

# *Redox-Switchable Behavior of Transition-Metal Complexes Supported by Amino-Decorated N- Heterocyclic Carbenes*

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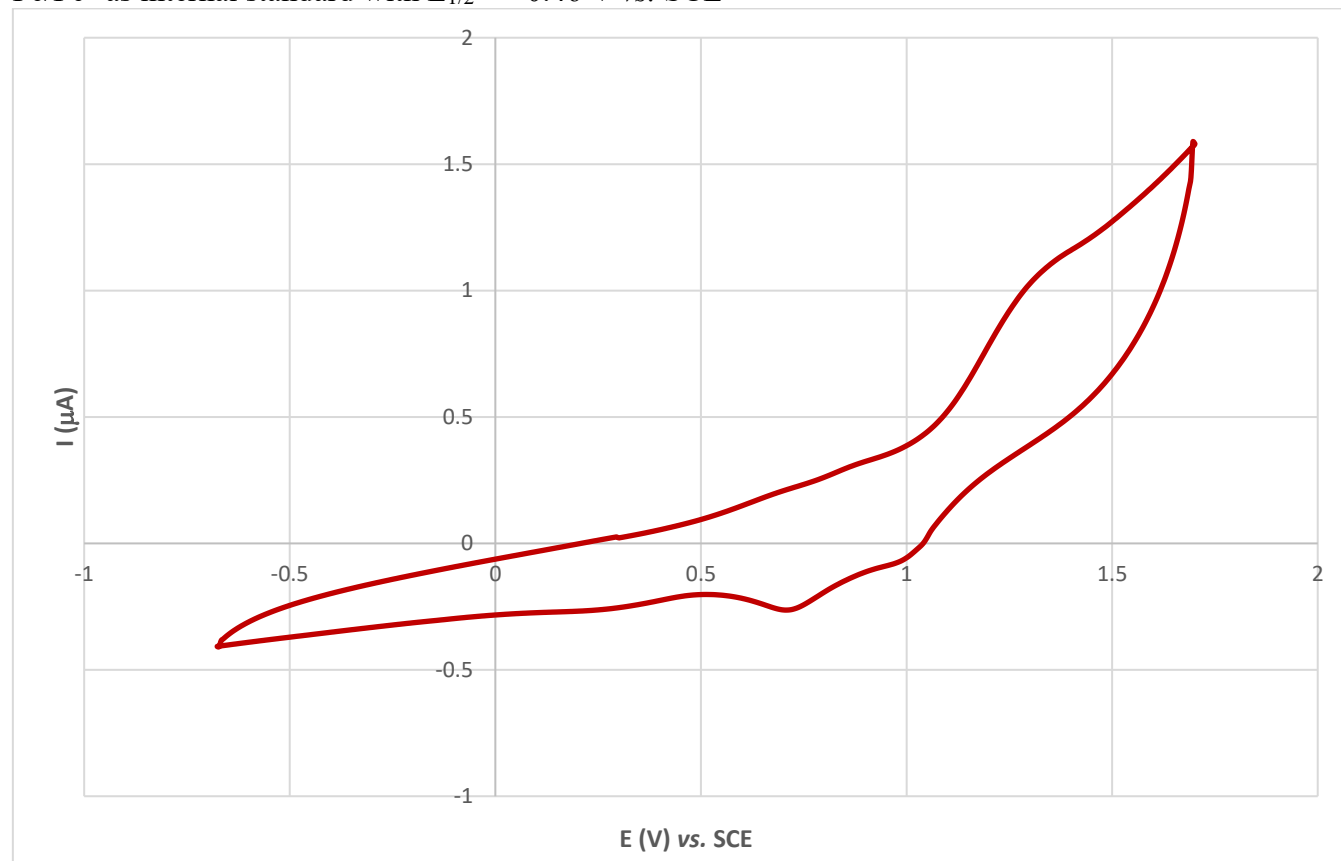
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## **Supporting Information**

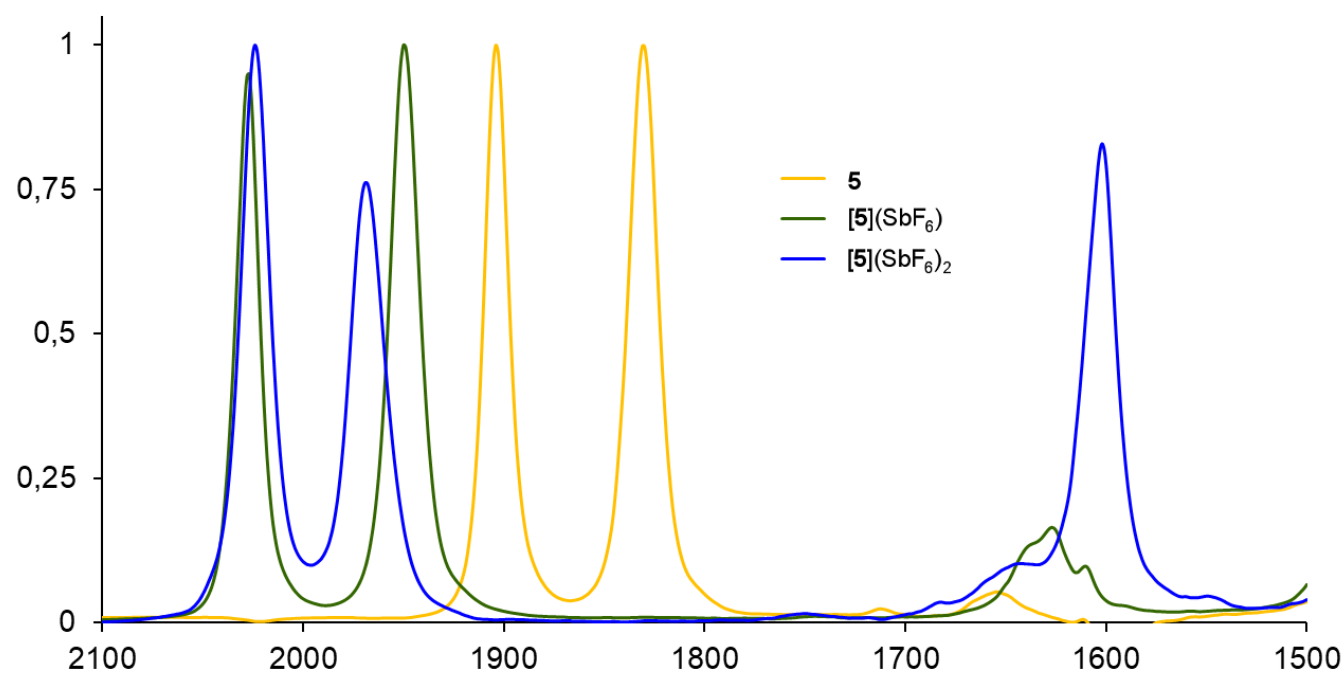
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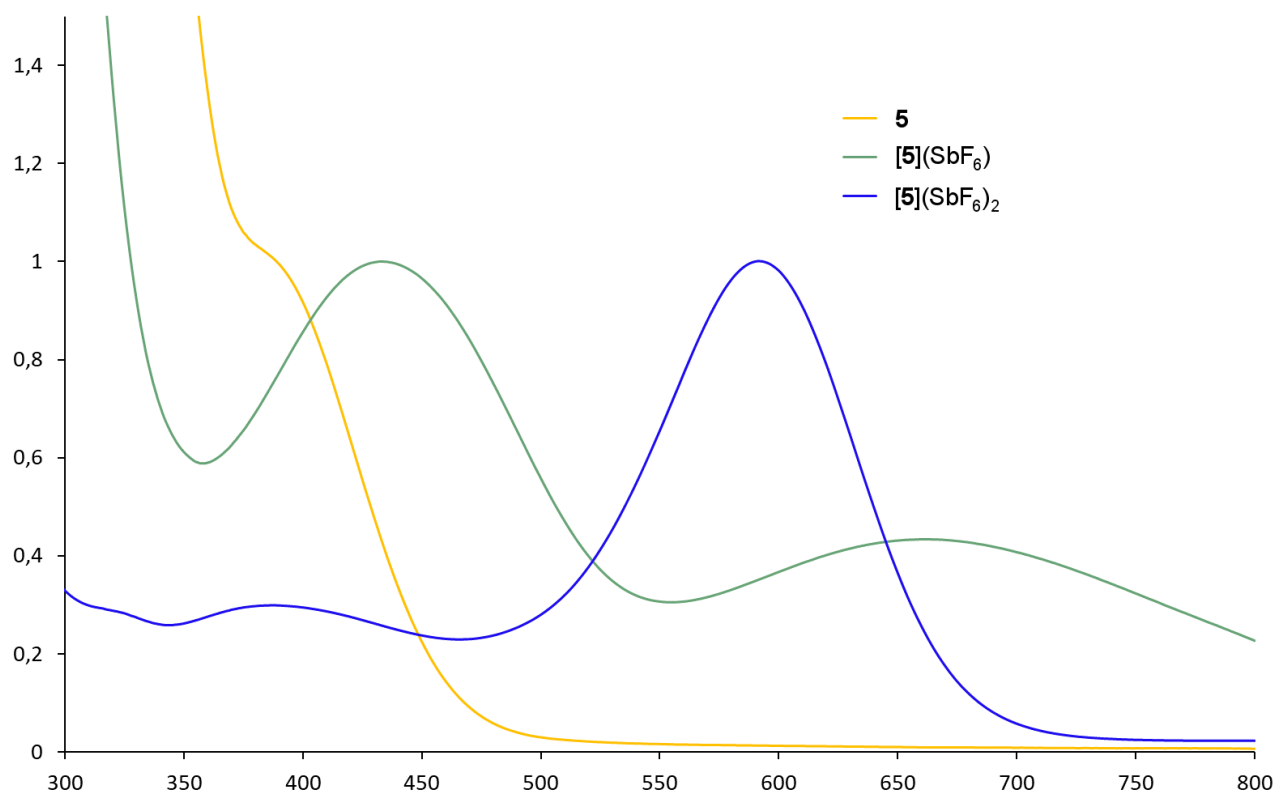
**Figure S1.** Cyclic voltammogram of complex [CuCl(IMes)]. Pt working electrode, 1 mM in CH<sub>2</sub>Cl<sub>2</sub> with 0.1 M Bu<sub>4</sub>NPF<sub>6</sub> as the supporting electrolyte, 200 mV.s<sup>-1</sup> scan rate, potentials were calibrated against Fc/Fc<sup>+</sup> as internal standard with E<sub>1/2</sub> = +0.46 V vs. SCE



