Investigations on the Spin States of Two Mononuclear Iron(II) Complexes Based on N-Donor Tridentate Schiff Base Ligands Derived from Pyridine-2,6-Dicarboxaldehyde

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Supplementary Information

Table S1. Experimental and computed ^{1}H NMR shifts (in ppm vs. TMS) in free ligands L^1, L^2 and corresponding $[Fe(L^1)_2]^{2+}$ and $[Fe(L^2)_2]^{2+}$ complexes (all in CD_3CN) [a]

	H-imine	**py-3,5**	**py-4**	**CH_2**	**H-2 / H-6**	**H-3 / H-5**	**H-4**	
L^1								
Expt.	8.42	7.97	7.79	4.79	7.30	7.29	7.21	
Calcd.	8.32	8.13	7.55	4.61	6.86	7.03	6.94	
$[Fe(L^1)_2]^{2+}$								
Expt.	7.73	8.13	8.38	3.68	6.47	7.16	7.29	
Calcd.	7.10	7.74	7.90	3.45	6.00	6.94	7.00	
	H-imine	**py-3,5**	**py-4**	**CH_2**	**H-2**	**H-4**	**H-5**	**H-6**
L^2								
Expt.	8.43	8.00	7.81	4.77	7.34	7.25	7.25	7.25
Calcd.	8.30	8.13	7.56	4.56	7.00	6.87	6.95	6.77
$[Fe(L^2)_2]^{2+}$								
Expt.	7.84	8.23	8.50	3.74	6.48	7.17	7.33	6.48
Calcd.	7.23	7.67	8.06	3.50	5.98	6.97	6.82	6.17

[a] Calculations done at the TPSSh-D3(BJ)/def2-TZVP/PCM(CH_3CN) level.

Table S2. Experimental and computed ^{13}C NMR shifts (in ppm vs. TMS) in free ligands L^1, L^2 and corresponding $[Fe(L^1)_2]^{2+}$ and $[Fe(L^2)_2]^{2+}$ complexes (all in CD_3CN) [a]

	C-imine	py-2,6	py-3,5	py-4	CH_2	C-1	C-2/C-6	C-3/C-5	C-4		
L^1											
Expt.	162.4	154.6	121.8	137.5	64.3	139.3	128.5	128.2	127.1		
Calcd.	166.9	154.9	122.2	135.9	67.0	142.0	125.4	126.8	124.9		
$[Fe(L^1)_2]^{2+}$											
Expt.	170.1	160.3	128.5	137.4	62.4	133.3	128.7	129.3	129.3		
Calcd.	167.7	157.4	128.7	136.3	65.6	133.4	127.3	128.2	128.6		
	C-imine	**py-2,6**	**py-3,5**	**py-4**	**CH_2**	**C-1**	**C-2**	**C-3**	**C-4**	**C-5**	**C-6**
L^2											
Expt.	163.0	154.4	122.0	133.8	63.4	141.8	128.0	137.6	127.0	130.1	126.6
Calcd.	167.1	154.8	122.4	136.0	66.3	144.5	126.4	139.9	125.7	128.5	123.2
$[Fe(L^2)_2]^{2+}$											
Expt.	171.1	160.4	128.6	135.5	61.8	134.5	128.7	137.8	130.9	129.6	127.3
Calcd.	167.4	157.3	128.7	137.6	65.1	135.1	128.8	140.3	129.8	125.7	125.7

[a] Calculations done at the TPSSh-D3(BJ)/def2-TZVP/PCM (CH_3CN) level.

