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Supporting Information for

Reactions of Aromatic N-Heterocycles with a Lutetium Benzyl Complex Supported by a Ferrocene-Diamide Ligand

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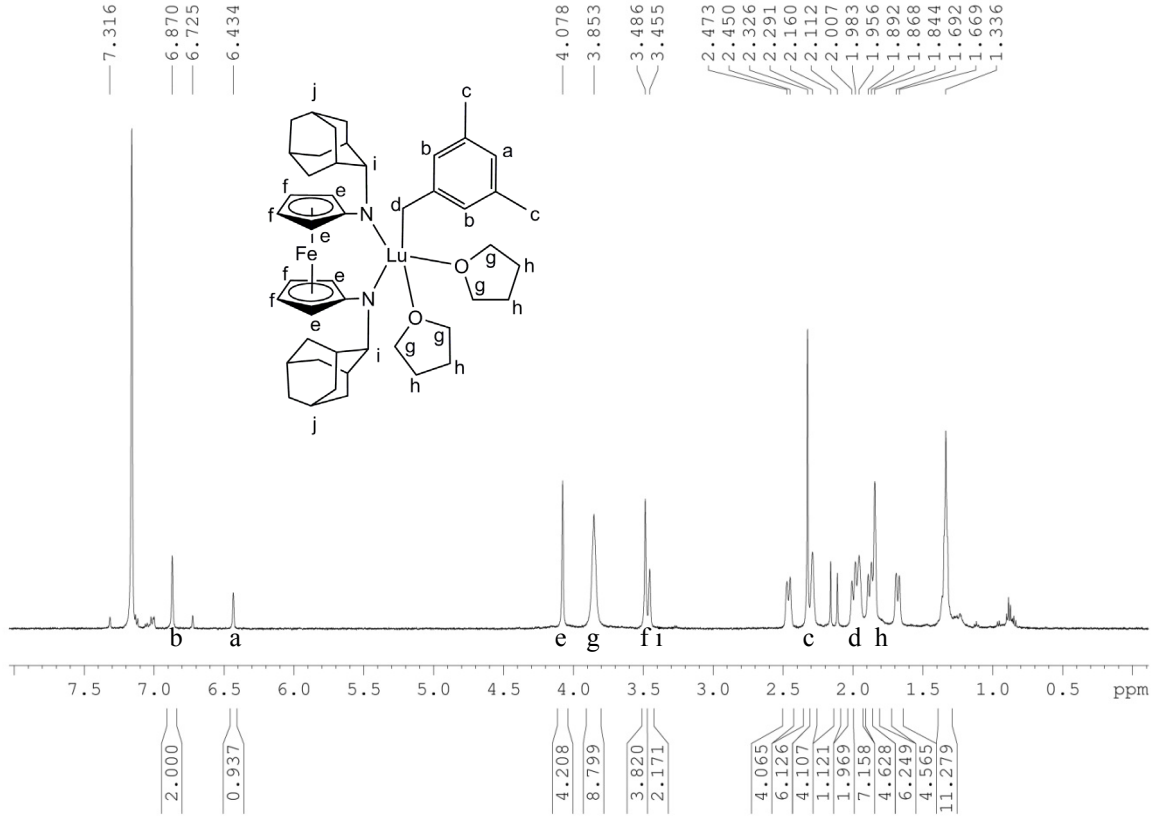
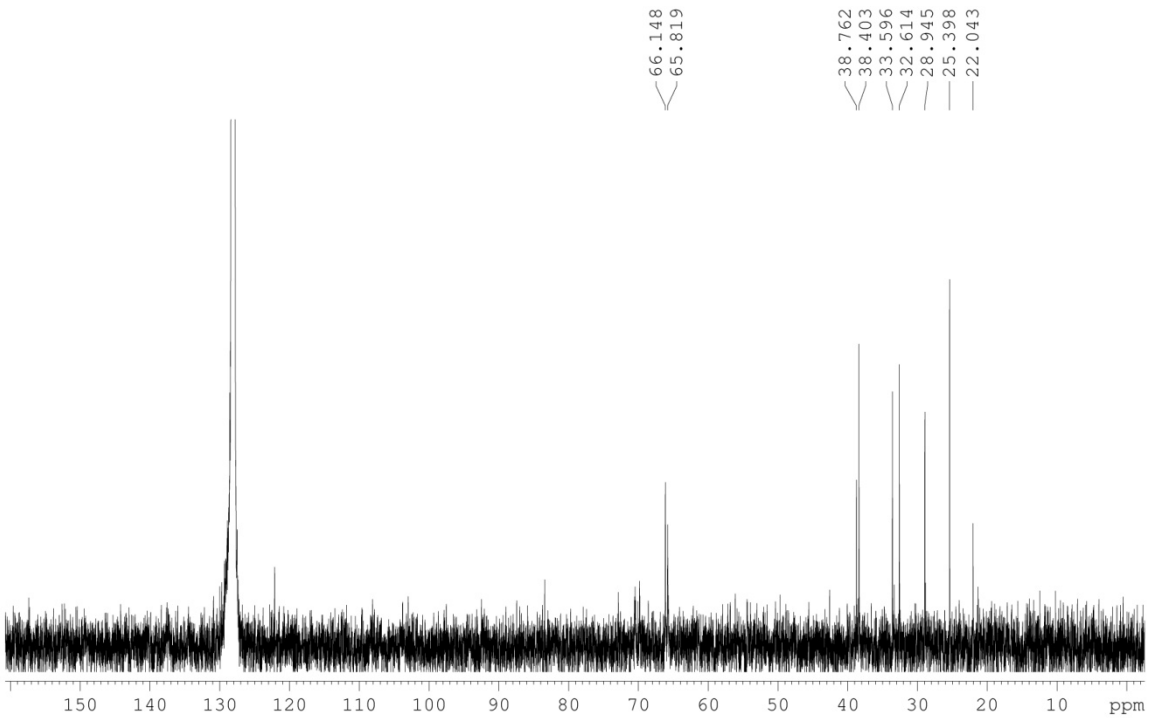
NMR spectra

