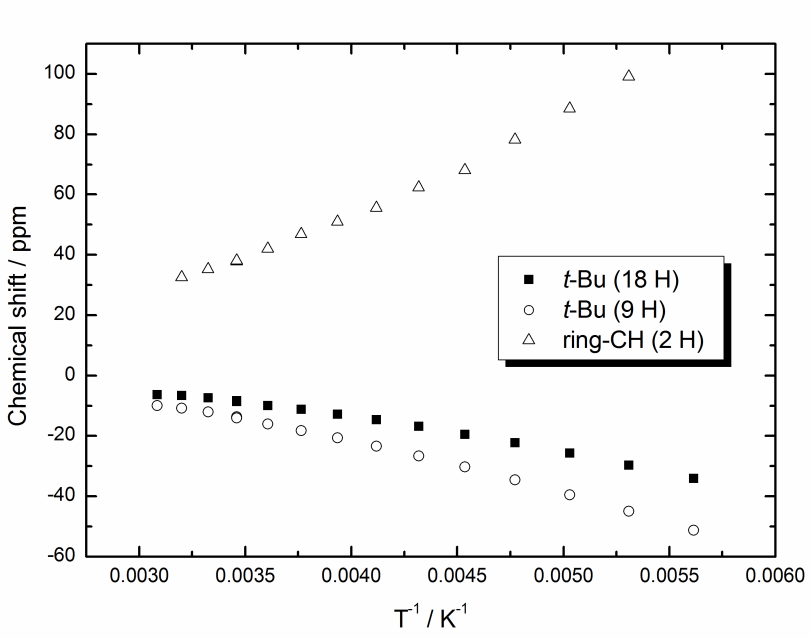

Figure S3. Chemical Shift (δ) vs. T^{-1} plot of ^{1}H NMR resonances of [Cp'FeI]$_2$ (**1-I**) in toluene-d_8 from 192 K to 312 K.

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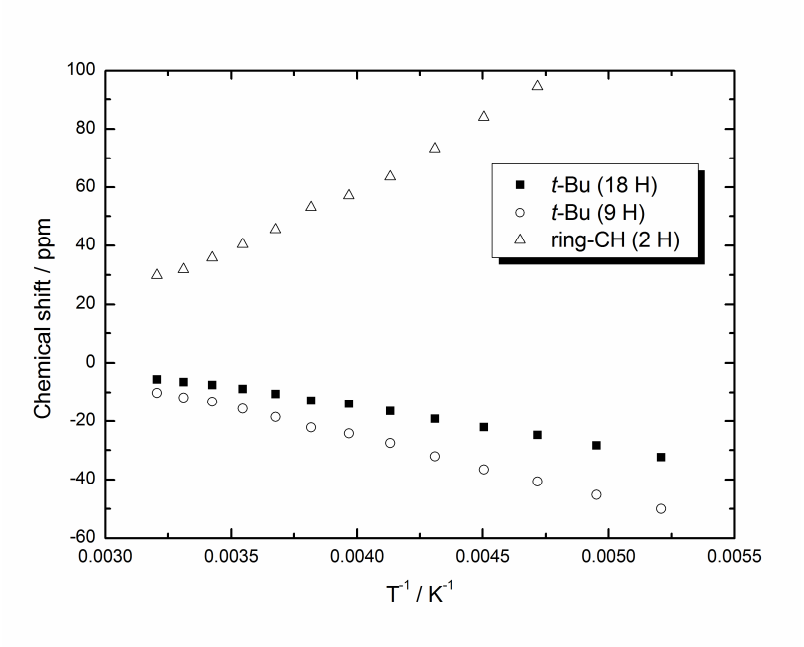

Figure S4. Chemical Shift (δ) vs. T^{-1} plot of ^{1}H NMR resonances of $[Cp'FeI]_2$ (**1-I**) in CD_2Cl_2 from 192 K to 312 K.

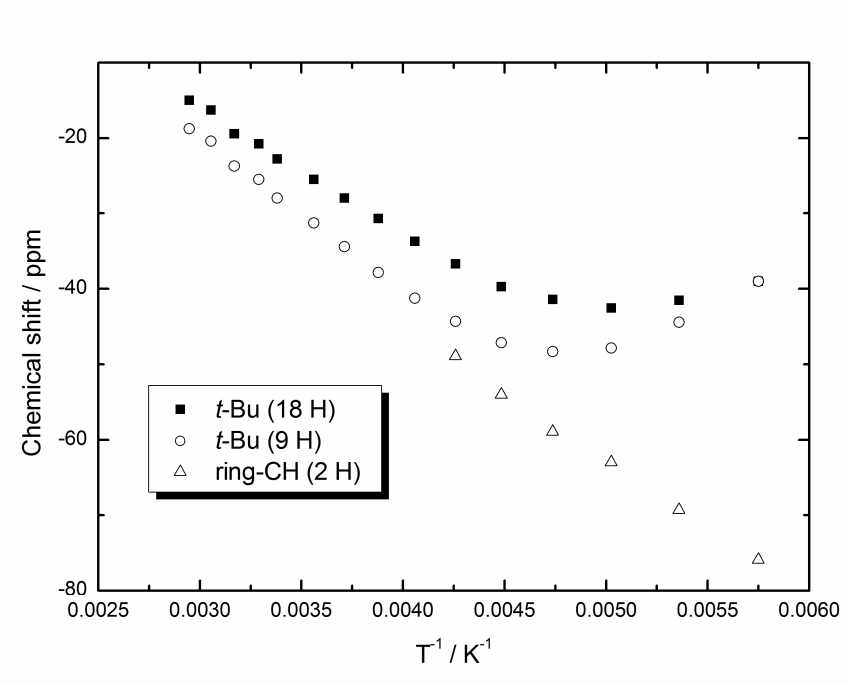

Figure S5. Chemical Shift (δ) vs. T^{-1} plot of ^{1}H NMR resonances of $[Cp'FeI]_2$ (**1-I**) in thf-d_8 from 186 K to 340 K.