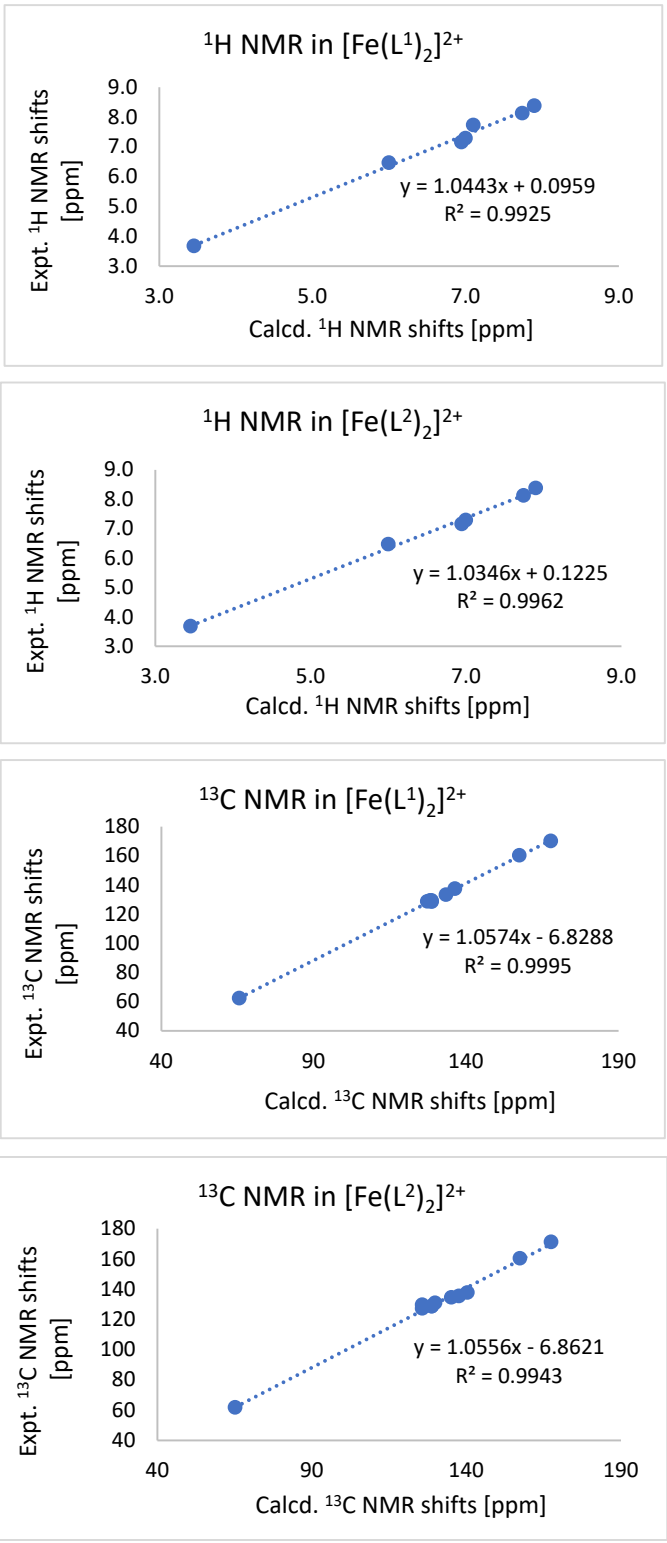
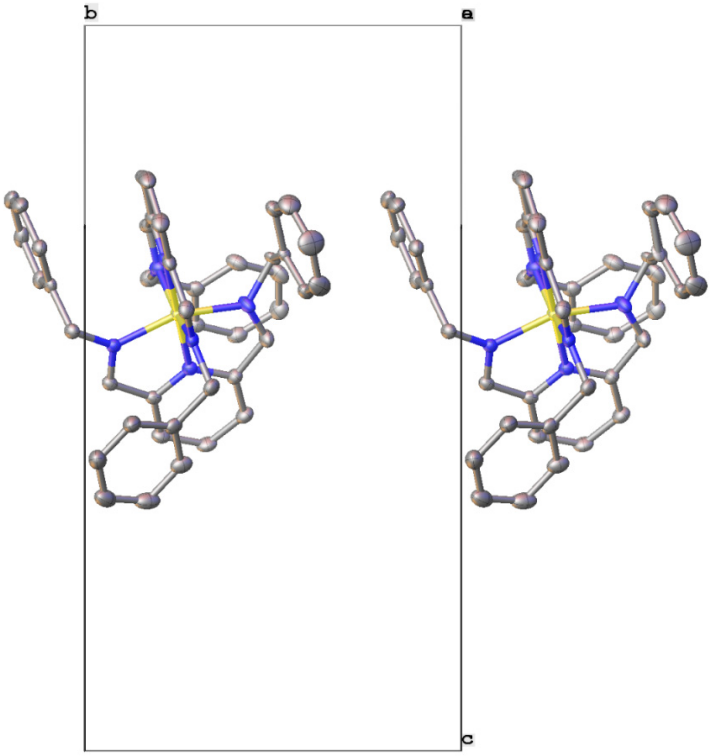
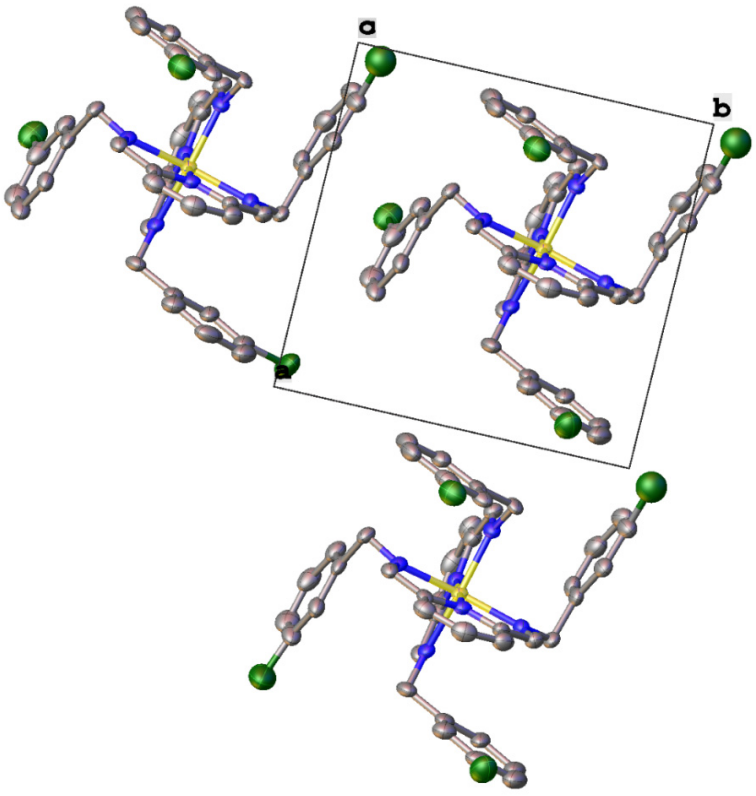


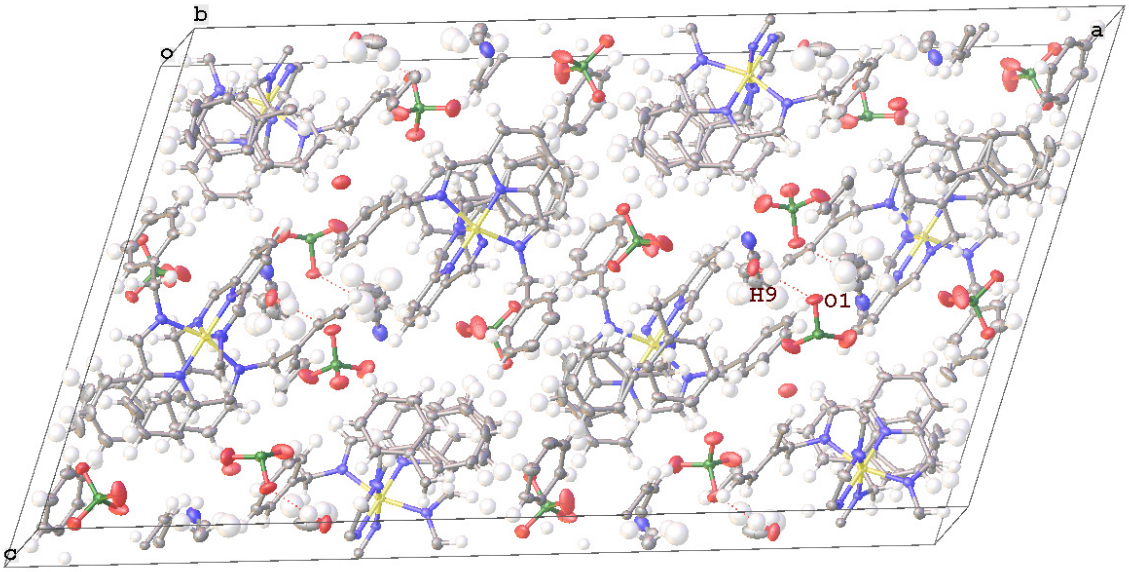
Figure S1. Comparison of calculated and experimental NMR shifts in $[FeL_2]^{2+}$ (S=0) complexes (cf. Tables S1 and S2 for numeric data)



