

Supporting Information for

Iron piano-stool complexes containing NHC ligands outfitted with pendent arms: synthesis, characterization, and screening for catalytic transfer hydrogenation

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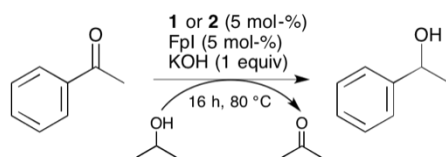
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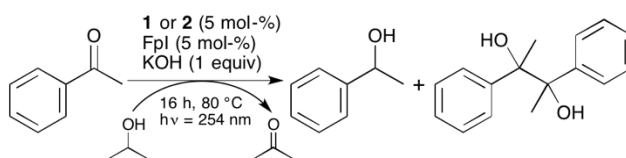
Table S1: Catalytic transfer hydrogenation of acetophenone catalysed by FpI and **1** and **2**



Imidazolium salt	%Conversion	%Selectivity	%Yield
None ^a	56	79	44
1	56	70	39
2	>99	>99	>99

^aNeither Fe nor imidazolium salt was present in this blank reaction.

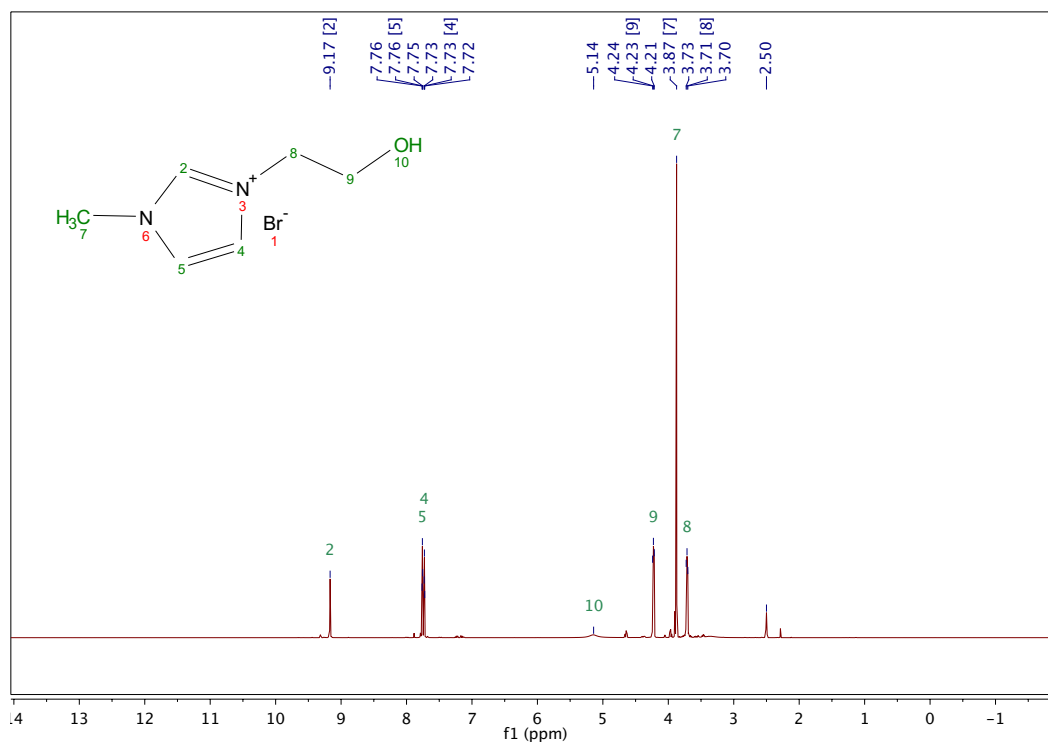
Table S2: UV-assisted CTH of acetophenone catalysed by FpI and **1** and **2**