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*3. Optical Spectra of **1-I**, **1-Br**, **1-Cl** and **2***

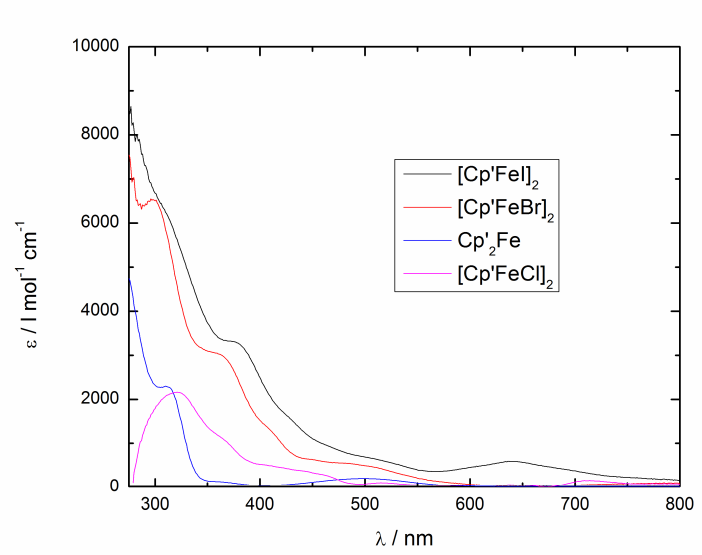

Figure S6. Optical Spectra of **1-I**, **1-Br**, **1-Cl** and **2**.

*4. ORTEP Diagram of **6***

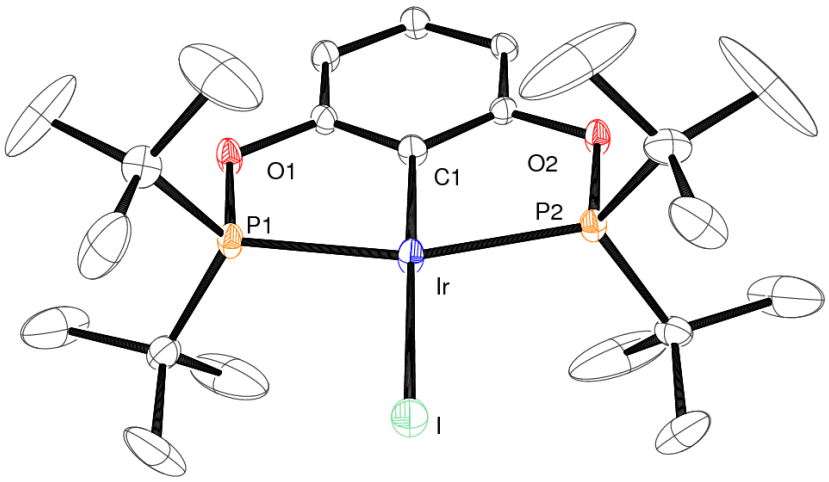

Figure S7. ORTEP diagram of **6** (50 % probability ellipsoids). Hydrogen atoms have been omitted for clarity. Selected bond distances (Å): Ir-I 2.7048(3), Ir-P1 2.3008(9), Ir1-P2 2.2997(9), Ir1-C1 2.007(3).

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5. Catalytic Transfer Dehydrogenation

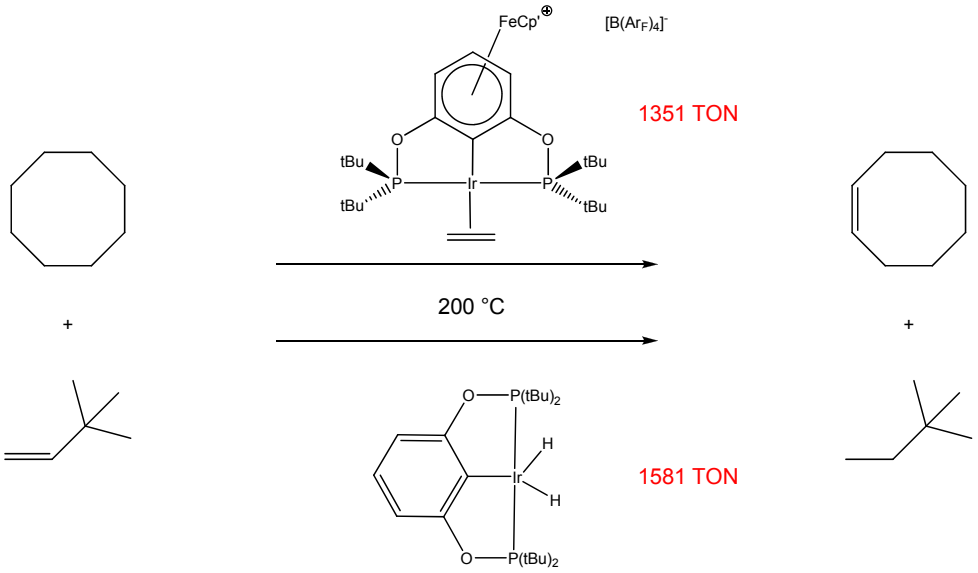

Table S1.