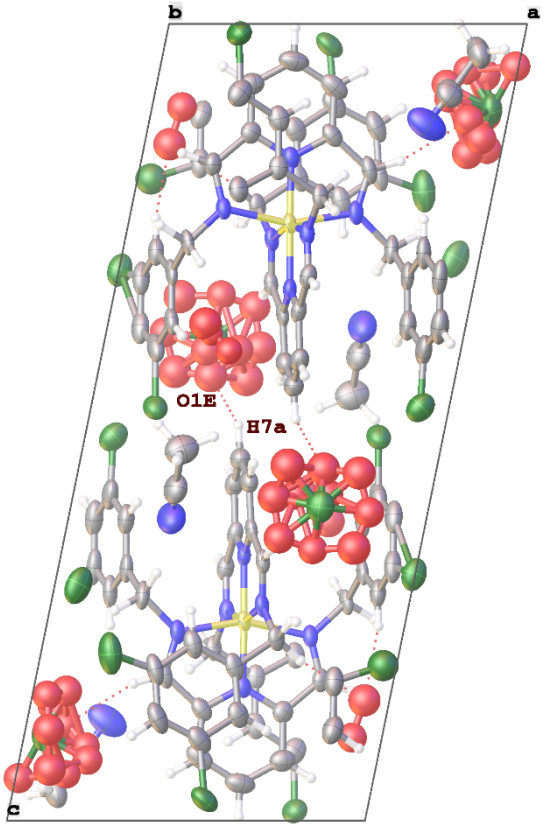
(a)



(b)



(c)

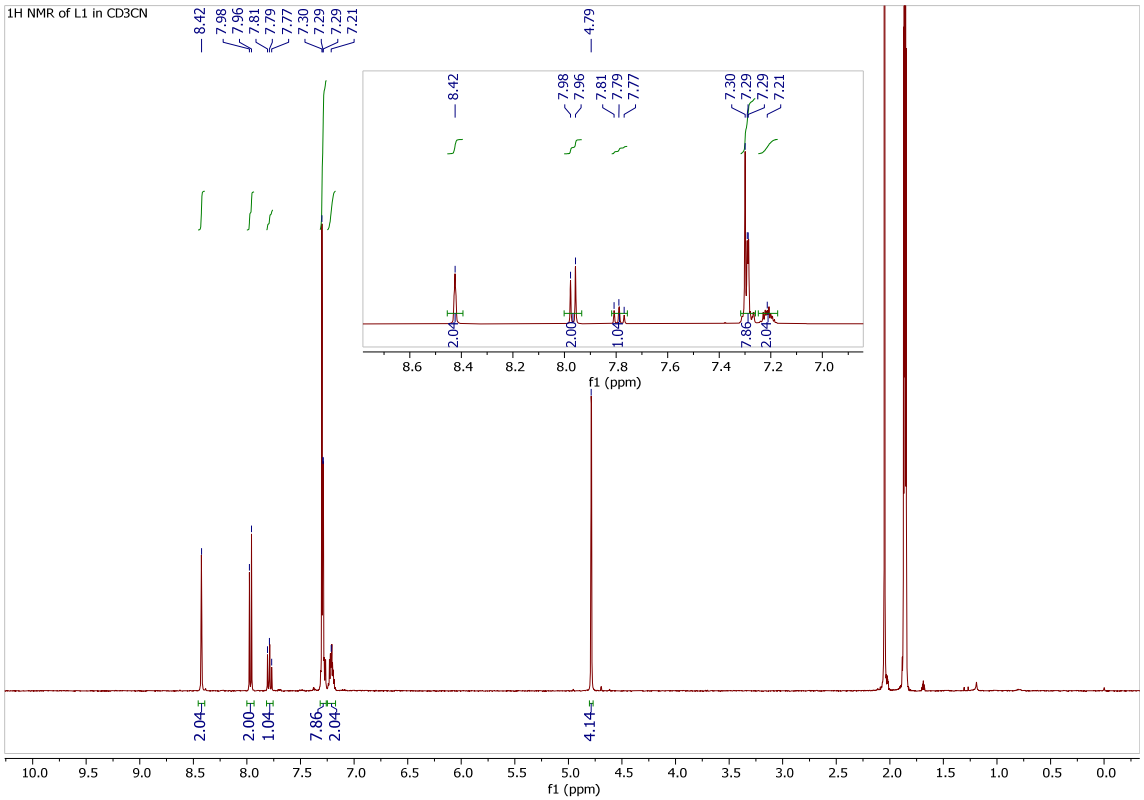


(d)

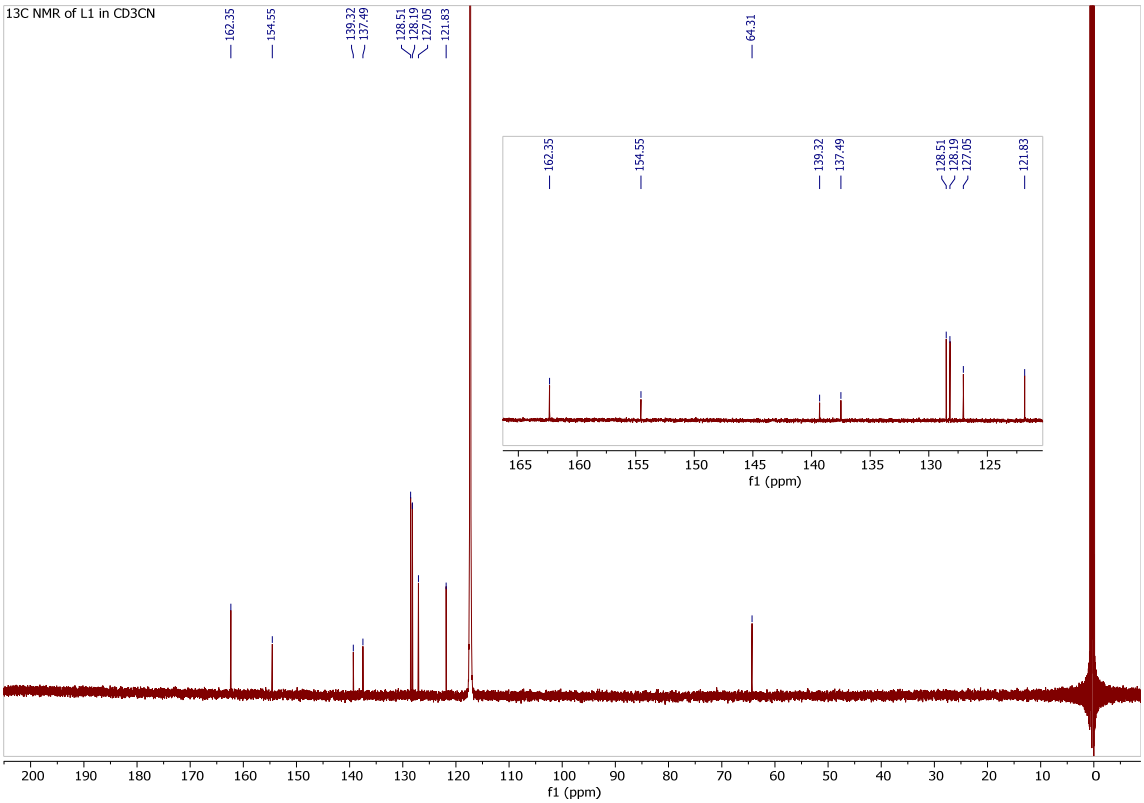
Figure S2. Projection of the π-π interaction through phenyl rings of **1** (a) along the bc plane and **2** (b) along the ab plane. ClO_4^- ions, solvents and hydrogen atoms have been omitted for clarity. Short intermolecular contacts and H-bonding **1** (c) and **2** (d) both in b-direction.