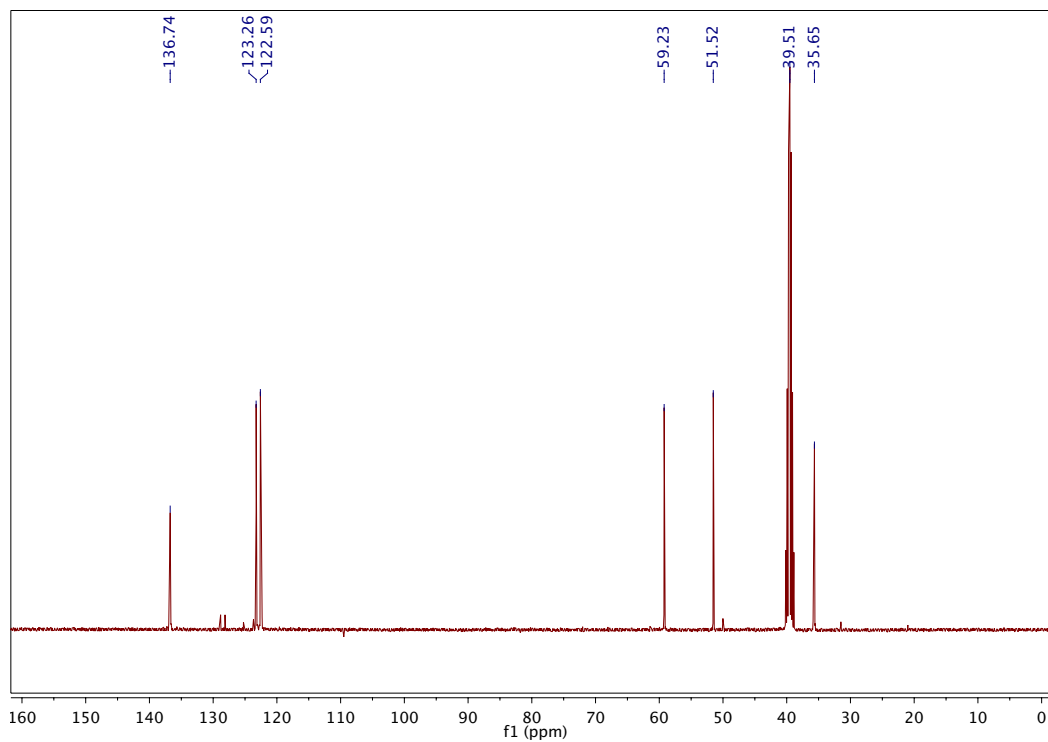
Imidazolium salt	%Conversion	%Selectivity ^a	%Yield ^a
1	100	40	40
2	77	29	22

^aReported for 1-phenylethanol.

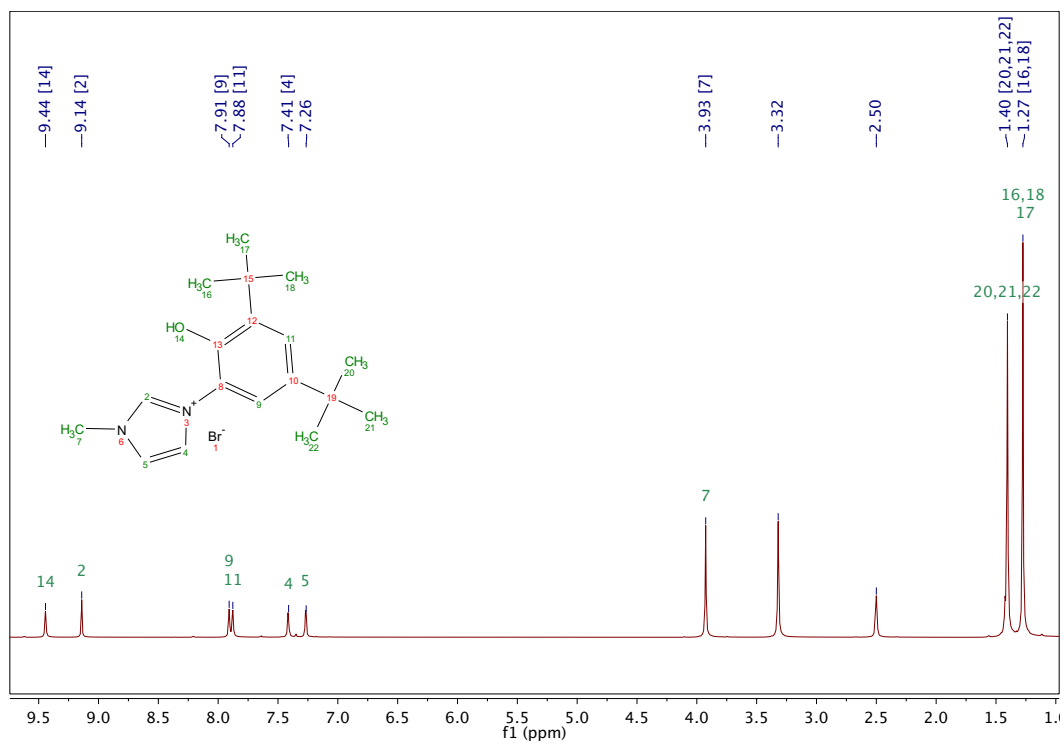
^1H NMR spectrum of **1**.