**Figure S2.** Normalized IR spectra of manganese NHC complexes **5**, [5](SbF<sub>6</sub>) and [5](SbF<sub>6</sub>)<sub>2</sub> in (CH<sub>2</sub>Cl<sub>2</sub> solution, 2200-1500 cm<sup>-1</sup> region).



**Figure S3.** Normalized UV/Vis spectra of manganese NHC complexes **5**, **[5](SbF<sub>6</sub>)** and **[5](SbF<sub>6</sub>)<sub>2</sub>** (CH<sub>2</sub>Cl<sub>2</sub> solution, 10<sup>-4</sup> M level of concentrations).

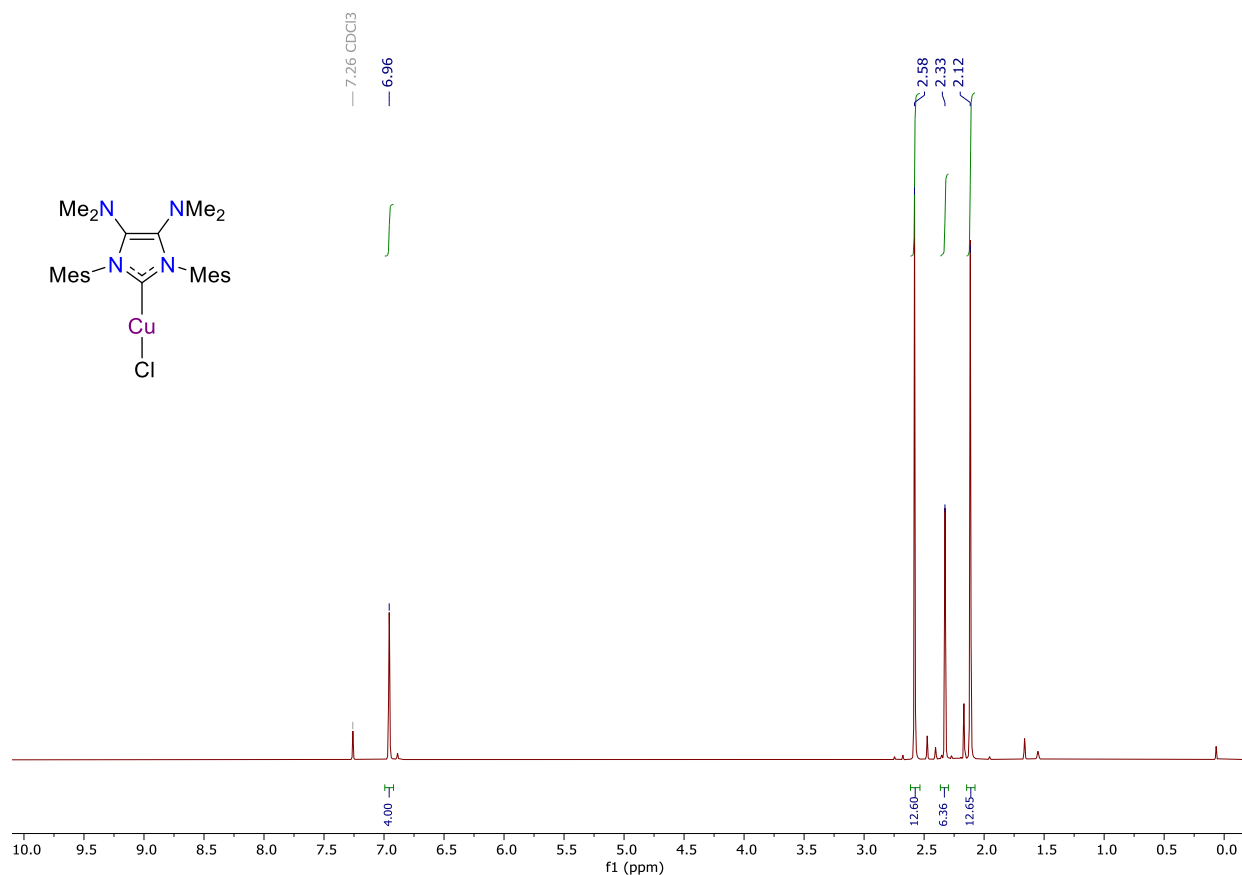


**Table S1.** Crystal data and structure refinement for NHC complexes **[4]**(BF<sub>4</sub>), **5**, **[5]**(SbF<sub>6</sub>) and **[5]**(SbF<sub>6</sub>)<sub>2</sub>