Table S3. Coordination bond angles for **1** and **2** at 120 K.

N–Fe1–N bond angles (°) at 120 K			
1		**2**	
N(2)–Fe(1)–N(5)	178.92(6)	N(5)–Fe(1)–N(5)	178.8(2)
N(2)–Fe(1)–N(3)	79.61(6)	N(5)–Fe(1)–N(4)	79.2(2)
N(5)–Fe(1)–N(3)	101.48(6)	N(2)–Fe(1)–N(4)	99.6(2)
N(2)–Fe(1)–N(4)	100.43(6)	N(2)–Fe(1)–N(3)	79.6(2)
N(5)–Fe(1)–N(4)	79.54(6)	N(5)–Fe(1)–N(3)	100.2(2)
N(3)–Fe(1)–N(4)	91.08(6)	N(4)–Fe(1)–N(6)	158.5(2)
N(2)–Fe(1)–N(6)	100.44(6)	N(5)–Fe(1)–N(1)	100.7(2)
N(5)–Fe(1)–N(6)	79.61(6)	N(5)–Fe(1)–N(6)	79.3(2)
N(3)–Fe(1)–N(6)	91.68(6)	N(3)–Fe(1)–N(6)	91.68(19)
N(4)–Fe(1)–N(6)	159.10(6)	N(4)–Fe(1)–N(1)	92.01(19)
N(2)–Fe(1)–N(1)	79.61(6)	N(2)–Fe(1)–N(6)	101.9(19)
N(5)–Fe(1)–N(1)	99.31(6)	N(2)–Fe(1)–N(1)	79.6(2)
N(3)–Fe(1)–N(1)	159.21(6)	N(4)–Fe(1)–N(3)	91.87(19)
N(4)–Fe(1)–N(1)	92.57(6)	N(6)–Fe(1)–N(1)	92.17(19)
N(6)–Fe(1)–N(1)	92.16(7)	N(3)–Fe(1)–N(1)	159.2(2)

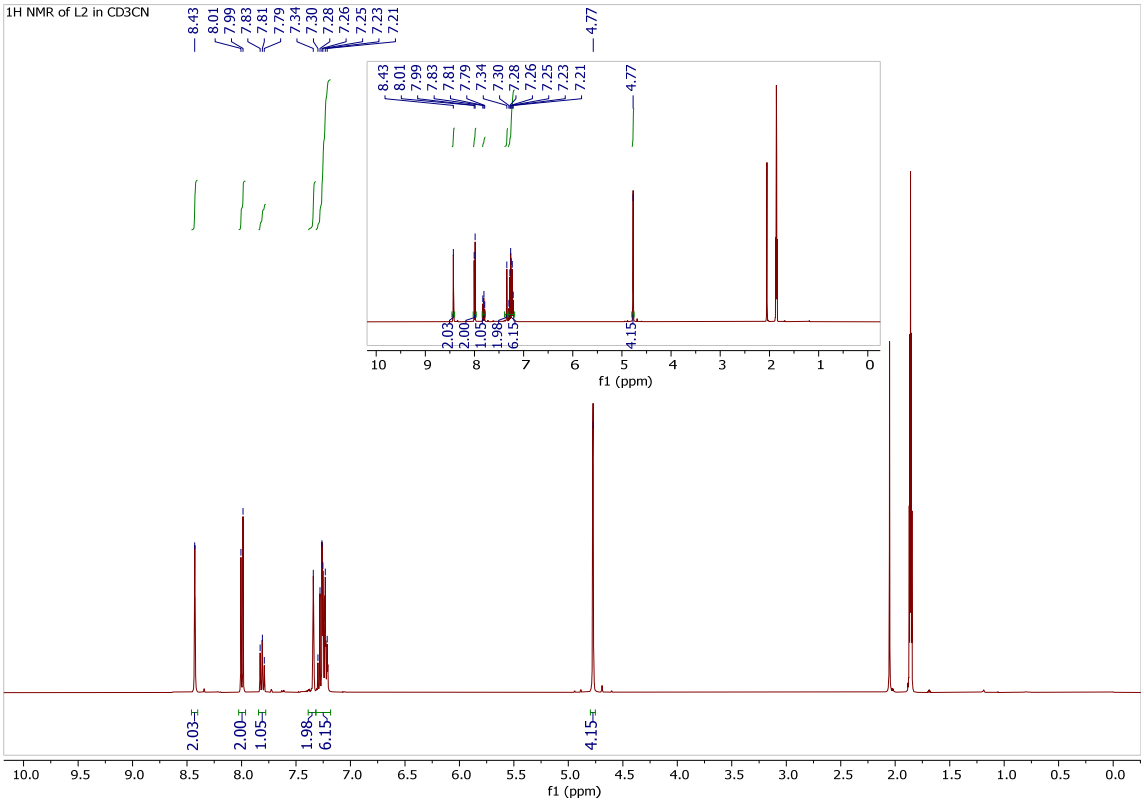


(a)