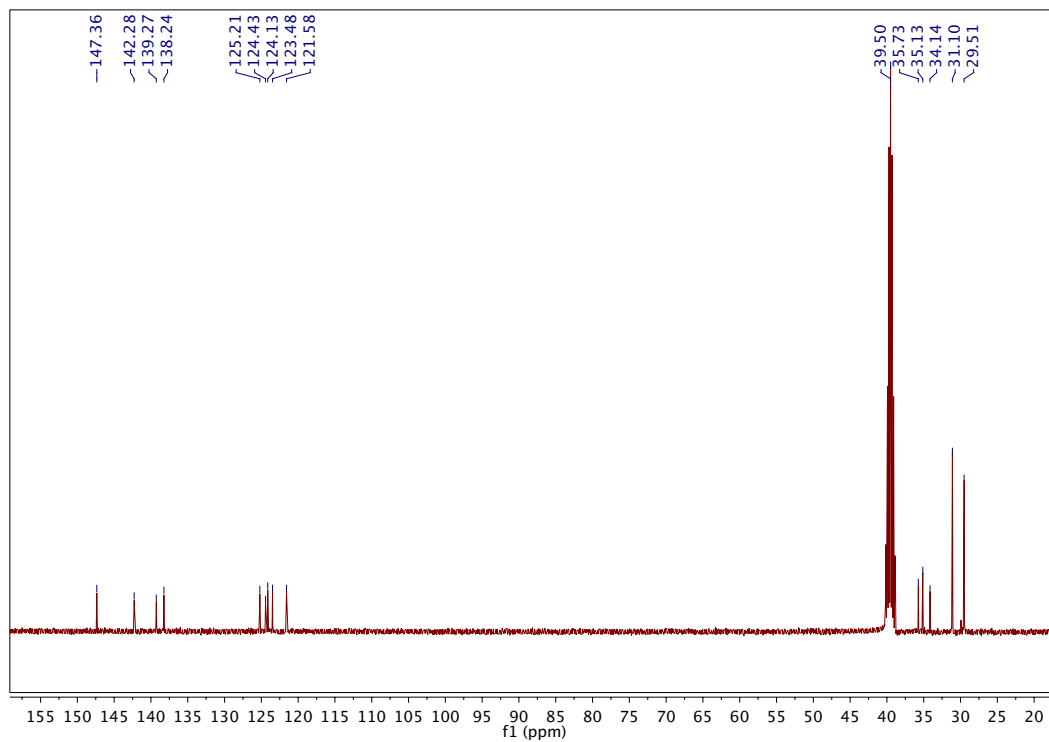
^{13}C NMR spectrum of **1**.