Time / min	(POCOP)Ir(H)(Cl)/NaOtBu TON	[**7**]$^+$ TON
8	922	101
31	1194	434
90	-	883
178	1514	-
918	1512	-
960	-	1299
1365	-	1301
2400	1581	1351
6170	1609	-
20305	1603	-

6. Cartesian Coordinates of Fully Optimized Structures

6.1 C_2H_4

C	-0.66734	0.02583	-0.01469
C	0.66734	-0.02583	0.01469
H	-1.20089	0.86244	-0.47559
H	1.28355	0.76630	-0.42090

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H	-1.28355	-0.76630	0.42090
H	1.20089	-0.86244	0.47559

6.2 (POCOP)Ir(H)(I)

I	3.53422	0.26722	-0.30019
P	0.14693	2.10968	-0.97654
P	0.62818	-1.98800	1.03847
O	-1.56196	2.03714	-0.98776
O	-1.05571	-2.27329	1.13209
C	-0.60919	3.06843	-3.59289
C	0.43047	0.79483	-3.36937
C	1.87497	2.84235	-3.10938
C	0.47236	2.25430	-2.85367
C	0.87966	-3.02989	-1.48869
C	-0.25147	4.94321	-0.75913
C	-3.50699	0.72988	-0.46316
C	-2.11367	0.86972	-0.46302
C	0.39630	3.74553	-0.03549
C	1.14582	-3.48348	-0.03229
C	-4.06267	-0.43875	0.07785
C	2.65092	-3.77071	0.14230
C	1.90376	3.98711	0.18645
C	0.30760	-4.74714	0.25032
C	-1.25208	-0.12384	0.04699
C	-3.25071	-1.45136	0.60951
C	-1.86196	-1.27352	0.59096
C	-0.29603	3.56023	1.33520
C	1.09165	-2.17440	2.87533
C	2.59092	-1.86241	3.06242
C	0.74810	-3.57221	3.42807
C	0.25415	-1.12003	3.63678
H	-0.42911	2.97755	-4.67868
H	0.60178	0.79558	-4.46042
H	2.10915	2.74371	-4.18401
H	-0.58136	4.13781	-3.34328
H	-1.61845	2.68854	-3.37946
H	-0.54618	0.31997	-3.18391
H	1.92513	3.91363	-2.86034
H	1.22271	0.18182	-2.90837
H	2.65670	2.30824	-2.54537
H	1.14732	-3.85298	-2.17462
H	0.26949	5.19419	-1.69483
H	1.49793	-2.15744	-1.75825
H	-0.18120	-2.78510	-1.65698
H	-1.31403	4.76022	-0.97981
H	-4.13451	1.52334	-0.87361
H	2.43481	4.22209	-0.74706
H	2.96006	-4.51024	-0.61719
H	0.56674	-5.51019	-0.50473
H	-0.18973	5.82901	-0.10272
H	3.26419	-2.86631	-0.00117
H	-5.14843	-0.56203	0.08647
H	-0.76996	-4.54298	0.17633
H	2.39563	3.11383	0.64085
H	2.02740	4.84793	0.86684
H	-3.67834	-2.36060	1.03652

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H	2.87719	-4.20152	1.12996
H	0.51140	-5.18017	1.23905
H	-1.37015	3.34762	1.22931
H	0.64125	0.76628	1.40479
H	-0.18440	4.49528	1.91098
H	0.16498	2.75017	1.92028
H	3.23971	-2.63408	2.62404
H	2.86742	-0.89703	2.61225
H	1.39037	-4.35682	3.00139
H	-0.30508	-3.83489	3.24680
H	0.50052	-0.09527	3.32005
H	-0.82650	-1.27713	3.50337
H	2.81017	-1.81652	4.14364
H	0.91392	-3.57178	4.51984
H	0.48473	-1.20317	4.71290
Ir	0.76640	0.09938	0.01886

6.3 (POCOP)Ir(C_2H_4)

C	2.55697	-0.03573	-2.72248
C	3.76834	2.10888	-2.28755
C	-1.53260	-2.77301	-1.97257
C	3.32634	0.77375	-1.65135
C	-2.31902	3.00536	-1.59546
C	-0.93242	3.18331	-1.49643
C	4.56656	-0.01346	-1.18049
C	-2.93099	1.81472	-1.18010
C	-3.70985	-3.16576	-0.80512
C	-0.16297	2.13744	-0.96820
C	-2.18857	-3.03101	-0.59416
C	-2.12108	0.79754	-0.65711
C	-0.71897	0.91548	-0.52880
C	-1.61688	-4.32103	0.02906
C	1.73462	-2.40146	0.06932
C	3.65131	3.14145	0.89477
C	2.82946	1.89960	1.28822
C	1.54268	-2.13434	1.44297
C	3.69424	0.93134	2.12038
C	-3.96484	-1.82711	2.21636
C	1.61747	2.34063	2.14164
C	-2.45315	-1.52723	2.21819
C	-2.22421	-0.09337	2.75248
C	-1.72303	-2.51869	3.14734
H	3.22369	-0.21528	-3.58500
H	4.34633	1.88408	-3.20203
H	1.67636	0.51893	-3.08170
H	-1.72625	-3.64066	-2.62838
H	2.90329	2.72326	-2.57286
H	-1.96017	-1.87964	-2.45326
H	2.20438	-1.00268	-2.33615
H	5.16945	-0.29522	-2.06188
H	-2.93513	3.81027	-2.00533
H	-0.45085	4.10774	-1.82062
H	-0.44613	-2.61964	-1.89227
H	-3.89016	-3.91974	-1.59229
H	4.41448	2.70419	-1.62849
H	-4.01047	1.67053	-1.25595