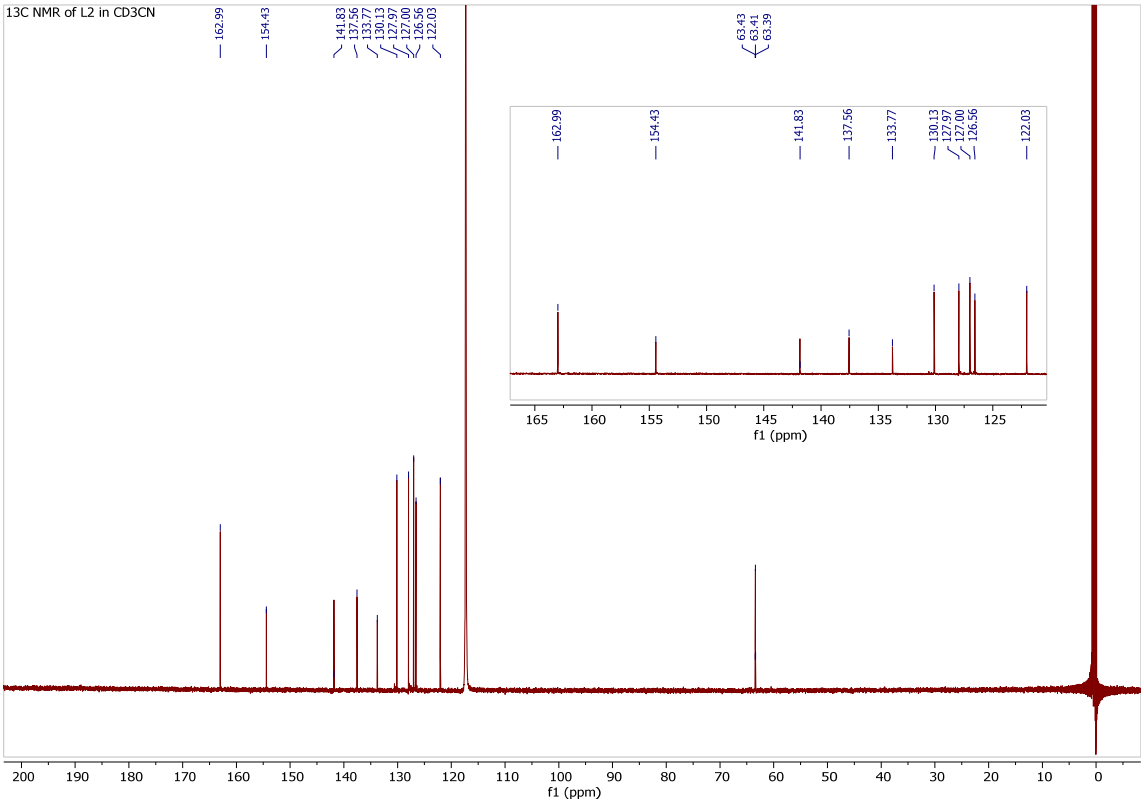


(b)

Figure S3. (a) ^{1}H NMR and (b) ^{13}C NMR of L^{1}.

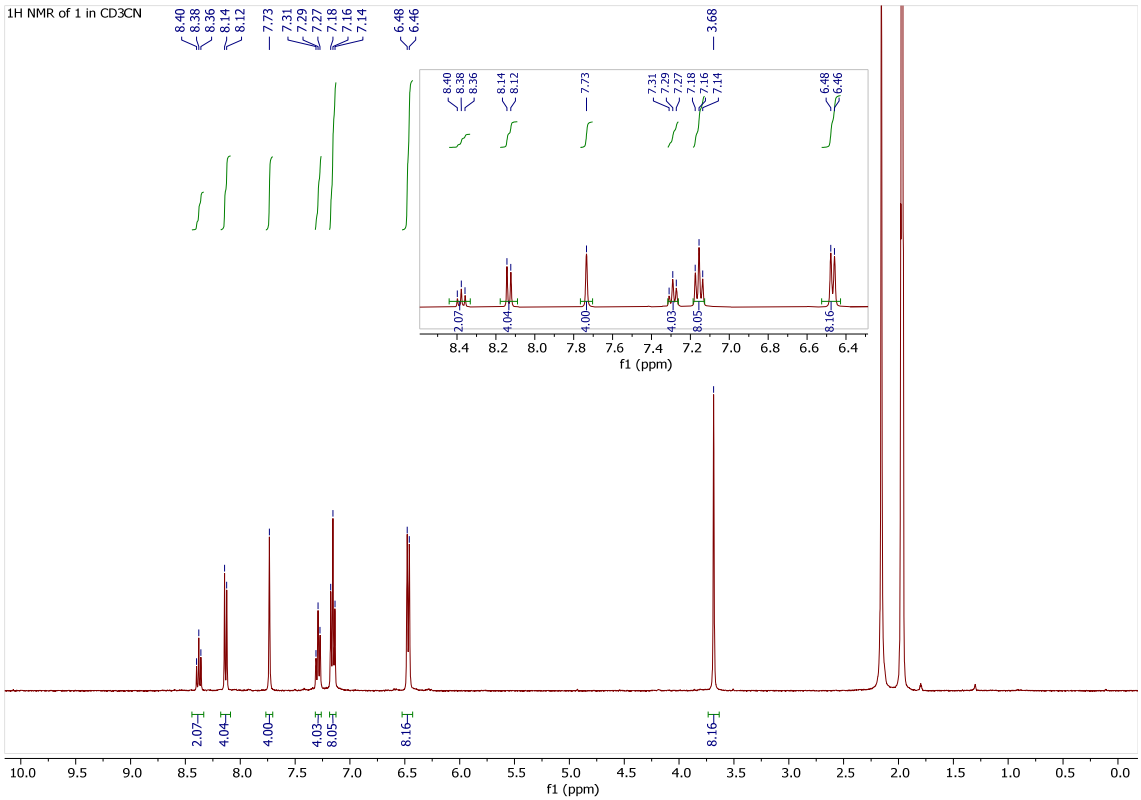


(a)