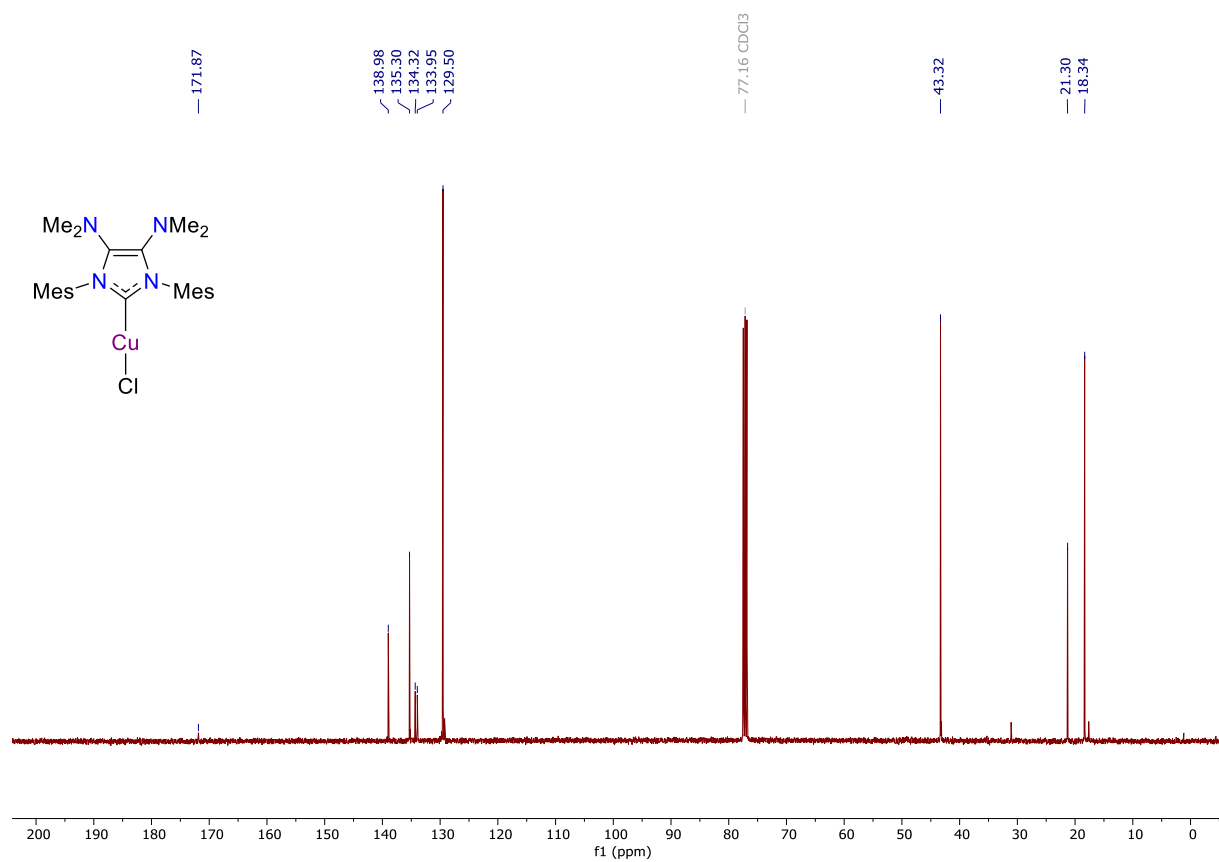
Complex	<b>[4]</b> (BF <sub>4</sub> )	<b>5</b>	<b>[5]</b> (SbF <sub>6</sub> )	<b>[5]</b> (SbF <sub>6</sub> ) <sub>2</sub>
Empirical formula	C <sub>12</sub> H <sub>13</sub> BF <sub>4</sub> FeN <sub>2</sub> O <sub>2</sub>	C <sub>32</sub> H <sub>39</sub> MnN <sub>4</sub> O <sub>2</sub>	C <sub>32</sub> H <sub>39</sub> F <sub>6</sub> MnN <sub>4</sub> O <sub>2</sub> Sb	C <sub>32</sub> H <sub>39</sub> F <sub>12</sub> MnN <sub>4</sub> O <sub>2</sub> Sb <sub>2</sub>
<i>M<sub>r</sub></i>	654.33	566.61	802.36	1038.13
<i>T</i> /K	173	123	150	100
$\lambda$ /Å	0.71073	0.71073	1.54184	0.71073
Crystal system	orthorhombic	monoclinic	monoclinic	triclinic
Space group (no.)	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (#19)	P2 <sub>1</sub> /c (#14)	P2 <sub>1</sub> /n (#14)	P1 bar (#2)
<i>a</i> /Å	9.1166(3)	16.9220(6)	12.95920(10)	8.8818(13)
<i>b</i> /Å	18.2281(5)	16.4516(3)	17.97800(10)	16.660(2)
<i>c</i> /Å	19.4675(5)	21.2589(6)	15.77180(10)	19.335(3)
$\alpha$ /°	90	90	90	97.327(4)
$\beta$ /°	90	90.000(3)	97.8330(10)	101.687(4)
$\gamma$ /°	90	90	90	99.991(4)
<i>V</i> /Å <sup>3</sup>	3235.08(16)	5918.3(3)	3640.24(4)	2719.7(7)
<i>Z</i>	4	4	4	2
<i>D<sub>c</sub></i> /g.cm <sup>-3</sup>	1.343	1.272	1.464	1.268
$\mu$ /mm <sup>-1</sup>	0.524	0.481	9.262	1.281
<i>F</i> (000)	1368	2400	1620	1020
$\theta_{\max}$ /°	26.4	26.4	71.4	26.4
Completeness				
to $\theta_{\max}$ (%)	0.997	0.984	0.997	0.981
Index range, <i>hkl</i>	-11< <i>h</i> <11 -22< <i>k</i> <22 -24< <i>l</i> <24	-21< <i>h</i> <20 -20< <i>k</i> <20 -26< <i>l</i> <26	-15< <i>h</i> <15 -22< <i>k</i> <22 -19< <i>l</i> <19	-10< <i>h</i> <11 -20< <i>k</i> <20 -24< <i>l</i> <24
Reflections				
collected	6600	11898	7059	38907
Independent				
reflections	6172	10775	6497	10900
Parameters	407	724	425	491
<i>GOF</i>	1.03	1.03	1.04	1.11
<i>R</i> (all data)	0.0328	0.0392	0.027	0.1413
<i>R</i> [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	0.0289	0.0328	0.024	0.1191
<i>R<sub>w</sub></i> (all data)	0.0845	0.0845	0.063	0.26
<i>R<sub>w</sub></i> [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	0.0813	0.0803	0.0612	0.2484
$\Delta\rho_{\max/\min}$ /e.Å <sup>-3</sup>	-0.16/0.44	-0.38/0.30	-0.61/0.44	-2.20/1.38