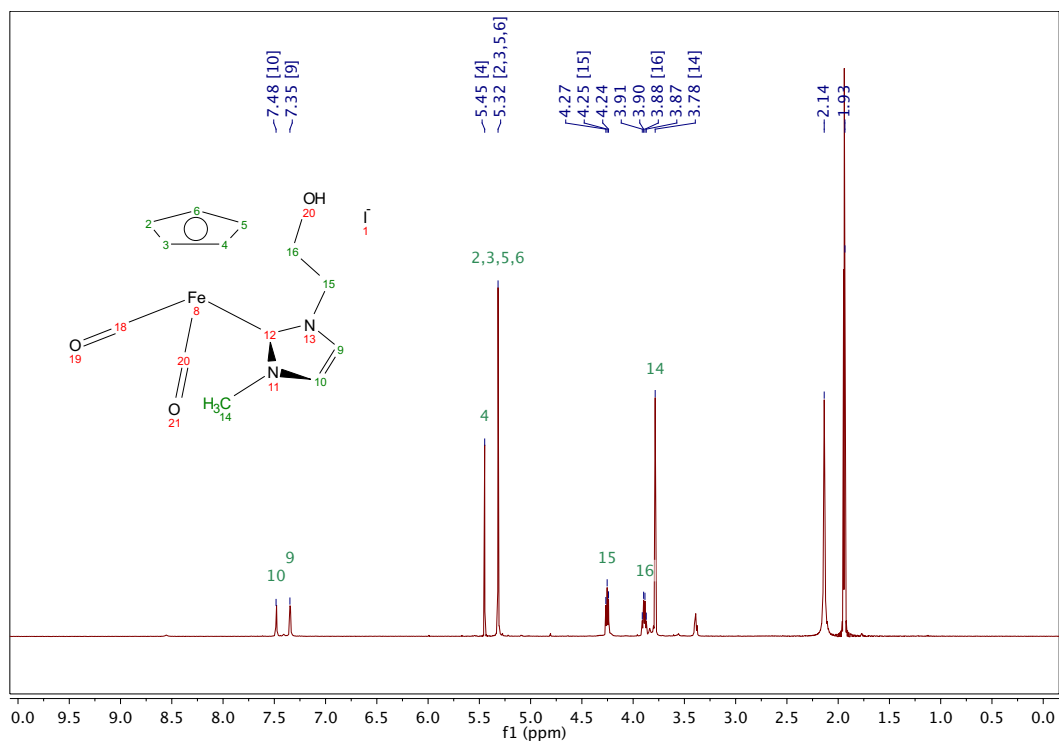
^1H NMR spectrum of **2**.



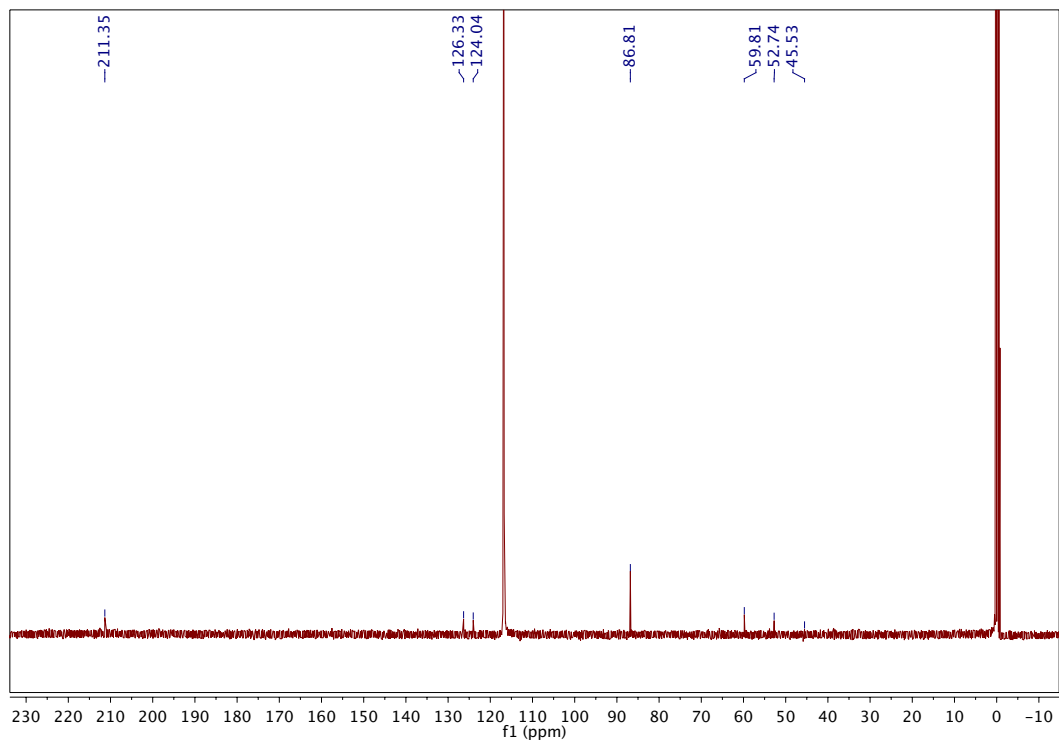
^{13}C NMR spectrum of **2**.