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H	-4.15277	-2.21593	-1.13720
H	-1.73265	-5.15230	-0.68844
H	4.30950	-0.94329	-0.64914
H	5.21140	0.59050	-0.52351
H	1.20529	-3.22920	-0.41326
H	2.69123	-2.16605	-0.40393
H	-4.23581	-3.50327	0.09789
H	3.09570	3.79469	0.20602
H	-0.54418	-4.23578	0.26556
H	4.61330	2.87244	0.43275
H	-2.15064	-4.60589	0.94918
H	-4.50452	-1.21999	1.47497
H	4.55085	0.52805	1.55999
H	3.87765	3.72228	1.80694
H	0.99673	3.08046	1.61498
H	-4.17701	-2.89017	2.02931
H	0.86674	-2.76256	2.02598
H	2.34064	-1.67471	2.02998
H	-2.78129	0.65435	2.16844
H	0.98118	1.47859	2.39828
H	3.09832	0.08962	2.50147
H	-1.78088	-3.56011	2.79578
H	-1.15614	0.17447	2.72335
H	4.09643	1.47530	2.99329
H	-4.37305	-1.58408	3.21386
H	1.98681	2.80098	3.07532
H	-0.66549	-2.24678	3.27385
H	-2.57437	-0.04406	3.79888
H	-2.19732	-2.48193	4.14421
O	1.20842	2.31740	-0.88746
O	-2.73603	-0.37679	-0.24951
P	2.06731	0.98767	-0.21633
P	-1.67315	-1.52162	0.46446
Ir	0.44405	-0.61395	0.20793

6.4 [Cp'Fe(POCOP)Ir(H)(I)]$^{+}$-endo

Ir	1.99429	-1.20137	1.03142
I	4.41655	-1.70010	2.23576
Fe	-1.54040	0.39804	-0.66565
P	2.72944	-1.28167	-1.18836
P	0.63000	-1.32125	2.92654
O	1.26675	-0.84261	-2.04624
O	-0.95430	-1.09625	2.22731
C	-3.11250	1.33428	-4.17996
C	-0.64695	1.56792	-4.24893
C	-2.12281	3.60335	-3.91590
C	-1.91934	2.10582	-3.55529
C	3.10462	-3.05427	-3.42332
C	3.63872	0.35657	-3.35561
C	1.07989	3.41997	-2.09467
C	5.40493	-0.66440	-1.84321
C	-1.94731	1.98586	-2.01042
C	2.96171	-3.05257	-1.88801
C	3.98783	-0.04941	-1.90753
C	-1.12182	-1.18172	-1.97523
C	1.68536	-3.83817	-1.50605

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C	4.17337	-3.74426	-1.22483
C	-3.13526	1.48025	-1.35624
C	0.11504	-0.96712	-1.30585
C	-2.29680	-1.41936	-1.20691
C	3.96766	1.19493	-0.99390
C	-0.47641	4.88533	-0.77732
C	-1.08126	2.48857	-0.93776
C	0.12385	3.45170	-0.88935
C	-3.06299	1.65487	0.06255
C	0.21443	-1.01075	0.11747
C	-2.24940	-1.34712	0.21416
C	-1.76777	2.20890	0.30371
C	0.96732	3.20260	0.38581
C	-5.31830	0.57889	0.57710
C	-4.83098	2.98018	1.11975
C	-1.00234	-1.11207	0.85520
C	-4.21713	1.54991	1.05543
C	0.69346	-4.02037	2.37859
C	-3.74050	1.15861	2.46988
C	0.42808	-3.10113	3.59448
C	0.37652	1.34661	3.55948
C	-0.98836	-3.38737	4.13374
C	0.60593	0.00369	4.28255
C	1.49130	-3.38110	4.67751
C	1.98997	0.03892	4.97040
C	-0.51408	-0.22135	5.31769
H	-3.05136	1.40935	-5.27641
H	-0.74471	1.71265	-5.33688
H	-2.23439	3.70892	-5.00720
H	3.70238	-0.48334	-4.06049
H	-4.08622	1.75248	-3.88168
H	-0.51369	0.49270	-4.06753
H	3.08833	-4.10124	-3.77184
H	2.27537	-2.52475	-3.91588
H	-3.09593	0.26263	-3.92286
H	4.05639	-2.61776	-3.75809
H	0.26807	2.07351	-3.93144
H	4.36582	1.11987	-3.68107
H	-1.27319	4.22686	-3.60601
H	-3.03234	4.00547	-3.44175
H	2.63191	0.79042	-3.43097
H	0.60928	3.79510	-3.01281
H	-1.15535	-1.19650	-3.06407
H	5.54725	-1.47871	-2.56729
H	6.12911	0.12835	-2.09566
H	1.46325	2.40717	-2.28306
H	1.80646	-4.88099	-1.84443
H	0.78126	-3.43663	-1.98667
H	1.94181	4.07408	-1.88819
H	-3.98076	1.03607	-1.87312
H	4.18487	-4.79783	-1.55261
H	-1.08474	5.14656	-1.65555
H	5.13402	-3.30042	-1.51512
H	-3.24979	-1.58857	-1.71007
H	4.66865	1.94138	-1.40449
H	5.65500	-1.02898	-0.83458
H	2.97428	1.66020	-0.94916