## NMR Spectra

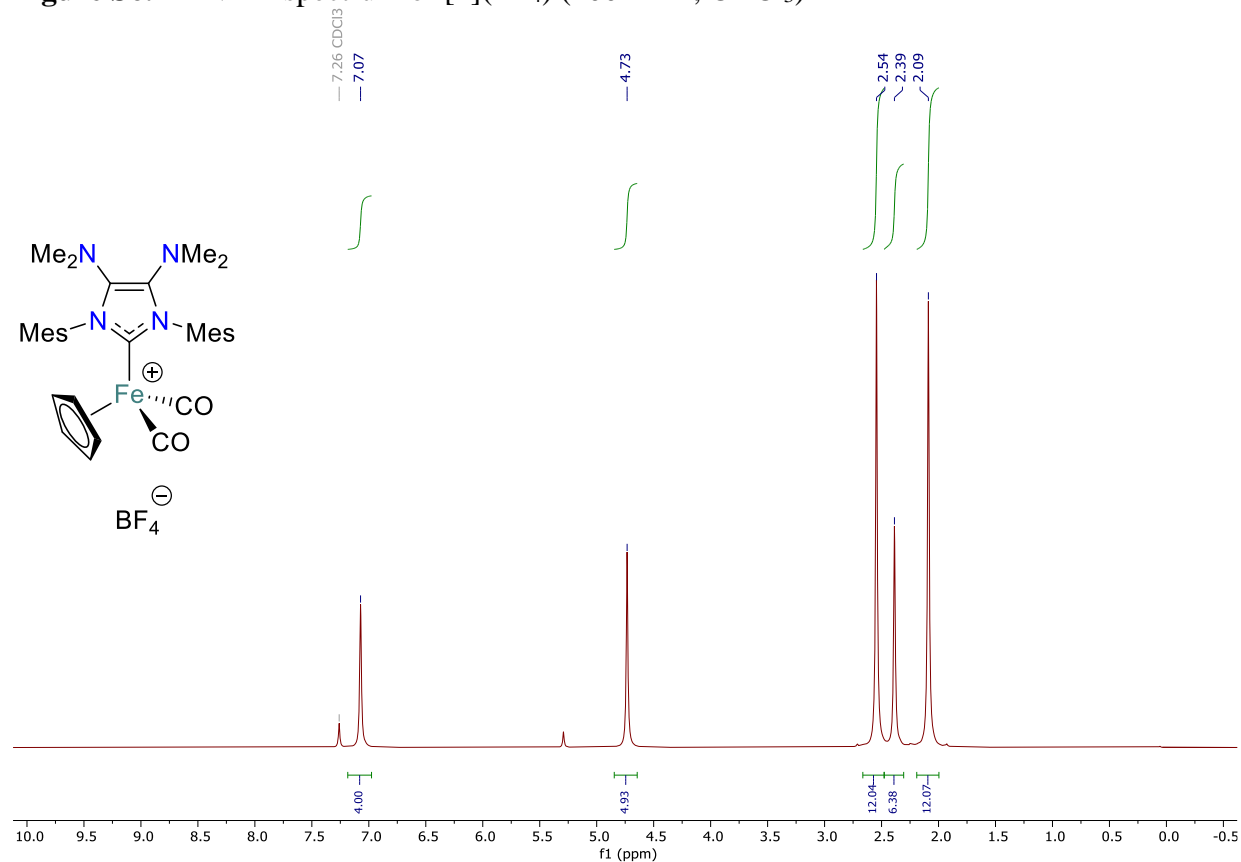
**Figure S4.**  $^1\text{H}$  NMR spectrum of **2** (400 MHz,  $\text{CDCl}_3$ )



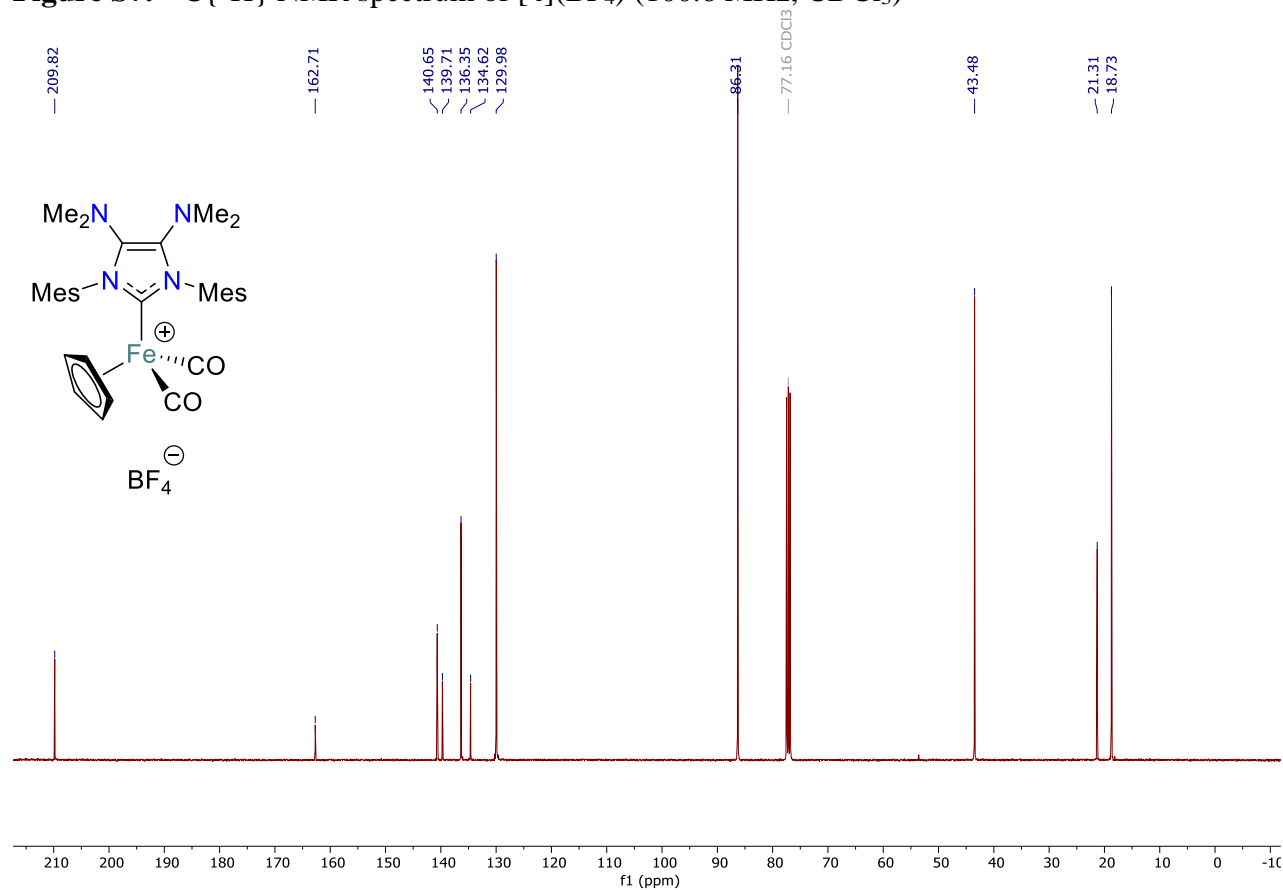
**Figure S5.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2** (100.6 MHz,  $\text{CDCl}_3$ )



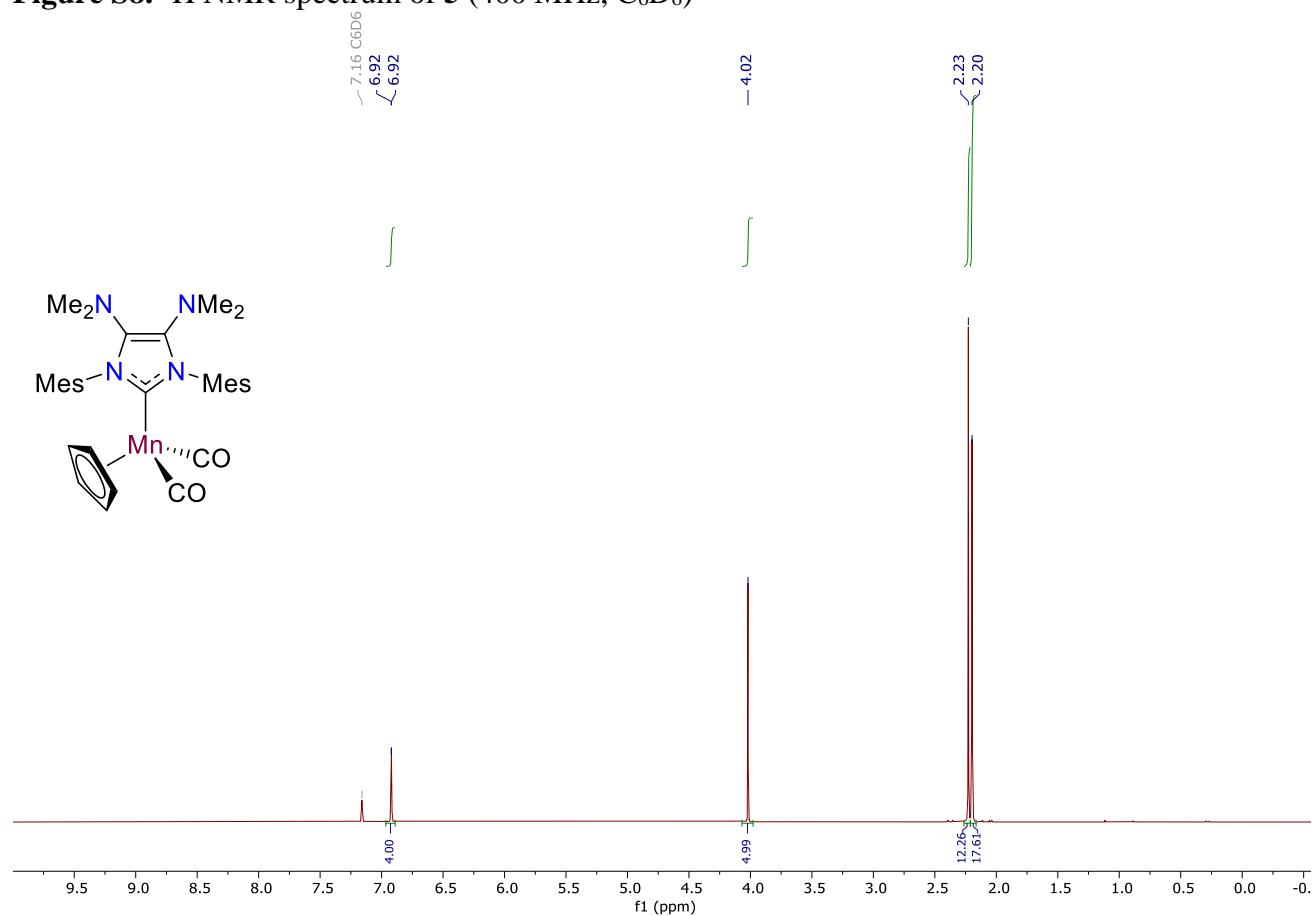
**Figure S6.**  $^1\text{H}$  NMR spectrum of **[4]**( $\text{BF}_4$ ) (400 MHz,  $\text{CDCl}_3$ )