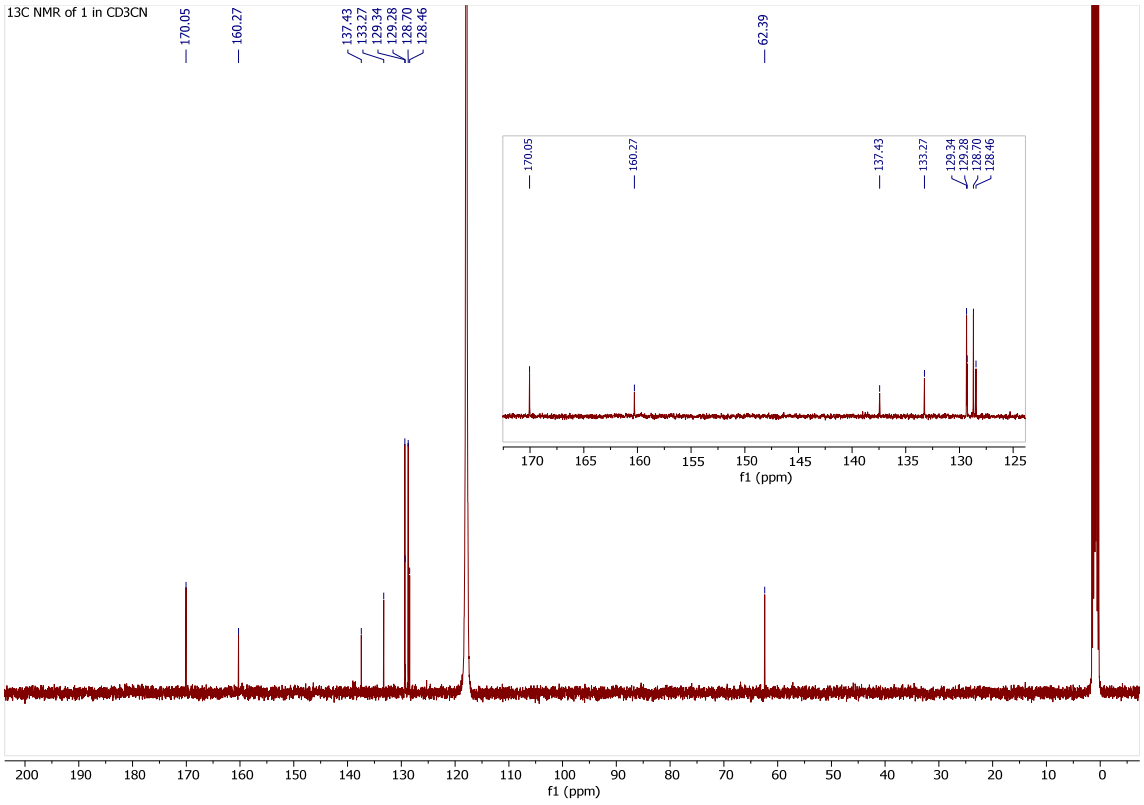


(b)

Figure S4. (a) ^{1}H NMR and (b) ^{13}C NMR of L^{2}.

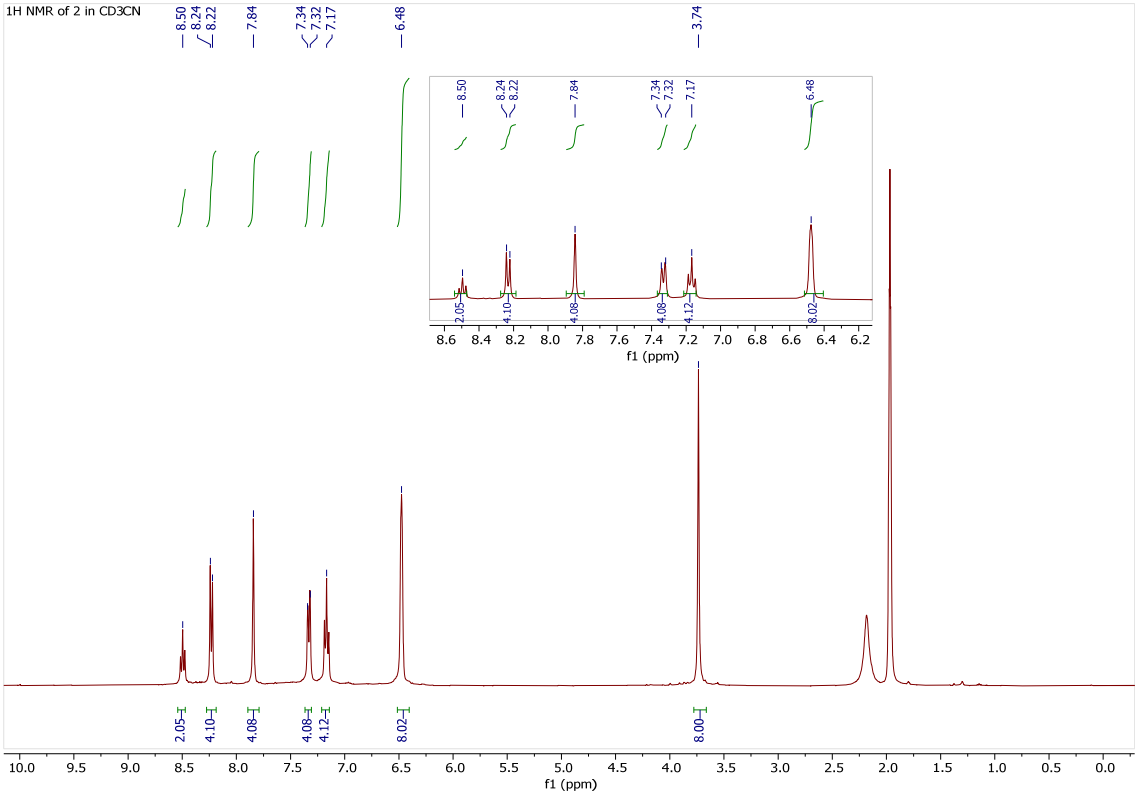


(a)