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H	0.34175	5.62006	-0.69853
H	-5.73456	0.88151	-0.39661
H	1.52513	-3.86404	-0.41688
H	4.11352	-3.73117	-0.12597
H	-5.19142	3.30749	0.13189
H	4.28820	0.94874	0.02933
H	-1.11094	4.98422	0.11710
H	1.85854	3.84872	0.36938
H	-4.95745	-0.45698	0.48769
H	1.30085	2.15511	0.44815
H	-3.14855	-1.47357	0.81566
H	-6.14994	0.57776	1.29897
H	2.08025	0.34267	1.06445
H	-4.09399	3.71617	1.47730
H	0.41585	3.44296	1.30638
H	-1.37556	2.45013	1.28780
H	-5.68592	2.98648	1.81522
H	-0.04110	-3.86803	1.57170
H	1.71393	-3.87907	1.98062
H	-3.25512	0.17164	2.48925
H	0.61404	-5.07294	2.70092
H	-3.02673	1.89473	2.87309
H	1.18029	1.56113	2.84041
H	-4.60073	1.13115	3.15754
H	-0.58852	1.35934	3.03201
H	-1.76421	-3.18257	3.38271
H	2.51054	-3.13757	4.33788
H	-1.04316	-4.45780	4.39599
H	2.80965	0.17377	4.24849
H	0.37183	2.15335	4.31157
H	1.46948	-4.45877	4.91329
H	-1.50402	-0.31296	4.84652
H	-1.22317	-2.81481	5.04053
H	2.19825	-0.86715	5.55536
H	1.28573	-2.84049	5.61323
H	2.00344	0.89374	5.66761
H	-0.33195	-1.10821	5.94122
H	-0.54361	0.65009	5.99395

6.5 [Cp'Fe(POCOP)Ir(H)(I)]$^{+}$-exo

I	-0.18492	5.13144	0.39242
Fe	0.06400	-1.70713	-0.23926
P	-0.33975	2.33536	-2.29365
P	-1.44694	1.94239	2.17363
O	-0.40698	0.61025	-2.56048
O	-1.40881	0.19136	2.13906
C	-1.47542	2.69256	-4.91627
C	1.71686	1.89261	-4.26286
C	1.62879	-2.11370	-3.79698
C	-1.77533	2.90520	-3.41861
C	1.47722	4.23978	-3.30754
C	0.36112	-4.24607	-3.29395
C	-2.05656	4.39607	-3.12788
C	-3.02056	2.06927	-3.04613
C	2.83770	-4.13151	-2.90349
C	1.37622	2.72787	-3.01128

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C	1.51006	-3.31883	-2.84186
C	2.35976	2.36144	-1.87857
C	-1.35620	-1.44074	-1.73896
C	-0.85230	-0.13477	-1.49668
C	1.37350	-2.88939	-1.38430
C	2.06321	-1.82077	-0.73171
C	-1.87544	-2.19772	-0.65134
C	0.75347	-3.63220	-0.32977
C	-0.90103	0.46383	-0.20325
C	-1.82648	-1.67463	0.67188
C	1.98281	-1.95298	0.70731
C	3.20425	0.25968	0.95878
C	1.10752	-3.10100	0.96872
C	-1.34451	-0.35360	0.87925
C	4.34435	-1.91619	1.44965
C	-4.10484	1.43802	1.42760
C	2.99016	-1.15261	1.55852
C	-0.28251	-5.02102	1.90285
C	-3.62979	3.72244	2.36529
C	0.73118	-3.89610	2.24504
C	-3.31314	2.21619	2.50363
C	2.01744	-4.60122	2.75725
C	2.65186	-0.98658	3.05059
C	1.07145	2.40432	3.20974
C	0.09179	-3.07337	3.38688
C	-0.38665	2.31387	3.70972
C	-3.74744	1.68807	3.88749
C	-0.77968	3.69128	4.29162
C	-0.49824	1.21053	4.78388
H	-2.38180	2.94802	-5.49138
H	-0.66881	3.34546	-5.27803
H	1.11505	2.16744	-5.13825
H	-1.22098	1.64669	-5.14478
H	1.77040	-2.46879	-4.83011
H	2.77434	2.07752	-4.51928
H	0.53388	-4.56959	-4.33234
H	0.86069	4.54061	-4.16765
H	3.00624	-4.48965	-3.93200
H	1.59500	0.81578	-4.07982
H	-2.92896	4.70919	-3.72642
H	-3.86735	2.42216	-3.65818
H	2.52580	4.47300	-3.55948
H	0.73285	-1.47582	-3.77445
H	-1.21543	5.04848	-3.40124
H	2.49904	-1.48621	-3.54633
H	-0.62013	-3.74870	-3.26226
H	-2.88012	0.99781	-3.25140
H	0.30359	-5.15628	-2.67648
H	3.69995	-3.51219	-2.61107
H	-1.34331	-1.84280	-2.75113
H	1.20136	4.85525	-2.43617
H	2.80323	-5.00798	-2.23747
H	3.39240	2.52730	-2.23010
H	-2.28558	4.57291	-2.06652
H	-3.30826	2.19071	-1.99039
H	2.26304	1.30312	-1.59229
H	2.62981	-1.04991	-1.24799