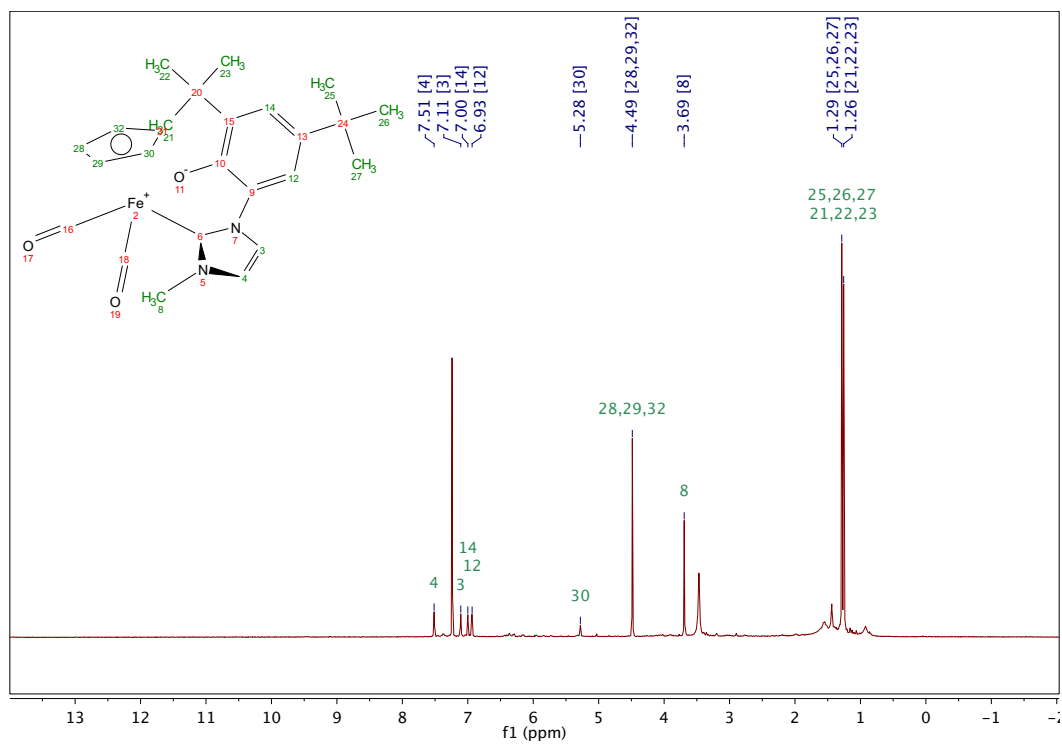
^1H NMR spectrum of a single crystal of **3**.



^{13}C NMR spectrum of a single crystal of **3**.



^1H NMR spectrum of a single crystal of **4**.



^{13}C NMR spectrum of a single crystal of **4**.