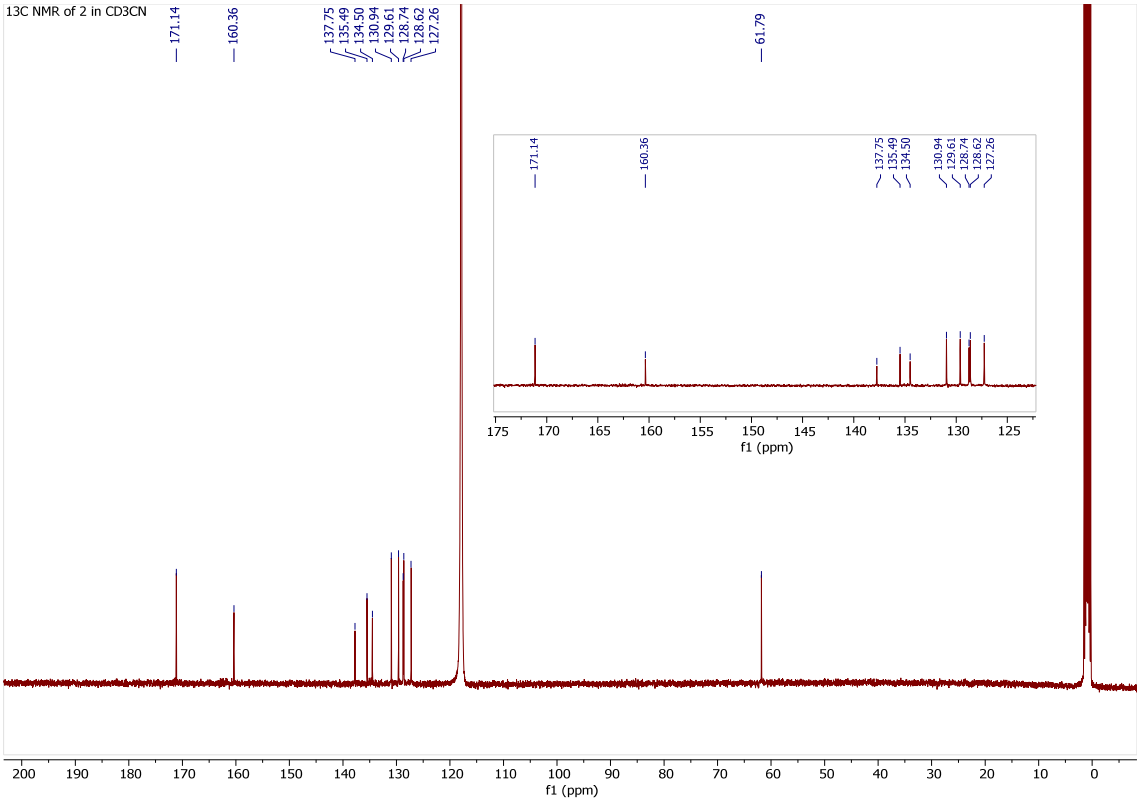


(b)

Figure S5. (a) ^{1}H NMR and (b) ^{13}C NMR of **1**.

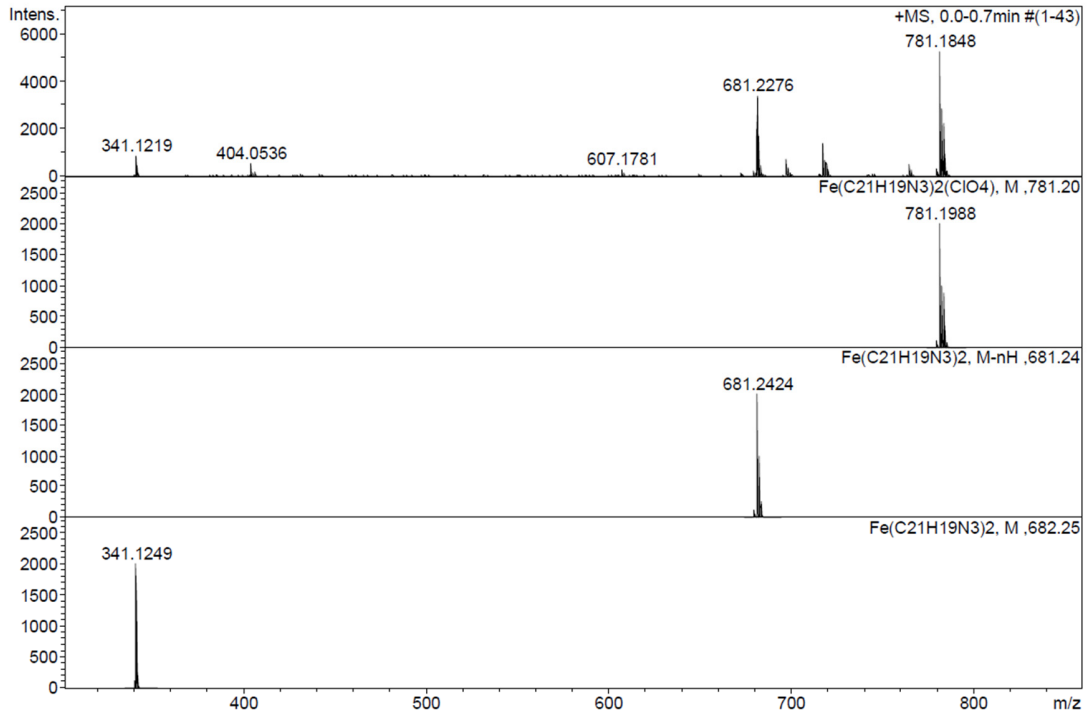


(a)