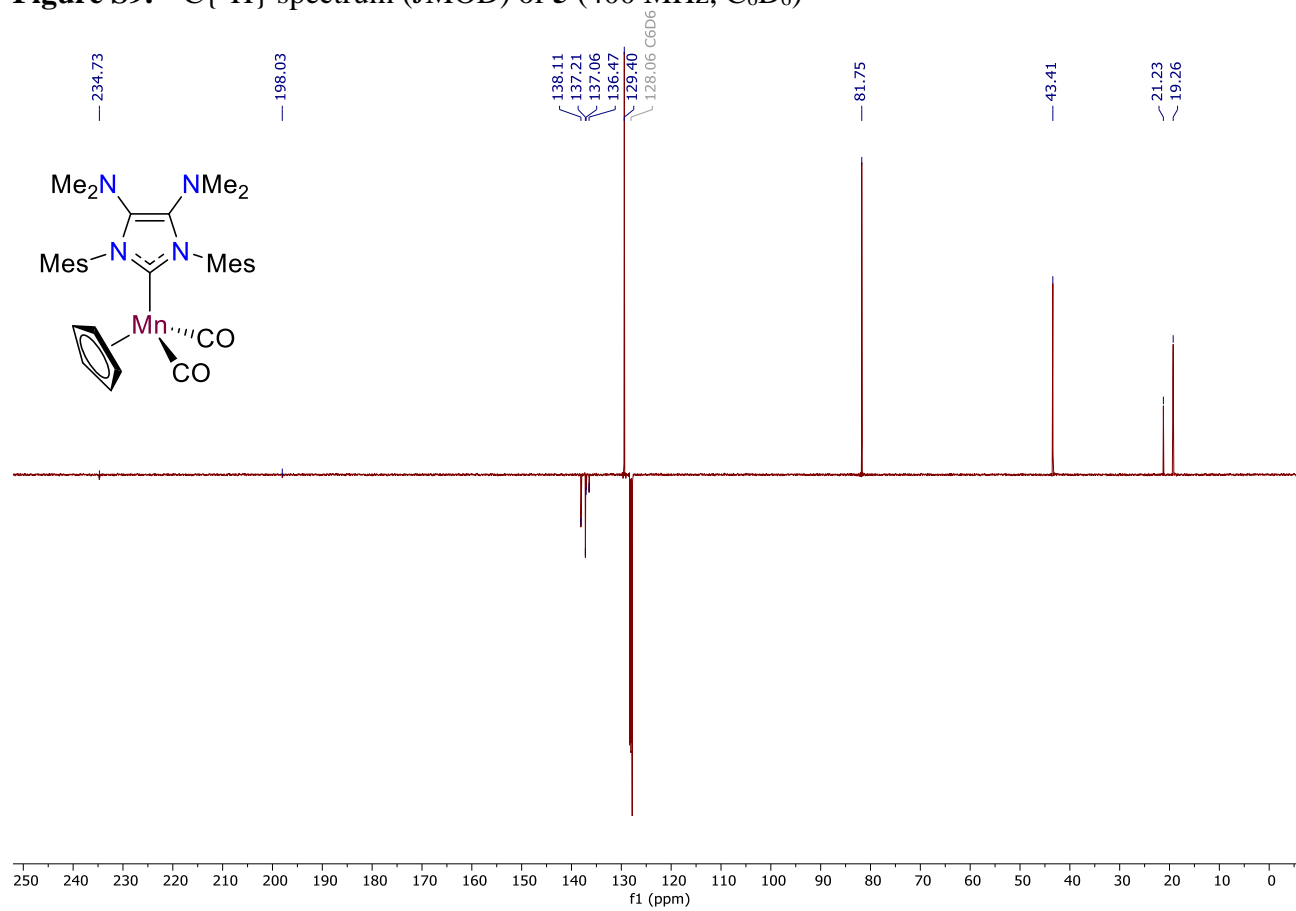
**Figure S7.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **[4]**( $\text{BF}_4$ ) (100.6 MHz,  $\text{CDCl}_3$ )