1^{Ad}-THF: 1^{Ad}-DME is not soluble in C_6D_6.

^{1}H NMR (500 MHz, C_6D_6): Peaks for free mesitylene are also present at 2.16 and 6.72 ppm.

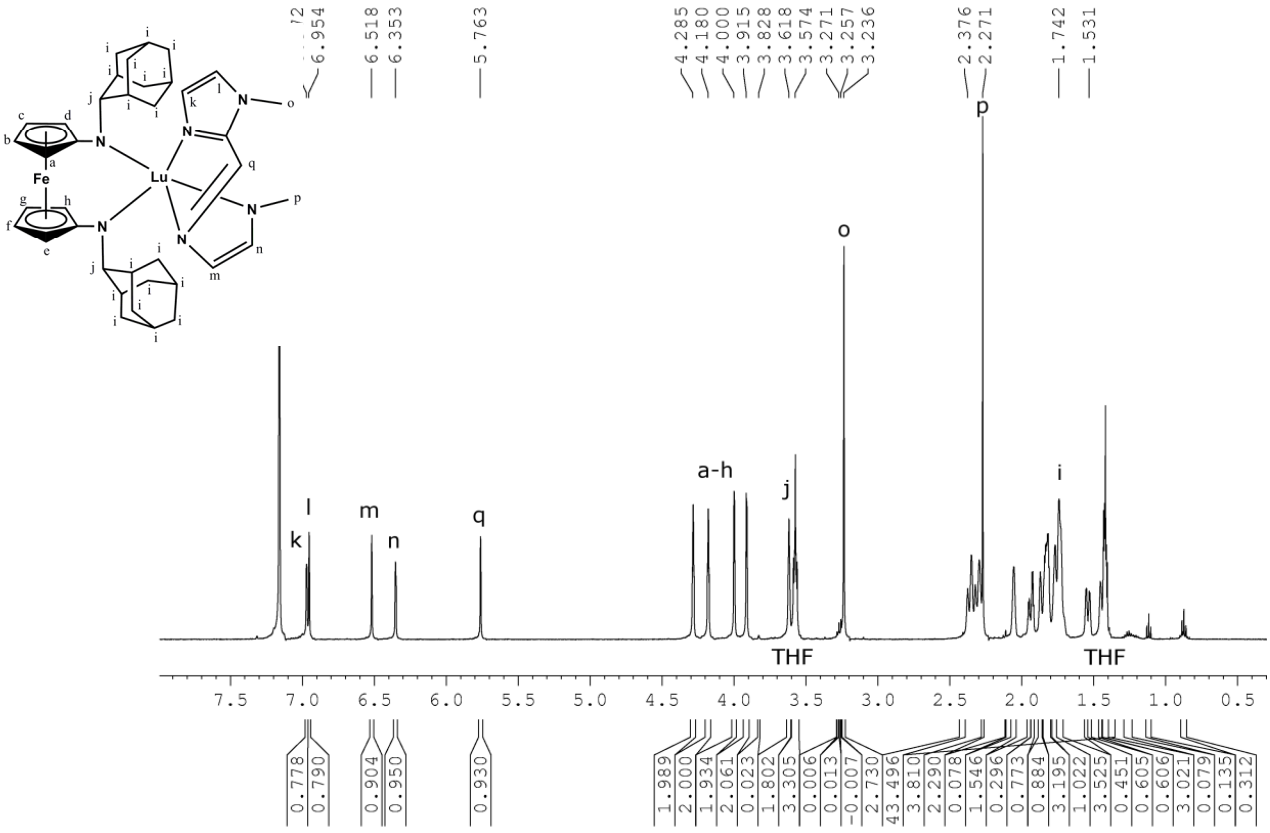


^{13}C NMR (126 MHz, C_6D_6)