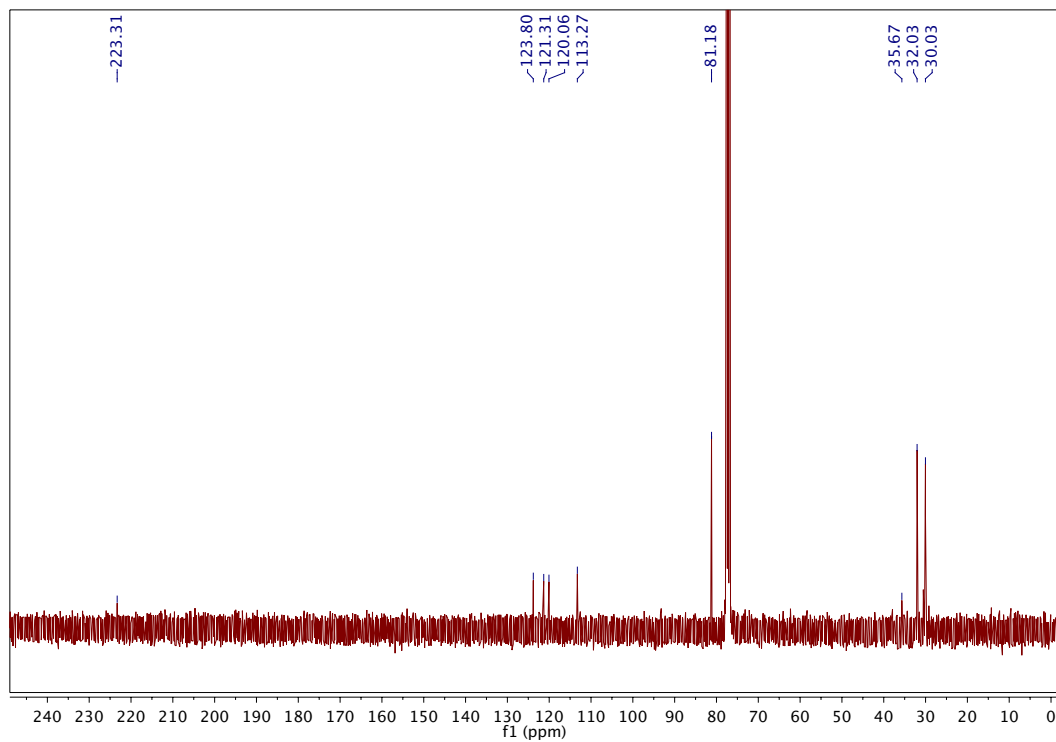


Table S1 Optimized coordinates of **3**.

Symbol	X	Y	Z
N	0.8976100	2.0603918	-0.4364358
N	1.9154311	0.4237445	0.4910252
C	0.6874224	0.8246259	0.0783092
C	2.8677173	1.3964607	0.2477761
C	2.2835988	-0.8934528	1.0090034
H	2.7875862	-0.7678828	1.9695713
C	2.2255152	2.4285658	-0.3354137
C	-0.1078310	2.9301126	-1.0390835
Fe	-1.0602685	-0.1962449	0.1490153
H	3.9041755	1.2711764	0.5113228
C	3.1757514	-1.6492714	0.0399598
H	1.3716031	-1.4646774	1.1594797
H	2.5868576	3.3812034	-0.6836483
H	-0.8561400	2.3221271	-1.5417865
H	0.3807208	3.5632452	-1.7774011
H	-0.5788204	3.5607353	-0.2844555
C	-0.7969452	-0.6525719	1.9606694
C	-2.0377108	-2.0885261	-0.3095449
C	-0.6816729	-2.1139303	-0.7636022
C	-0.5411716	-1.1085253	-1.7507237
C	-1.7750917	-0.4274800	-1.8761223
C	-2.0808292	1.3216551	0.6158967
C	-2.7079958	-1.0528897	-0.9869484
O	2.4248949	-1.8629166	-1.1391249
H	4.0862258	-1.0771324	-0.1692267
H	3.4650018	-2.5948180	0.5106301
O	-0.6408109	-0.9403887	3.0346834
H	-2.4726601	-2.7397692	0.4343794
H	0.0904216	-2.8060158	-0.4672730
H	0.3812537	-0.8700833	-2.2573802
H	-1.9978468	0.3720989	-2.5661144
O	-2.7294830	2.1992749	0.8803996
H	-3.7438333	-0.7767137	-0.8551113
H	2.9698168	-2.3164877	-1.7882397

Table S2 Optimized coordinates of **3z**.

Symbol	X	Y	Z
N	1.1579631	1.8839324	-0.4271318
N	1.9593825	0.1767330	0.5968463
C	0.8061830	0.6867392	0.1157469
C	3.0161844	1.0235161	0.3373235
C	2.2177332	-1.2165526	0.9717509
H	2.8945445	-1.2166817	1.8321879
C	2.5161526	2.1027562	-0.2986301
C	0.2766322	2.8271972	-1.0938528
Fe	-1.0488933	-0.0996891	0.1667951
H	4.0262255	0.7609468	0.5997811
C	2.7852594	-1.9680647	-0.2787372
H	1.2715584	-1.6750148	1.2491816
H	2.9928530	2.9899435	-0.6781174
H	-0.5349469	2.2855218	-1.5735377
H	0.8454321	3.3505561	-1.8612746
H	-0.1291267	3.5573808	-0.3909620
C	-0.8024259	-0.6348148	1.9351541
C	-2.2355273	-1.8516261	-0.3176122
C	-0.9003967	-2.0208750	-0.7986126
C	-0.6523411	-1.0150011	-1.7628233
C	-1.8025021	-0.1925464	-1.8490294
C	-1.8103704	1.5105010	0.6713471
C	-2.7920000	-0.7228244	-0.9544939
O	1.9689077	-1.8571052	-1.3210492
H	3.8148663	-1.5479477	-0.4282161
H	2.9592179	-3.0070450	0.0993207
O	-0.6819597	-0.9621951	3.0057829
H	-2.7308552	-2.4589454	0.4260872
H	-0.1623701	-2.7630419	-0.5357517
H	0.3233072	-0.9050587	-2.2209749
H	-1.9443898	0.6486290	-2.5107973
O	-2.3030175	2.4822519	0.9646573
H	-3.7834390	-0.3260362	-0.7919143