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H	2.20317	2.98674	-0.98480
H	-2.25450	-3.20601	-0.82319
H	0.11110	-4.49319	-0.48855
H	-2.19731	2.53611	-0.35687
H	3.70482	0.22404	-0.01988
H	4.67308	-2.00131	0.40220
H	-3.87374	1.77573	0.40606
H	2.25255	0.79941	0.83852
H	0.13778	-5.77114	1.21538
H	-3.31366	4.12264	1.39029
H	-1.21350	-4.62483	1.46589
H	-5.17952	1.61949	1.59641
H	-3.93732	0.35269	1.48553
H	-2.18982	-2.25929	1.51653
H	3.85274	0.84905	1.62506
H	4.27841	-2.93111	1.86836
H	2.47904	-5.20950	1.96302
H	5.12046	-1.36692	2.00766
H	-4.72132	3.85639	2.45292
H	1.20983	3.24288	2.51065
H	-0.55445	-5.54963	2.82932
H	1.39737	1.47725	2.72052
H	-3.15868	4.33207	3.14799
H	2.77012	-3.88789	3.11964
H	-0.85394	-2.61320	3.06948
H	1.65797	-0.54176	3.19734
H	1.76308	-5.27234	3.59356
H	-0.75175	4.48535	3.52925
H	3.39268	-0.31690	3.51547
H	2.69581	-1.93769	3.59719
H	-4.84324	1.78828	3.96778
H	0.73852	-2.27787	3.76446
H	-3.50123	0.62325	4.01792
H	1.73237	2.57194	4.07739
H	-0.13156	-3.74612	4.23038
H	-0.24738	0.21872	4.38163
H	-3.30995	2.25849	4.71814
H	-1.76818	3.68734	4.77194
H	-0.04045	3.95447	5.06702
H	-1.49654	1.15364	5.23745
H	0.21878	1.44382	5.58942
Ir	-0.70124	2.45832	0.01406

6.6 [Cp'Fe(POCOP)Ir(C_2H_4)]$^+$

C	-2.37697	0.67255	-5.21471
C	3.34482	0.77679	-4.74886
C	-2.01102	2.89243	-4.14993
C	-0.54789	-2.54782	-4.18060
C	-2.11758	1.37267	-3.85272
C	3.22603	2.84708	-3.33531
C	3.03337	1.31529	-3.32133
C	0.41428	1.65530	-3.39462
C	-0.77455	0.83595	-3.29595
C	-3.34446	1.20124	-2.92714
C	1.58710	0.91376	-3.04533
C	-0.93384	-1.89608	-2.81908

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C	-0.31858	-0.48140	-2.83663
C	-2.46302	-1.98040	-2.67412
C	1.11051	-0.37284	-2.64374
C	4.01691	0.66452	-2.32748
C	-0.29826	-2.74664	-1.68899
C	0.25458	2.93219	-0.63501
C	-1.02134	2.35562	-0.38872
C	1.42428	2.23709	-0.22294
C	2.62820	-2.90683	0.50572
C	-4.78265	-0.87348	0.64351
C	-1.10854	1.14013	0.34389
C	1.29381	1.00823	0.47879
C	4.67777	-1.53422	0.92852
C	-3.12422	-2.74698	0.88807
C	0.03323	0.45740	0.87085
C	3.40106	-2.11205	1.57939
C	-3.77687	-1.54552	1.60545
C	3.79642	-3.05214	2.73849
C	-4.52337	-2.06413	2.85548
C	-4.36207	1.51593	3.03421
C	4.41449	0.53798	3.51057
C	-1.95221	2.11970	3.32639
C	-2.96447	0.95343	3.36772
C	0.35911	-2.80881	3.51424
C	2.90747	0.24673	3.64734
C	2.14228	1.58837	3.66299
C	-0.96087	-2.42261	3.80193
C	-2.94684	0.34892	4.78836
C	2.62403	-0.49466	4.97132
H	-1.52904	0.82294	-5.90178
H	-3.27648	1.09991	-5.68704
H	2.66930	1.21730	-5.49883
H	4.37993	1.03380	-5.02687
H	-2.53751	-0.40892	-5.10582
H	-0.97882	-1.99948	-5.03208
H	-1.26829	3.11738	-4.93094
H	3.24003	-0.31851	-4.79419
H	-2.98412	3.25378	-4.51608
H	0.54452	-2.57960	-4.31498
H	-0.92669	-3.58267	-4.21471
H	2.59077	3.33105	-4.09391
H	4.27134	3.08709	-3.58575
H	0.41915	2.69731	-3.70015
H	-2.98832	-1.56640	-3.54472
H	-4.22354	1.65864	-3.40952
H	-1.76101	3.47540	-3.24881
H	5.04943	0.95672	-2.57700
H	-3.59114	0.15649	-2.72294
H	-2.75807	-3.03899	-2.59605
H	3.00552	3.30741	-2.36034
H	3.96889	-0.43505	-2.37673
H	1.74459	-1.18141	-2.28839
H	-3.19415	1.70406	-1.96160
H	0.76057	-2.96805	-1.88945
H	-2.81803	-1.46474	-1.77185
H	-0.81571	-3.71704	-1.62735
H	3.81574	0.96514	-1.28841