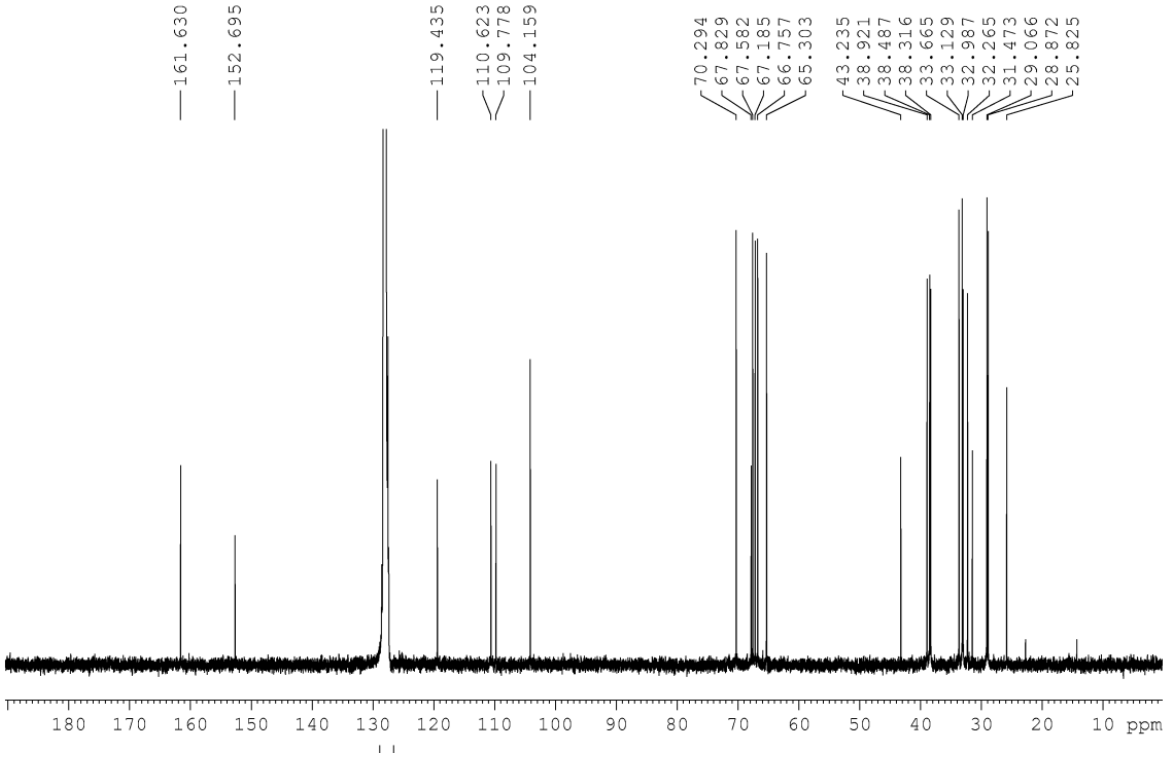


2$^{\mathbf{Ad}}$

^{1}H NMR (500 MHz, C_6D_6): Solvent peaks for THF are also present at 1.40 and 3.57 ppm.