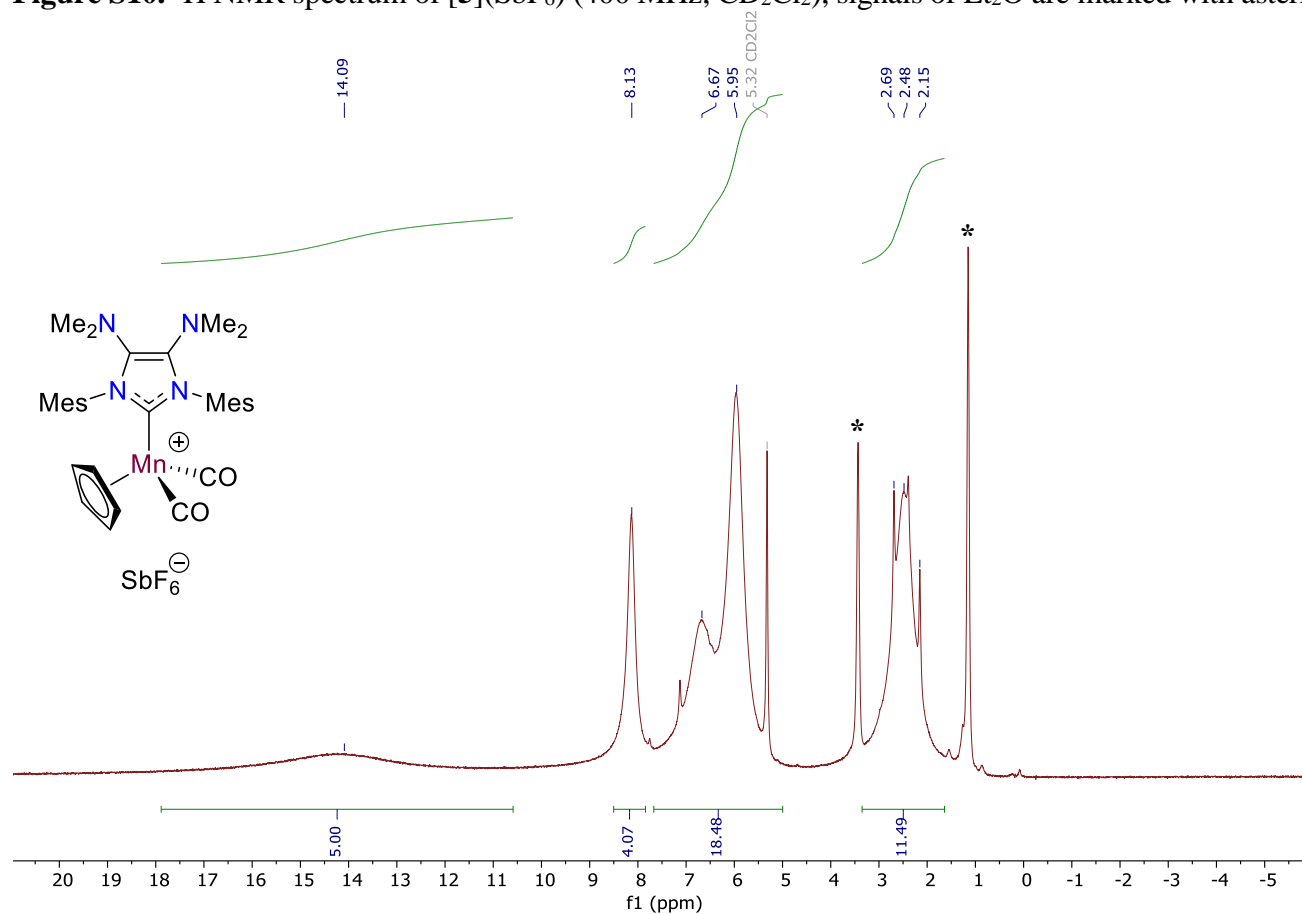
**Figure S8.**  $^1\text{H}$  NMR spectrum of **5** (400 MHz,  $\text{C}_6\text{D}_6$ )



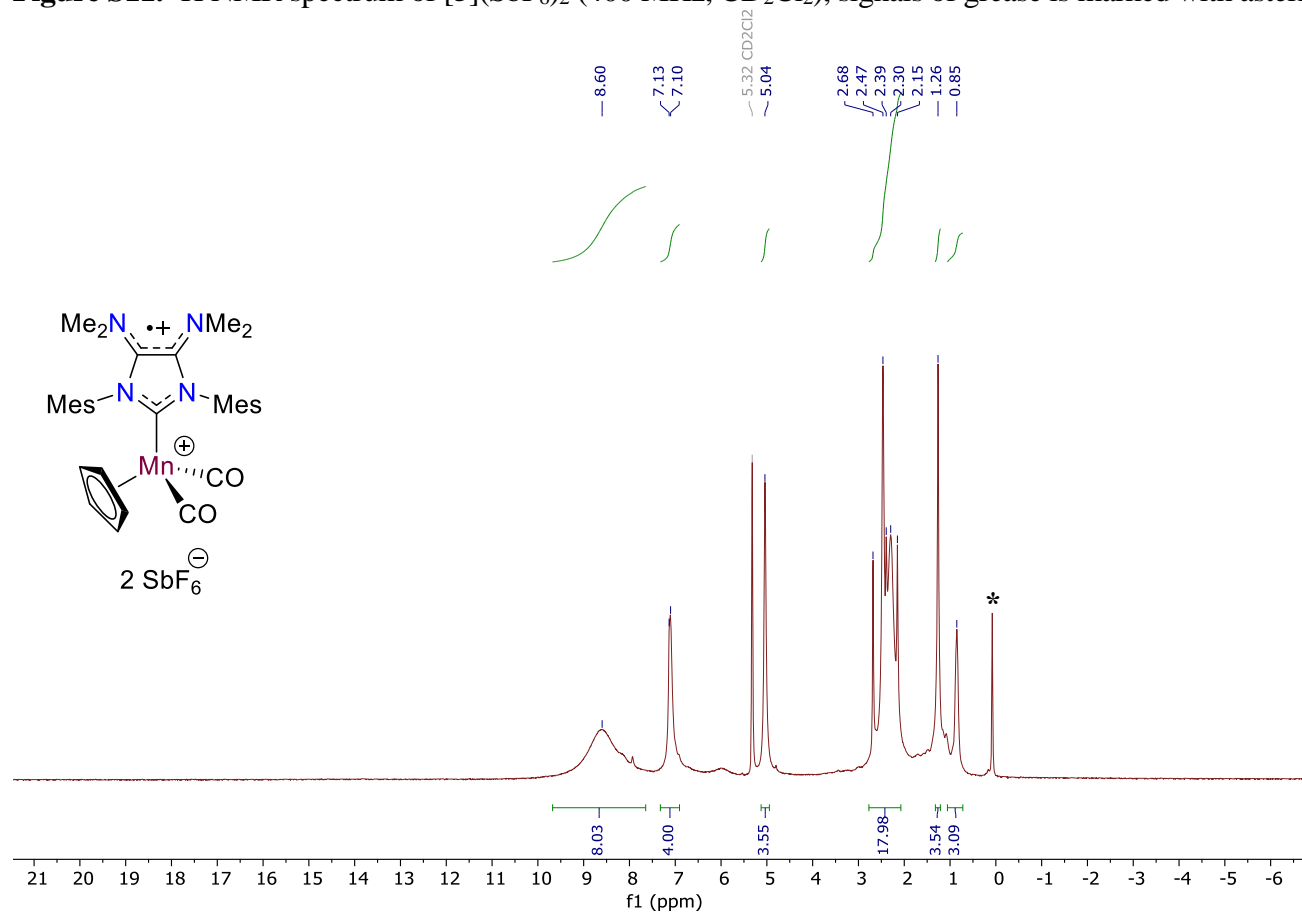
**Figure S9.**  $^{13}\text{C}\{^1\text{H}\}$  spectrum (JMOD) of **5** (400 MHz,  $\text{C}_6\text{D}_6$ )



**Figure S10.**  $^1\text{H}$  NMR spectrum of  $[\mathbf{5}](\text{SbF}_6)$  (400 MHz,  $\text{CD}_2\text{Cl}_2$ ), signals of  $\text{Et}_2\text{O}$  are marked with asterisk



**Figure S11.**  $^1\text{H}$  NMR spectrum of  $[\mathbf{5}](\text{SbF}_6)_2$  (400 MHz,  $\text{CD}_2\text{Cl}_2$ ), signals of grease is marked with asterisk

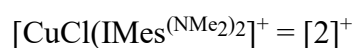




## DFT-optimized geometries

All DFT calculations were performed with the ADF (Amsterdam Density Functional) code developed by E. J. Baerends and co-workers<sup>[1]</sup> using triple-zeta (TZ2P) basis sets (no frozen core) (relativistic ZORA/TZ2P for Rhodium). Geometry optimizations were performed *in vacuo* relying on the Generalized Gradient Approximation (GGA) VBP exchange-correlation (XC) potential (VWN + BP: Vosko, Wilk & Nusair<sup>[2]</sup> + corrective terms by Becke<sup>[3]</sup> for the exchange, and Perdew<sup>[4]</sup> for the correlation) with ADF grid precision 6 throughout.

- [1] G. te Velde, E. J. Baerends, J. Comput. Phys. 1992, 99, 84–98.
- [2] S. H. Vosko, L. Wilk, M. Nusair, Can. J. Phys. 1980, 58, 1200–1211.
- [3] A. D. Becke, Phys. Rev. A 1988, 38, 3098–3100.
- [4] J. P. Perdew, Phys. Rev. B 1986, 33, 8822–8824.