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H	0.33762	3.86830	-1.18895
H	-1.93361	2.84936	-0.72243
H	-0.36265	-2.25146	-0.70519
H	2.41842	2.62486	-0.44142
H	-4.29350	-0.49415	-0.26339
H	2.37487	-2.26595	-0.35152
H	3.26465	-3.73055	0.13937
H	4.44258	-0.81517	0.13286
H	-5.52659	-1.63081	0.34270
H	-2.49955	-2.43258	0.04374
H	5.23377	-2.37221	0.47389
H	-3.92135	-3.40261	0.49743
H	-5.32534	-0.04175	1.11018
H	1.69241	-3.33393	0.89332
H	5.34723	-1.05198	1.65113
H	-2.49439	-3.34639	1.56027
H	-4.41022	1.90877	2.00770
H	4.42081	-3.86397	2.32803
H	-5.24060	-2.83596	2.52778
H	4.66007	0.99891	2.54246
H	-1.99700	2.67608	2.37882
H	2.38118	2.21051	2.78795
H	0.53759	-3.65583	2.84488
H	-5.16846	0.78207	3.17316
H	2.92924	-3.52364	3.22089
H	-5.10065	-1.28157	3.36677
H	4.39559	-2.54364	3.50866
H	-1.78233	-3.01401	3.39561
H	5.03569	-0.35860	3.64940
H	-3.85374	-2.53798	3.58850
H	-4.56866	2.35583	3.71968
H	-0.92278	1.76333	3.47692
H	1.05501	1.42182	3.69237
H	4.70072	1.25371	4.30040
H	-2.19735	2.82417	4.13909
H	1.13745	-2.62622	4.25656
H	2.43417	2.15039	4.56633
H	-1.18267	-1.89706	4.73312
H	-3.59661	-0.53068	4.89931
H	3.10380	-1.48361	5.02274
H	-1.92554	0.07671	5.09368
H	1.54284	-0.61330	5.13801
H	-3.30895	1.11490	5.49522
H	3.02682	0.10745	5.80342
O	-2.35835	0.67332	0.67157
O	2.44208	0.38441	0.90034
P	-2.35842	-0.34083	2.08032
P	2.18812	-0.75654	2.17792
Fe	0.23127	1.05667	-1.44606
Ir	-0.12482	-1.01977	2.25586

6.7 [Cp'Fe(POCOP)Ir]$^+$

C	4.283371	-2.232391	-0.581493
C	1.530252	0.208820	-2.755024
C	3.967669	0.314643	-0.938064
C	1.140479	-1.057747	-2.236159

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C	3.670733	-0.871290	-0.162240
C	3.886837	2.937797	-0.603046
C	1.022767	1.402192	-2.169208
C	3.503699	1.496729	-0.277735
C	0.175745	-1.122894	-1.195279
C	2.966304	-0.401653	1.037274
C	0.085083	1.315286	-1.107030
C	2.838189	1.031237	0.898920
C	-2.917455	-2.876233	-1.611790
C	-0.457695	0.057257	-0.680232
C	-2.862860	2.404761	-2.352979
C	2.642247	-1.020065	2.413603
C	-1.801703	-3.636521	1.241534
C	-3.136582	4.562946	-1.096463
C	-3.182269	3.028847	-0.976308
C	-4.586758	2.559892	-0.528710
C	-1.646179	3.375404	1.770448
H	2.268560	0.265647	-3.556124
H	4.481267	0.310792	-1.894942
H	1.553212	-1.979528	-2.645633
H	1.354276	2.382307	-2.510141
H	-1.900969	2.759817	-2.751909
H	-3.653474	2.695790	-3.065170
H	-2.837708	1.305272	-2.296939
H	2.343292	1.675664	1.621190
H	-2.133880	4.927414	-1.366014
H	-3.826528	4.871397	-1.900907
H	-3.465126	5.070438	-0.177846
H	-5.330123	2.899589	-1.270174
H	-4.638928	1.459034	-0.479476
H	-4.884009	2.969239	0.448281
O	-0.283459	-2.353466	-0.784813
O	-0.426328	2.479187	-0.577970
P	-1.892135	-2.288266	-0.105782
P	-1.936052	2.267386	0.257089
Fe	1.933161	0.184653	-0.751103
Ir	-2.060662	-0.037697	0.388945
C	-2.566211	-1.931565	-2.782978
H	-2.734194	-0.878292	-2.511512
H	-1.524684	-2.050081	-3.116212
H	-3.219998	-2.176287	-3.637227
C	-4.415384	-2.690010	-1.276093
H	-4.628723	-1.652761	-0.968116
H	-5.008921	-2.895106	-2.183494
H	-4.772286	-3.368929	-0.489936
C	-2.611112	-4.325320	-2.036827
H	-2.936670	-5.069689	-1.296230
H	-3.152503	-4.541512	-2.973973
H	-1.537934	-4.470014	-2.234551
C	-0.806172	-4.758832	0.883744
H	0.202735	-4.365118	0.697375
H	-0.748257	-5.458132	1.735374
H	-1.116493	-5.334033	0.001076
C	-3.207505	-4.223551	1.500334
H	-3.579305	-4.833794	0.665938
H	-3.146209	-4.879391	2.385272
H	-3.952301	-3.443632	1.728088