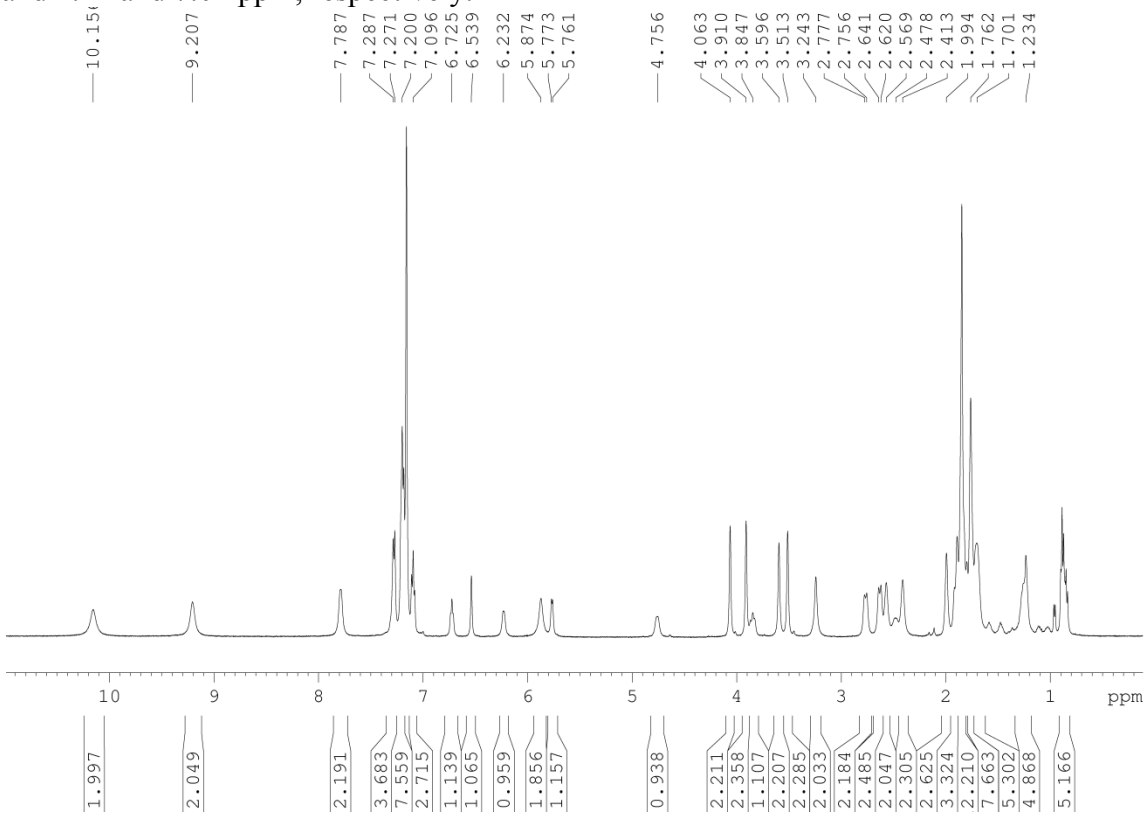


^{13}C NMR (126 MHz, C_6D_6): Solvent peaks for THF are also present at 25.72 and 67.80 ppm.

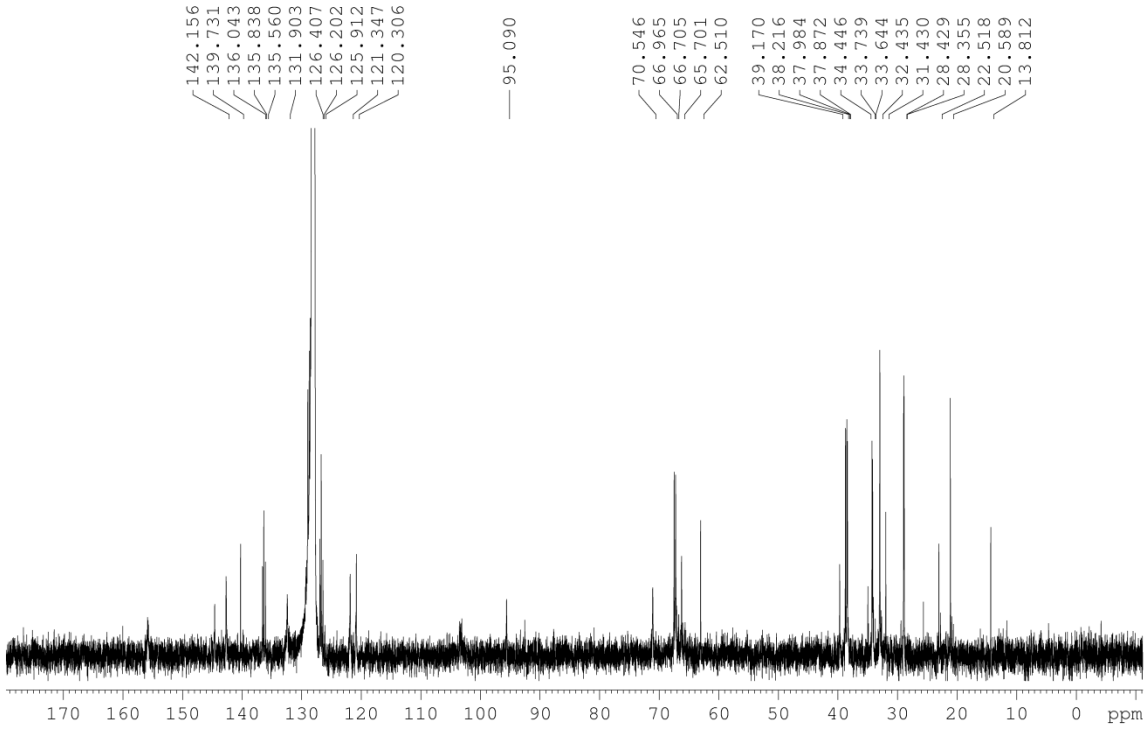


3^{Ad}-(iqn)$_2$

^{1}H NMR (500 MHz, C_6D_6): Solvent peaks for hexane and toluene are also present at 0.89 and 1.24 ppm and 2.11 and 7.02 ppm, respectively.