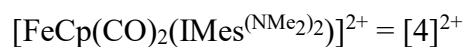
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H	5.548225	-1.301127	14.969302
H	4.733403	0.221405	15.442415
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H	6.724217	-0.001179	11.729689
H	6.999206	-1.234191	12.987015
H	7.746029	0.380267	13.144055
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H	1.335375	0.190498	15.691110
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C	7.274426	3.323089	12.570540
C	8.510041	3.701207	12.035575
H	9.209324	4.243081	12.674227
C	8.862588	3.431227	10.707898
C	7.931810	2.767955	9.899943
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C	6.915146	3.688880	13.988495
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H	-3.092115	3.961166	12.910747
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H	1.949913	1.699496	10.177676
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N	2.958931	2.481169	12.758906
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N	2.596638	0.424708	14.050497
Cl	3.807782	6.388941	9.933897



Rh	3.909596	4.862127	10.937715
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O	6.341381	6.350589	12.143054
C	2.262823	4.458257	9.954440
O	1.352228	4.381450	9.265321
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H	5.467757	-1.267253	14.927009
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C	6.832141	-0.129486	12.801481
H	6.728671	0.068691	11.731601
H	6.928628	-1.215175	12.949613
H	7.749674	0.355499	13.168720
C	2.762374	-1.031144	13.720435
H	3.614069	-1.228079	13.064120
H	1.857867	-1.457079	13.258108
H	2.919003	-1.534793	14.684987
C	1.393957	0.778613	14.688325
H	0.461600	0.608398	14.128219
H	1.440460	1.827669	14.991540
H	1.376577	0.152500	15.592548
C	6.446628	2.735213	11.900778
C	7.319125	3.250564	12.874740
C	8.625801	3.559517	12.477483
H	9.311429	3.972075	13.219112

C	9.069826	3.373698	11.164834
C	8.161027	2.864881	10.226898
H	8.484290	2.718705	9.194887
C	6.845416	2.538500	10.564497
C	6.886190	3.504158	14.297342
H	7.602190	4.161064	14.802829
H	6.826721	2.574096	14.881828
H	5.898322	3.981822	14.345902
C	10.474524	3.735001	10.756020
H	10.942889	2.924797	10.181859
H	11.105705	3.950741	11.625182
H	10.472855	4.626550	10.112539
C	5.902020	2.011889	9.514580
H	5.157890	2.778240	9.248250
H	5.344621	1.128514	9.857364
H	6.447456	1.738590	8.605201
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H	-0.607402	5.144288	13.842499
C	-1.146435	3.638437	12.396191
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C	0.684763	2.186219	11.660563
C	2.031243	4.731087	14.218272
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H	1.466462	5.389174	14.886871
H	2.714409	5.355114	13.621914
C	-2.588757	4.065901	12.309274
H	-3.221570	3.271730	11.897052
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H	-2.982998	4.349004	13.293165
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H	0.433865	0.865600	9.981410
H	1.303765	0.127421	11.331897
H	2.123569	1.303284	10.294063
N	5.099111	2.373455	12.294071
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N	5.643294	0.318490	13.530254
N	2.578732	0.409651	13.910318
Cl	3.834763	6.854779	9.690506



Fe	11.650658	4.347856	6.015645
C	10.485754	3.228739	5.283479
C	10.791642	5.731090	5.301255
C	9.885196	3.847308	9.830887
C	9.977707	5.269858	9.791691
C	9.900098	3.476751	12.263819
H	10.487689	4.397564	12.266036
H	10.503063	2.670318	12.706030
H	9.000545	3.603829	12.880637
C	8.930997	1.743201	10.817967
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H	8.371725	1.618362	9.889944

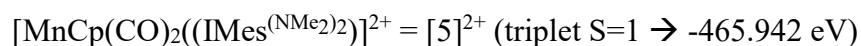
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C	8.189805	5.888867	11.364235
H	7.743884	4.955114	11.013870
H	7.504916	6.717092	11.130304
H	8.322768	5.857282	12.453746
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H	13.864671	4.260658	7.928854
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H	13.296946	2.002126	6.546402
C	13.101594	3.381851	4.785286
H	12.867256	2.703534	3.971042
C	13.247584	4.791020	4.676104
H	13.146618	5.371913	3.765054
C	13.571148	5.306973	5.976901
H	13.760099	6.347815	6.213244
C	10.410232	1.991762	8.218347
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C	12.072418	7.566378	8.361593
C	12.227687	8.894080	7.944376
H	13.187007	9.385877	8.116761
C	11.189399	9.616680	7.345266
C	9.956771	8.972313	7.172995
H	9.130101	9.519147	6.716998
C	9.744357	7.646137	7.558934
C	13.208162	6.900376	9.102602
H	13.418881	7.432357	10.041614
H	14.140647	6.934699	8.524915
H	12.999710	5.856045	9.355166
C	11.390169	11.036831	6.888080
H	11.666683	11.060753	5.823384
H	12.192238	11.532619	7.446329
H	10.472855	11.627379	6.996154
C	8.384373	7.022011	7.363062
H	7.828062	7.552903	6.583349

H	7.780109	7.076745	8.281478
H	8.441325	5.965603	7.071453
C	10.816155	4.447482	7.814034
N	10.342850	3.398143	8.587003
N	10.608449	5.583331	8.582935
N	9.540421	3.079341	10.893632
N	9.471216	6.149390	10.690285
O	9.796314	2.557183	4.649799
O	10.283586	6.561407	4.685973



Mn	11.594456	4.337599	5.928137
C	11.406497	2.576236	5.593136
C	9.966949	4.519418	5.199679
C	9.747850	3.910667	9.755246
C	9.923400	5.293109	9.750350
C	9.774202	3.380886	12.146061
H	10.687973	3.983838	12.133391
H	9.991352	2.431121	12.657812
H	9.003625	3.906929	12.735958
C	8.162994	2.225292	10.701464
H	7.300658	2.690570	11.212303
H	8.374738	1.263201	11.187912
H	7.892604	2.033852	9.661673
C	10.153166	7.135089	11.422911
H	10.343126	6.683848	12.414071
H	9.604349	8.074254	11.573082
H	11.108325	7.374171	10.950645
C	7.994805	6.031180	11.054604
H	7.434785	5.418429	10.340558
H	7.496025	7.007720	11.140570
H	7.957720	5.551512	12.048057
C	13.553990	5.254953	6.293957
H	14.007088	5.376935	7.269685
C	13.697276	4.113893	5.453268
H	14.269490	3.219555	5.675280
C	12.970679	4.364444	4.244254
H	12.887747	3.692653	3.397148
C	12.383769	5.654456	4.353415
H	11.767881	6.135773	3.600885
C	12.749143	6.212847	5.610312
H	12.471913	7.197925	5.969104
C	10.304750	2.034809	8.214842
C	11.429252	1.297738	8.639728
C	11.452958	-0.072440	8.375680
H	12.324509	-0.650032	8.688558
C	10.398124	-0.722836	7.721701
C	9.298308	0.042391	7.327591
H	8.470499	-0.442477	6.806611
C	9.222909	1.421121	7.561753
C	12.583392	1.955849	9.350736
H	12.266944	2.396691	10.307071
H	13.016439	2.764576	8.745227
H	13.373284	1.227031	9.562514
C	10.443003	-2.208701	7.471417
H	9.864592	-2.483714	6.581588