Table S3 Optimized coordinates of **4**.

Symbol	X	Y	Z
O	0.4488704	-0.5312738	-2.2044593
C	-0.4572541	-0.3741992	-1.5567289
Fe	-2.1919178	0.0419876	-0.8267167
C	-2.9382937	-1.5634066	-1.3788496
C	-3.8003922	1.4092488	-0.3364049
C	-3.7443122	1.2799231	-1.7516259
C	-2.4718060	1.7118789	-2.1864302
C	-1.8341225	-0.7531023	0.9771856
C	-2.5622635	1.9683356	0.0988847
C	-1.7443767	2.1478606	-1.0311484
O	-3.4116867	-2.5423151	-1.6782073
H	-4.6541965	1.1849422	0.2830723
H	-4.5244607	0.8785507	-2.3824533
H	-2.1209514	1.7277838	-3.2070623
N	-2.7167029	-1.1833149	1.9142971
N	-0.6271867	-0.8738976	1.5656355
H	-2.2280405	2.1423635	1.1108166
H	-0.7276679	2.5074334	-1.0004741
C	-4.1634163	-1.2230916	1.7882397
C	-2.0638564	-1.5396095	3.0818876
C	-0.7470057	-1.3360149	2.8590690
C	0.6245085	-0.4859678	0.9780270
H	-4.5382140	-2.1375464	2.2478576
H	-4.4379302	-1.2133278	0.7371905
H	-4.6127963	-0.3593992	2.2820658
H	-2.5936967	-1.8971676	3.9480840
H	0.1162661	-1.4667666	3.4878845
C	1.4909373	-1.4826060	0.5499591
C	0.9092345	0.9224036	0.9572615
H	1.1693436	-2.5174137	0.6417100
C	2.7086821	-1.1540583	-0.0245575
C	2.2043508	1.2409492	0.3849722
O	0.0825427	1.7663900	1.4026891
C	3.6349947	-2.2525419	-0.5526817
C	3.0180931	0.2200091	-0.0837883
C	2.6686954	2.7010360	0.3838281
C	2.9287918	-3.0266721	-1.6793054
C	3.9873839	-3.2289607	0.5824135
C	4.9428838	-1.6851956	-1.1141081
H	3.9708471	0.4974462	-0.5130643
C	2.7626127	3.1948108	1.8397122
C	1.6727055	3.5896135	-0.3821046
C	4.0452600	2.8782861	-0.2670694

H	2.0007684	-3.4824472	-1.3244714
H	2.6807590	-2.3559310	-2.5056283
H	3.5728788	-3.8254446	-2.0607443
H	4.4943040	-2.7028284	1.3950869
H	4.6478786	-4.0211343	0.2159763
H	3.0926267	-3.7018097	0.9941124
H	5.5710352	-2.5039260	-1.4750445
H	4.7593376	-1.0088912	-1.9529641
H	5.5046282	-1.1423254	-0.3495480
H	1.7983438	3.0940777	2.3379792
H	3.5089071	2.6134853	2.3884463
H	3.0658228	4.2468115	1.8599051
H	1.5475662	3.2273663	-1.4083888
H	0.7089885	3.5963706	0.1254589
H	2.0503179	4.6157904	-0.4317303
H	4.3218081	3.9353589	-0.2351330
H	4.0421231	2.5643935	-1.3151298
H	4.8204756	2.3170243	0.2612887