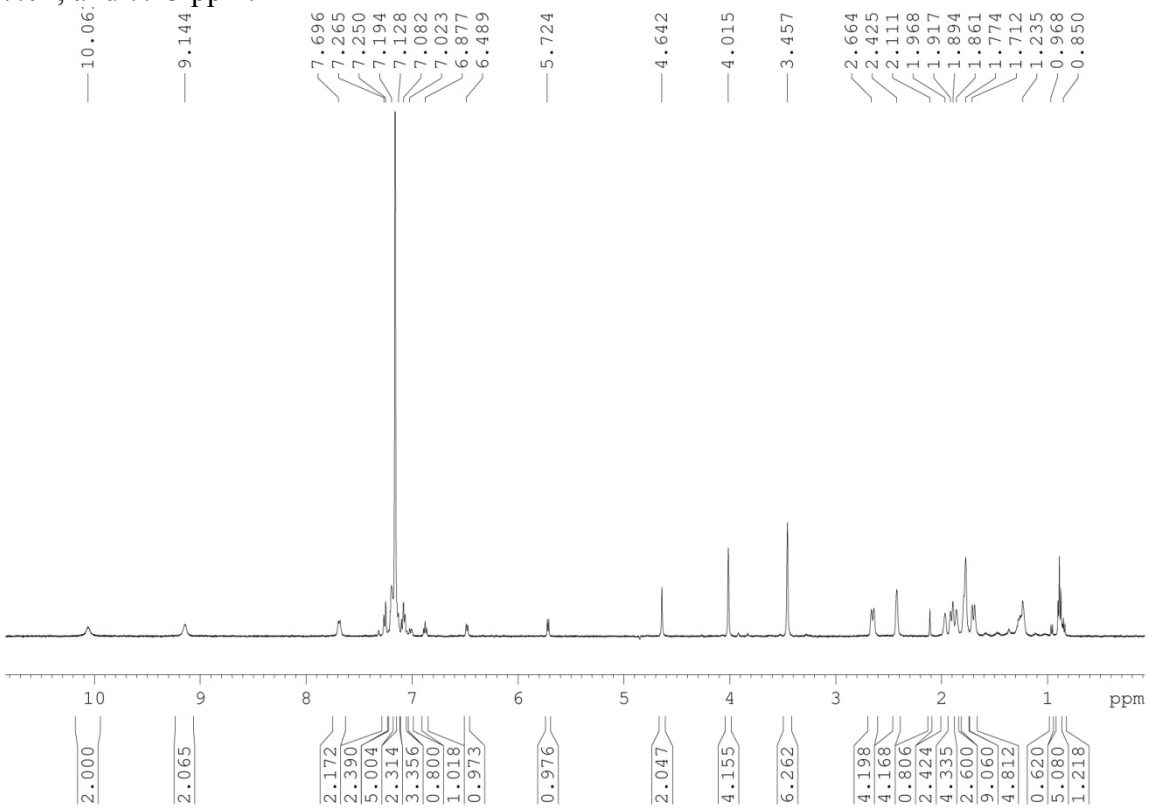


^{13}C NMR (126 MHz, C_6D_6):