H	10.017469	-2.759435	8.323729
H	11.472630	-2.561183	7.336768
C	8.015995	2.181884	7.069073
H	7.088305	1.667095	7.352893
H	8.019498	2.241916	5.972003
H	7.972270	3.206468	7.452973
C	11.049824	6.938272	8.258664
C	12.306498	7.392417	8.695007
C	12.674832	8.709435	8.385547
H	13.653934	9.067428	8.708776
C	11.832079	9.572120	7.681052
C	10.576985	9.087144	7.288205
H	9.895069	9.747137	6.748694
C	10.156216	7.785418	7.573312
C	13.257453	6.540518	9.502874
H	13.244595	6.834492	10.562984
H	14.290483	6.680163	9.160119
H	13.014025	5.474360	9.454872
C	12.244953	10.986519	7.360580
H	12.261651	11.158328	6.275411
H	13.240968	11.215747	7.755177
H	11.535544	11.708399	7.788168
C	8.767972	7.344933	7.188755
H	8.347420	8.008644	6.425229
H	8.101327	7.378999	8.063258
H	8.746327	6.320918	6.801605
C	10.831368	4.464784	7.788650
N	10.257750	3.445567	8.530041
N	10.636500	5.590677	8.575963
N	9.339386	3.092459	10.781646
N	9.359106	6.246184	10.572851
O	11.383353	1.498406	5.162525
O	8.931675	4.623809	4.681835

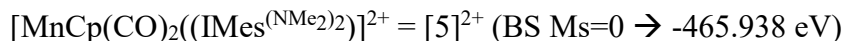


Note : both triplet (S=1 ; here) and BS (Ms=0 ; below) states have been geometry-optimized. They are quasi isoenergetic, meaning that both spin sources (Mn and NHC backbone) are isolated from one another (i.e. do not communicate with one another, magnetically speaking).

Mn	11.604509	4.387624	6.040636
C	10.039690	4.009047	5.204109
C	11.323487	6.097462	5.402653
C	9.771418	3.832382	9.860965
C	9.860357	5.254553	9.823010
C	9.652823	3.398921	12.282977
H	10.254180	4.309562	12.338073
H	10.222890	2.571998	12.731522
H	8.728211	3.525880	12.861909
C	8.696012	1.748056	10.721154
H	7.932037	1.661573	11.505930
H	9.406314	0.916112	10.834087
H	8.205198	1.683337	9.747981
C	9.938085	7.462652	10.997694
H	9.849790	7.636460	12.079108
H	9.399990	8.264415	10.471298
H	10.993908	7.492259	10.721332

C	8.064705	5.908906	11.376123
H	7.608882	4.979764	11.025736
H	7.392593	6.744975	11.132391
H	8.185613	5.879047	12.467300
C	13.495948	3.489520	6.619885
H	13.841790	3.366103	7.639252
C	12.758826	2.526784	5.859105
H	12.416098	1.556679	6.206237
C	12.568150	3.055474	4.551583
H	12.047702	2.564510	3.735227
C	13.174778	4.336824	4.496671
H	13.206083	4.988469	3.629392
C	13.753664	4.610235	5.779400
H	14.312142	5.502392	6.041964
C	10.526104	1.980154	8.322172
C	11.672976	1.358449	8.858555
C	11.913379	0.025984	8.509390
H	12.803978	-0.464137	8.906280
C	11.053867	-0.696367	7.668601
C	9.913115	-0.045905	7.186532
H	9.217956	-0.594164	6.548156
C	9.612381	1.284010	7.509839
C	12.621039	2.053856	9.805932
H	12.319214	1.893665	10.851968
H	12.670129	3.137673	9.645823
H	13.633659	1.645231	9.710387
C	11.328526	-2.138561	7.334005
H	10.876013	-2.425701	6.378217
H	10.903945	-2.796520	8.106917
H	12.404009	-2.345972	7.288941
C	8.297828	1.862525	7.046964
H	8.140785	1.684267	5.977089
H	8.209298	2.937970	7.228225
H	7.464113	1.365868	7.565607
C	10.744025	6.916199	8.143533
C	12.030002	7.475190	8.286082
C	12.215394	8.790318	7.848634
H	13.204524	9.239599	7.948525
C	11.172750	9.549801	7.301971
C	9.907412	8.953337	7.194927
H	9.084964	9.526366	6.764113
C	9.661701	7.641017	7.605006
C	13.168020	6.731272	8.939971
H	13.058523	6.705827	10.035506
H	14.122832	7.224871	8.729609
H	13.235314	5.690843	8.601284
C	11.403515	10.955034	6.817424
H	11.488149	10.971305	5.720472
H	12.325802	11.380406	7.227560
H	10.566616	11.612600	7.083010
C	8.287228	7.041918	7.440495
H	7.663661	7.680658	6.806485
H	7.766760	6.933930	8.403700
H	8.324685	6.046027	6.978330
C	10.761254	4.431371	7.877661
N	10.287951	3.379524	8.642818

N	10.506738	5.565198	8.622472
N	9.350235	3.052634	10.887266
N	9.356241	6.143676	10.714565
O	9.073459	3.806826	4.606108
O	11.202265	7.093905	4.840113



Mn	11.592669	4.377005	6.014325
C	9.967270	4.294387	5.219171
C	11.547074	6.134582	5.507733
C	9.773650	3.820815	9.837024
C	9.822939	5.251934	9.786210
C	9.597665	3.408188	12.260265
H	10.172010	4.335254	12.325928
H	10.180450	2.599438	12.725156
H	8.655791	3.509232	12.815133
C	8.742530	1.712058	10.689219
H	7.977646	1.599235	11.469374
H	9.485013	0.909952	10.810104
H	8.261163	1.625800	9.713055
C	9.820857	7.474105	10.937252
H	9.699527	7.664376	12.012419
H	9.264630	8.243446	10.382135
H	10.880897	7.537798	10.685160
C	8.003138	5.861961	11.329794
H	7.572500	4.919368	10.984214
H	7.313128	6.678861	11.072147
H	8.117665	5.847084	12.421511
C	13.436700	3.284679	6.450973
H	13.862872	3.144082	7.437679
C	12.558109	2.385792	5.778775
H	12.177995	1.445746	6.165683
C	12.279192	2.925418	4.491909
H	11.644260	2.473658	3.736226
C	12.992004	4.146949	4.353050
H	13.000784	4.784681	3.475348
C	13.709938	4.375560	5.571346
H	14.370497	5.213671	5.767743
C	10.600482	1.976379	8.344525
C	11.744954	1.384245	8.919370
C	12.004377	0.045322	8.615346
H	12.893541	-0.422840	9.040733
C	11.164627	-0.712199	7.784200
C	10.032512	-0.085548	7.253774
H	9.357833	-0.658411	6.615084
C	9.717289	1.253240	7.524477
C	12.671912	2.127894	9.850326
H	12.308328	2.091326	10.888386
H	12.784188	3.186038	9.582772
H	13.666483	1.668004	9.852544
C	11.457528	-2.162480	7.505803
H	10.954394	-2.510993	6.597253
H	11.104824	-2.789228	8.338400
H	12.533946	-2.343721	7.401286
C	8.430312	1.819891	6.977661
H	8.381423	1.709719	5.887296



H	8.288146	2.878501	7.214899
H	7.569609	1.265693	7.379324
C	10.711204	6.925607	8.135375
C	11.990701	7.486563	8.325562
C	12.180379	8.811220	7.926442
H	13.162862	9.263936	8.067305
C	11.150796	9.575110	7.357907
C	9.894542	8.974700	7.198507
H	9.082677	9.551708	6.753172
C	9.640645	7.654695	7.582556
C	13.118586	6.716408	8.965864
H	12.890855	6.436471	10.005946
H	14.033359	7.317573	8.984447
H	13.334783	5.785134	8.425483
C	11.394225	10.988326	6.904056
H	11.657733	11.003099	5.835618
H	12.221624	11.453237	7.451774
H	10.499697	11.610548	7.024526
C	8.265307	7.065416	7.391254
H	7.688537	7.662472	6.676999
H	7.693404	7.050713	8.331679
H	8.300874	6.035310	7.014488
C	10.783797	4.433003	7.862694
N	10.331956	3.374451	8.642132
N	10.471989	5.568893	8.595991
N	9.341374	3.043812	10.858691
N	9.292186	6.127760	10.672747
O	8.947272	4.263932	4.678297
O	11.590179	7.163767	4.988979