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C	-1.346952	-2.920899	2.532214
H	-0.374526	-2.428879	2.412217
H	-2.073839	-2.156061	2.849132
H	-1.256818	-3.665419	3.342150
C	-3.001521	3.591099	2.479797
H	-2.821267	4.103217	3.439913
H	-3.688478	4.220931	1.895568
H	-3.507309	2.638229	2.709642
C	-0.716925	2.563320	2.696490
H	-1.142754	1.577859	2.942113
H	0.264171	2.401176	2.226519
H	-0.559904	3.124845	3.633338
C	-0.972467	4.723586	1.441934
H	-1.628221	5.407276	0.888874
H	-0.705503	5.218964	2.391406
H	-0.046726	4.583418	0.865264
C	2.796526	3.942109	-0.174194
H	3.127155	4.968766	-0.398353
H	1.841028	3.767876	-0.690932
H	2.607440	3.891201	0.910047
C	5.171980	3.218420	0.230843
H	5.519408	4.247753	0.045375
H	4.979547	3.110808	1.309776
H	5.985139	2.527847	-0.042778
C	4.234007	3.132136	-2.094718
H	3.376350	2.937255	-2.756437
H	4.555136	4.171187	-2.268347
H	5.063595	2.479038	-2.408770
C	4.883652	-2.135004	-2.009736
H	4.126060	-1.864572	-2.763129
H	5.710999	-1.411023	-2.068492
H	5.293239	-3.116555	-2.292915
C	5.468424	-2.532085	0.377069
H	5.138326	-2.686346	1.413843
H	5.987274	-3.447846	0.050128
H	6.199376	-1.707861	0.371510
C	3.309583	-3.434431	-0.601290
H	2.939368	-3.707729	0.389989
H	2.436950	-3.242205	-1.240328
H	3.836668	-4.313102	-1.006740
C	2.410701	-2.540828	2.447096
H	1.623847	-2.851742	1.745871
H	3.325024	-3.105331	2.222291
H	2.095731	-2.833385	3.461418
C	3.862422	-0.697517	3.327019
H	4.031312	0.388147	3.400165
H	3.674537	-1.083120	4.342620
H	4.787827	-1.160765	2.953022
C	1.396748	-0.336035	3.031002
H	0.528604	-0.369706	2.352634
H	1.127237	-0.846238	3.969140
H	1.589789	0.715450	3.289402

6.8 [(POCOP)Ir]

C	1.89513	-0.47325	-4.16911
C	1.36604	2.80375	-2.86515

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C	3.92796	-1.01571	-2.74327
C	2.39390	-0.85912	-2.76192
C	3.79000	2.30826	-2.30033
C	1.75692	-2.20660	-2.34679
C	2.32965	2.18113	-1.83052
C	-4.32012	-1.38789	-0.77970
C	2.16047	2.92305	-0.48438
C	-3.69967	2.05824	-0.10275
C	-2.35518	-2.81167	-0.10437
C	-3.32797	-1.70119	0.35829
C	1.97667	-0.35657	0.99076
C	0.56166	-0.32928	0.94113
C	-3.20306	1.36694	1.18643
C	-4.06937	-2.19278	1.61809
C	-2.16817	2.28611	1.87612
C	-4.37383	1.10703	2.15123
C	2.67721	-0.70593	2.14975
C	-0.12166	-0.66537	2.13500
C	1.95544	-1.03751	3.30592
C	0.55299	-1.01859	3.30823
H	2.12631	-1.29107	-4.87401
H	2.38158	0.43827	-4.55060
H	0.80277	-0.32106	-4.18642
H	1.43250	2.32264	-3.85307
H	4.20288	-1.88080	-3.37275
H	3.94176	1.91082	-3.31567
H	4.45278	-0.13772	-3.14307
H	2.07624	-2.98865	-3.05904
H	1.61461	3.87175	-2.99679
H	4.06649	3.37760	-2.32440
H	0.32204	2.73891	-2.51517
H	0.65717	-2.14778	-2.34580
H	4.29536	-1.20881	-1.72464
H	4.48405	1.79969	-1.61407
H	-3.80447	-0.99932	-1.67401
H	-4.83987	-2.31626	-1.07501
H	2.07771	-2.51071	-1.33829
H	-1.79971	-2.50926	-1.00600
H	-2.85679	2.27095	-0.78164
H	-4.44353	1.45792	-0.64890
H	2.37009	3.99623	-0.63952
H	-5.09006	-0.66130	-0.47597
H	-2.93430	-3.72599	-0.32658
H	-4.17514	3.01973	0.16032
H	1.13278	2.81732	-0.10059
H	2.85456	2.54080	0.27860
H	-1.61889	-3.05473	0.67751
H	-4.53860	-3.16753	1.39448
H	-1.29668	2.45979	1.22422
H	-5.20310	0.56521	1.67086
H	-4.86691	-1.50959	1.93931
H	-2.64412	3.25834	2.09468
H	3.76921	-0.71283	2.13570
H	-4.77515	2.07665	2.49667
H	-3.37366	-2.33743	2.45763
H	-1.81043	1.85436	2.82253
H	-4.05140	0.54386	3.04018

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H	2.49256	-1.31221	4.21677
H	-0.02091	-1.27061	4.20250
O	2.70345	-0.02575	-0.15454
O	-1.51775	-0.64688	2.14738
P	1.73181	0.40147	-1.49226
P	-2.21750	-0.17979	0.66146
Ir	-0.40502	0.17791	-0.69470