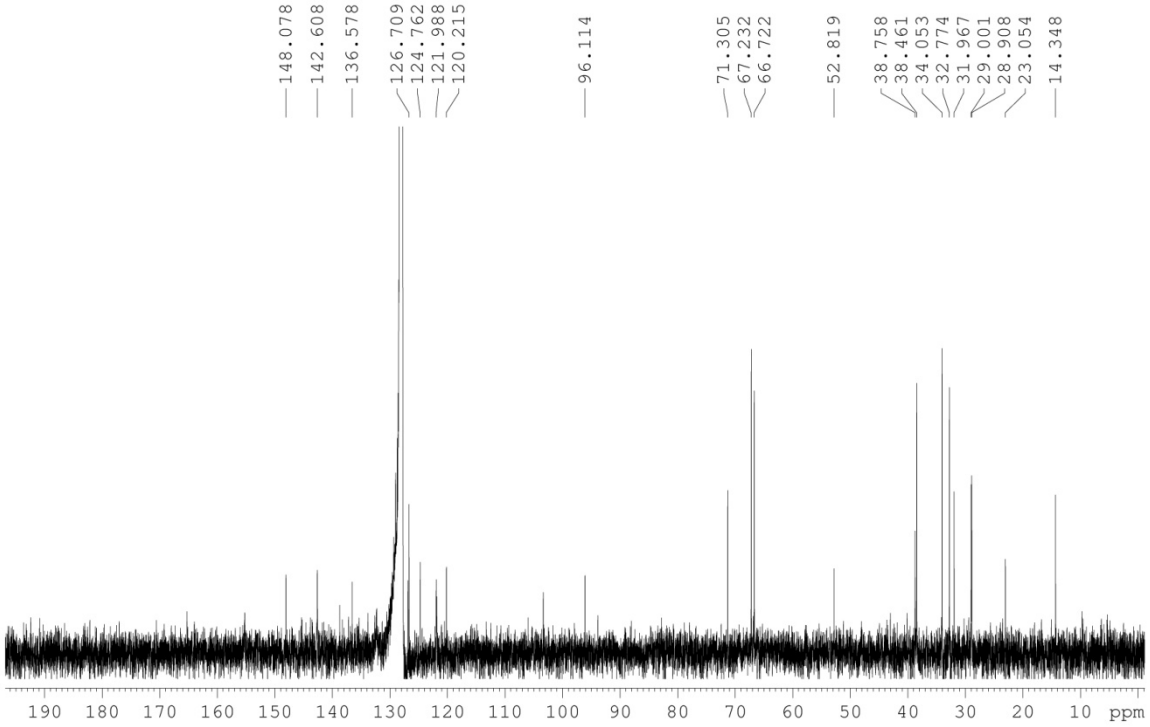


4^{Ad}-(iqn)$_2$

^{1}H NMR (500 MHz, C_6D_6): Solvent peaks for hexanes and toluene are also present at 0.85, 1.23, 2.11,7.02, and 7.13 ppm.



^{13}C NMR (126 MHz, C_6D_6):



X-ray crystal structure of 1^{Ad}-DME

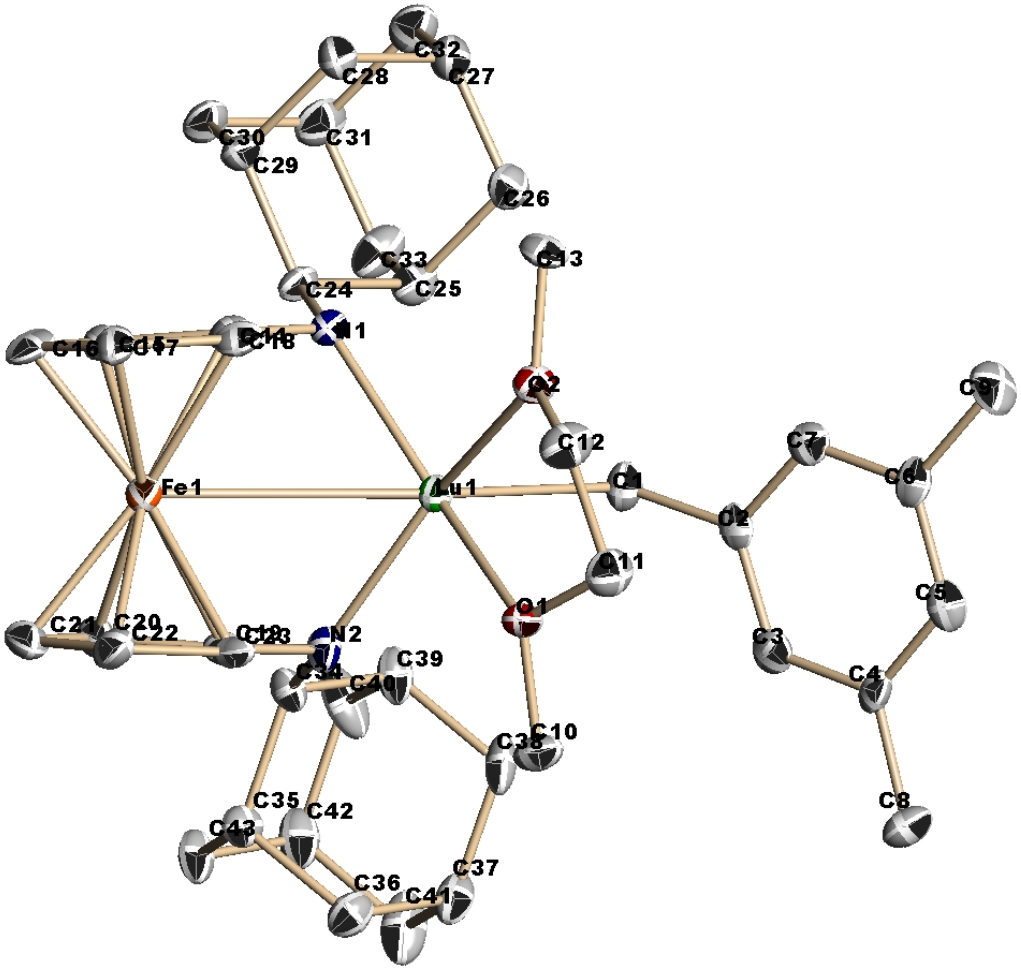


Figure S1. Thermal-ellipsoid (50% probability) representation of **1^{Ad}-DME**. Hydrogen atoms were omitted for clarity.

Computational details: XYZ coordinates

1^{Ad}-DME

1.Lu	20.064107	4.105036	1.819236
2.Fe	17.520306	6.229923	2.261498
3.N	19.458426	5.168533	-0.080687
4.N	18.220285	3.129127	2.680668
5.O	21.117396	4.263488	4.119700
6.O	22.062067	5.619966	2.010597
7.C	21.553896	2.334143	1.079696
8.H	20.962787	1.406197	1.041495
9.H	21.784617	2.634943	0.045781
10.C	22.795162	2.136185	1.841243
11.C	22.878955	1.215385	2.906537
12.H	22.008639	0.594588	3.132211
13.C	24.043628	1.040089	3.652929
14.C	25.173815	1.804179	3.343789
15.H	26.094973	1.665902	3.914308
16.C	25.144218	2.711902	2.278219
17.C	23.965450	2.870525	1.553100
18.H	23.950588	3.567524	0.711452
19.C	24.106281	-0.000413	4.739486
20.H	24.701156	0.348048	5.593715
21.H	24.574809	-0.922098	4.360434
22.H	23.105149	-0.266105	5.105324
23.C	26.392173	3.456904	1.885389
24.H	26.953722	3.801352	2.765933
25.H	26.160392	4.328306	1.258827
26.H	27.061478	2.802587	1.303508
27.C	20.847769	3.207492	5.073120
28.H	20.943227	3.604310	6.096065
29.H	21.551388	2.376474	4.916622
30.H	19.820089	2.876655	4.883356
31.C	22.491882	4.696723	4.180730
32.H	23.149128	3.877680	3.848239
33.H	22.747158	4.973691	5.218978
34.C	22.645682	5.908532	3.294708
35.H	22.142270	6.793008	3.723642
36.H	23.721432	6.123434	3.179846
37.C	22.545848	6.484644	0.963711
38.H	23.597952	6.246210	0.743279
39.H	22.456121	7.540875	1.263065
40.H	21.909669	6.294459	0.091814
41.C	18.700597	6.216031	0.440767
42.C	17.308879	6.537598	0.220222
43.H	16.629182	5.995844	-0.432108
44.C	16.975159	7.723908	0.951745
45.H	16.014687	8.232751	0.935348
46.C	18.126005	8.120482	1.699053
47.H	18.209120	8.986549	2.350712
48.C	19.171207	7.186534	1.407947
49.H	20.184875	7.251164	1.793787
50.C	17.521480	4.249045	3.133025
51.C	16.200849	4.709156	2.768037
52.H	15.520533	4.206597	2.085753

53.C	15.900201	5.905359	3.496797
54.H	14.959982	6.450445	3.465597
55.C	17.048393	6.250895	4.272686
56.H	17.143908	7.098369	4.946472
57.C	18.045838	5.252409	4.036912
58.H	19.017266	5.220374	4.523459
59.C	18.933516	4.631929	-1.345860
60.H	17.888261	4.282802	-1.208625
61.C	19.742294	3.413272	-1.831761
62.H	19.784966	2.661264	-1.025064
63.C	21.168771	3.821265	-2.233955
64.H	21.737707	2.926116	-2.542883
65.H	21.692353	4.263473	-1.372201
66.C	21.113665	4.845665	-3.378118
67.H	22.140220	5.135395	-3.665202
68.C	20.339663	6.079066	-2.888269
69.H	20.305400	6.851369	-3.677663
70.H	20.846754	6.523087	-2.015569
71.C	18.910848	5.674663	-2.496519
72.H	18.360799	6.568384	-2.158929
73.C	18.198823	5.061061	-3.713627
74.H	17.162280	4.785096	-3.447495
75.H	18.138030	5.806318	-4.526976
76.C	18.968531	3.820125	-4.192632
77.H	18.453572	3.373771	-5.061531
78.C	20.396412	4.230420	-4.591063
79.H	20.361021	4.960797	-5.419625
80.H	20.955429	3.349197	-4.954248
81.C	19.034323	2.794040	-3.049862
82.H	18.015595	2.471218	-2.770806
83.H	19.583639	1.894464	-3.379777
84.C	17.347942	2.057911	2.180839
85.H	16.670366	2.453983	1.395763
86.C	16.449060	1.441995	3.286405
87.H	15.889369	2.253600	3.781281
88.C	17.307262	0.707406	4.327275
89.H	16.661004	0.308955	5.130017
90.H	18.009175	1.419540	4.791376
91.C	18.084401	-0.432039	3.649248
92.H	18.698115	-0.964203	4.397933
93.C	18.997262	0.174733	2.572062
94.H	19.704280	0.875570	3.041893
95.H	19.591347	-0.615276	2.078146
96.C	18.145893	0.913721	1.528170
97.H	18.796949	1.333346	0.741535
98.C	17.164572	-0.079407	0.880502
99.H	16.562688	0.433388	0.109331
100.H	17.729580	-0.882089	0.373624
101.C	17.098734	-1.418051	3.000076
102.H	17.652022	-2.245517	2.519758
103.H	16.447000	-1.864190	3.772720
104.C	16.244680	-0.680288	1.955113
105.H	15.538895	-1.387310	1.484505
106.C	15.464649	0.451846	2.642618
107.H	14.793492	0.035027	3.414855
108.H	14.827493	0.973641	1.905595

1^{Si}-THF

1.Lu	-0.209173	9.876340	5.426325
2.Fe	0.973175	12.076498	3.172070
3.Si	-3.451391	10.268416	3.711034
4.Si	2.729017	10.609053	7.439003
5.N	1.599725	10.943795	6.151116
6.C	0.458873	7.385023	3.946165
7.H	-0.511159	7.630133	3.501834
8.C	-0.569774	7.609484	6.209848
9.H	-0.475653	7.277900	7.250405
10.H	-1.550995	7.336163	5.792749
11.C	2.757300	6.725299	3.656463
12.H	3.608187	6.509834	3.006279
13.C	0.543046	7.219897	5.353785
14.C	1.544061	7.124242	3.099150
15.C	2.886857	6.557260	5.043430
16.C	4.185374	6.061798	5.618056
17.H	4.168231	6.069738	6.716840
18.H	5.032467	6.680275	5.283542
19.H	4.379053	5.027548	5.289390
20.C	1.797604	6.810096	5.866874
21.H	1.895999	6.654143	6.942811
22.C	1.395412	7.220557	1.605619
23.H	1.616573	6.250787	1.133211
24.H	2.091640	7.959635	1.181636
25.H	0.374635	7.501078	1.317806
26.C	-2.497447	12.318255	8.645887
27.H	-3.256282	13.113523	8.625124
28.H	-1.741894	12.579557	9.403610
29.C	-2.003385	10.012091	8.405558
30.H	-1.163502	9.912380	9.110207
31.H	-2.350006	9.018073	8.100821
32.C	-3.085480	10.932106	8.940161
33.H	-3.284204	10.767118	10.008292
34.H	-4.021563	10.780548	8.379048
35.C	-1.841395	12.124384	7.283129
36.H	-2.524668	12.343819	6.450101
37.H	-0.903973	12.682593	7.157623
38.C	-0.184764	13.054661	1.768190
39.H	-0.012033	14.068794	1.415643
40.C	2.384390	13.506293	3.611982
41.H	2.399171	14.511260	3.197575
42.C	0.371553	11.862878	1.203117
43.H	1.037320	11.813489	0.344958
44.C	1.730713	13.101335	4.815491
45.H	1.169723	13.746895	5.487096
46.C	1.996902	11.703269	5.045818
47.C	-0.998561	12.677865	2.879924
48.H	-1.559616	13.354027	3.520259
49.C	-0.108079	10.755318	1.963516
50.H	0.117519	9.708962	1.779789
51.C	2.757961	11.245060	3.905077
52.H	3.106229	10.223333	3.768553
53.C	-1.005676	11.239169	2.989200
54.C	3.017956	12.353620	3.045736
55.H	3.596086	12.331308	2.125586

56.C	3.234443	12.186232	8.447754
57.C	4.310793	9.786291	6.794656
58.H	4.062273	8.822189	6.322307
59.H	5.037941	9.592725	7.600534
60.H	4.807844	10.410706	6.034957
61.C	3.986729	11.763003	9.724280
62.H	4.306739	12.659205	10.289934
63.H	4.895097	11.182958	9.492472
64.H	3.357749	11.156099	10.395825
65.C	1.851242	9.437714	8.648027
66.H	1.308348	8.639675	8.117967
67.H	1.131001	9.968944	9.289069
68.H	2.581402	8.949294	9.313423
69.C	1.981748	12.978604	8.856221
70.H	2.265574	13.875588	9.439405
71.H	1.306115	12.377350	9.486836
72.H	1.416171	13.314379	7.974176
73.C	4.155675	13.097982	7.617278
74.H	4.426314	13.998478	8.201584
75.H	3.675977	13.435072	6.685530
76.H	5.093316	12.588207	7.346746
77.C	-4.358550	11.943814	3.762536
78.H	-4.229412	12.432133	4.743680
79.H	-5.442929	11.817265	3.603067
80.H	-3.989921	12.641471	2.992714
81.C	-4.068152	9.239714	5.182053
82.H	-3.724840	9.681348	6.131460
83.H	-3.715192	8.196102	5.150759
84.H	-5.170055	9.217974	5.206185
85.C	-3.724448	10.279436	0.853921
86.H	-3.998135	9.745659	-0.076947
87.H	-2.670663	10.586835	0.764465
88.H	-4.339942	11.192499	0.902772
89.C	-3.961825	9.366629	2.073296
90.C	-3.135779	8.080243	1.901391
91.H	-3.431472	7.555462	0.972407
92.H	-3.283164	7.375882	2.736934
93.H	-2.061998	8.306092	1.831247
94.C	-5.454409	8.988723	2.120648
95.H	-5.748410	8.497504	1.173575
96.H	-6.101162	9.872834	2.242408
97.H	-5.677385	8.284852	2.938295
98.O	-1.523711	10.691508	7.203665
99.N	-1.726013	10.450776	3.894930