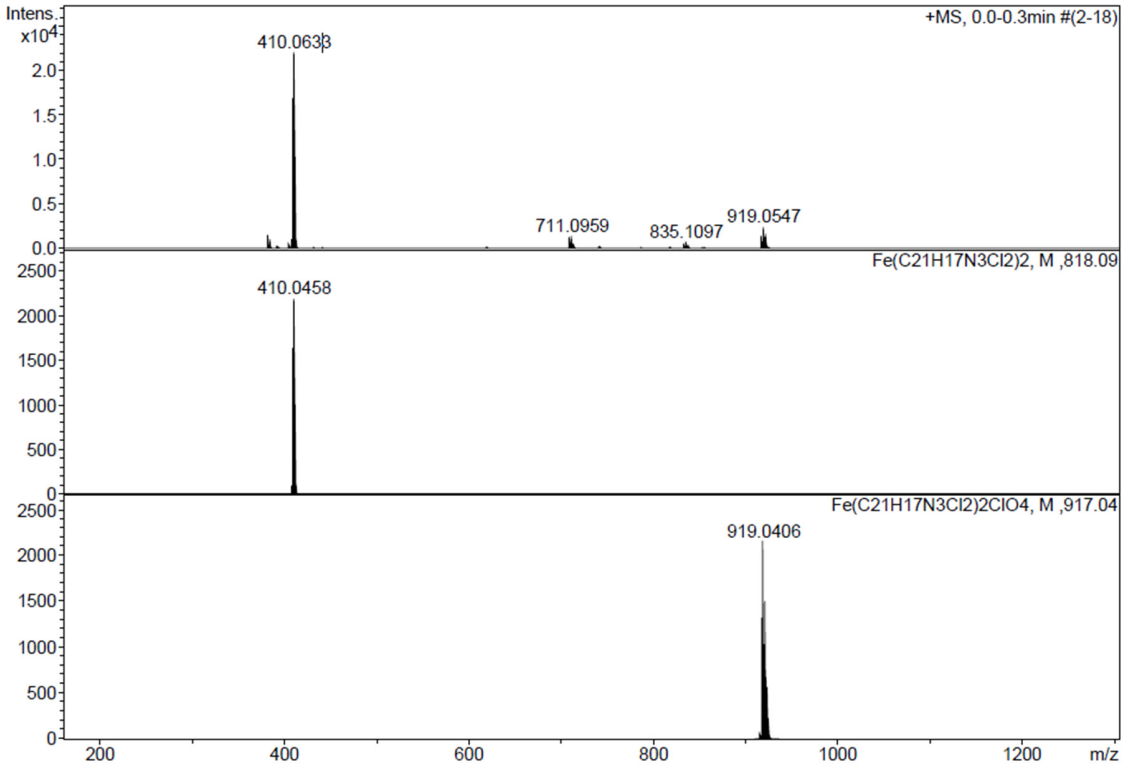


(b)

Figure S6. (a) ^{1}H NMR and (b) ^{13}C NMR of **2**.



(a)



(b)

Figure S7. ESI-MS molecular ion peaks of **1** (a) and **2** (b).

DFT optimized Cartesian coordinates of ligands (L^1, L^2) and their Fe(II) complexes ($[Fe(L^1)_2]^{2+}$, $[Fe(L^2)_2]^{2+}$) in S=0 and S=2 spin-states

TPSSh-D3(BJ)/def2-TZVP results *in vacuo*

L^1

43

Energy=-976.3794439730

N	3.48472	-0.56867	0.16722
N	0.00000	0.00000	-0.23258
N	-3.48472	0.56867	0.16722
C	1.13390	-0.18299	0.45708
C	6.64275	-2.23095	-0.90231
H	7.15958	-1.39756	-1.36808
C	4.61327	-0.75607	-0.72154
H	5.32033	0.05819	-0.53051
H	4.31292	-0.68849	-1.77998
C	-1.13390	0.18299	0.45708
C	5.32204	-2.07217	-0.48009
C	2.34392	-0.38360	-0.35808
H	2.17548	-0.36228	-1.44307
C	-6.64275	2.23095	-0.90231
H	-7.15958	1.39756	-1.36808
C	4.67521	-3.14653	0.12667
H	3.65490	-3.02713	0.47016
C	-5.32204	2.07217	-0.48009
C	-2.34392	0.38360	-0.35808
H	-2.17548	0.36228	-1.44307
C	1.18071	-0.18969	1.85357
H	2.13268	-0.34224	2.34550
C	7.30174	-3.44192	-0.73061
C	6.64848	-4.51182	-0.12515
H	7.16237	-5.45590	0.01372
C	0.00000	0.00000	2.55707
H	0.00000	0.00000	3.64084
C	-7.30174	3.44192	-0.73061
C	-1.18071	0.18969	1.85357
H	-2.13268	0.34224	2.34550
C	5.33527	-4.35883	0.30447
H	4.82066	-5.18505	0.78175
C	-4.61327	0.75607	-0.72154
H	-5.32033	-0.05819	-0.53051
H	-4.31292	0.68849	-1.77998
C	-4.67521	3.14653	0.12667
H	-3.65490	3.02713	0.47016
H	8.32788	-3.54903	-1.06339
C	-6.64848	4.51182	-0.12515
H	-7.16237	5.45590	0.01372
C	-5.33527	4.35883	0.30447
H	-4.82066	5.18505	0.78175
H	-8.32788	3.54903	-1.06339

L^2

43

Energy=-1895.641815306

N	3.48013	-0.59452	0.17739
N	0.00000	0.00000	-0.22071
N	-3.48013	0.59452	0.17739
C	1.13280	-0.18869	0.46899
C	6.62366	-2.24798	-0.95523
H	7.12489	-1.43773	-1.47152
C	4.60817	-0.77570	-0.71216
H	5.31044	0.04326	-0.52316
H	4.30921	-0.71372	-1.77096
C	-1.13280	0.18869	0.46899
C	5.32595	-2.08699	-0.46901
C	2.34146	-0.39358	-0.34702
H	2.17408	-0.35970	-1.43171
C	-6.62366	2.24798	-0.95523
H	-7.12489	1.43773	-1.47152
C	4.71203	-3.14349	0.19897
H	3.71034	-3.01560	0.58876
C	-5.32595	2.08699	-0.46901
C	-2.34146	0.39358	-0.34702
H	-2.17408	0.35970	-1.43171
C	1.17971	-0.19547	1.86549
H	2.13073	-0.35194	2.35802
C	7.27992	-3.45667	-0.77466
C	6.67625	-4.51835	-0.11062
H	7.20968	-5.45032	0.02135
C	0.00000	0.00000	2.56913

H	0.00000	0.00000	3.65284
C	-7.27992	3.45667	-0.77466
C	-1.17971	0.19547	1.86549
H	-2.13073	0.35194	2.35802
C	5.38631	-4.34762	0.37591
H	4.90353	-5.16451	0.89951
C	-4.60817	0.77570	-0.71216
H	-5.31044	-0.04326	-0.52316
H	-4.30921	0.71372	-1.77096
C	-4.71203	3.14349	0.19897
H	-3.71034	3.01560	0.58876
Cl	8.90084	-3.64347	-1.38895
C	-6.67625	4.51835	-0.11062
H	-7.20968	5.45032	0.02135
C	-5.38631	4.34762	0.37591
H	-4.90353	5.16451	0.89951
Cl	-8.90084	3.64347	-1.38895

$[Fe(L^1)_2]^{2+}$ (S=0)

87

Energy=-3216.281344199

Fe	0.00322	-0.03493	0.00687
N	1.86298	-0.47481	0.53070
N	0.19697	0.12461	-1.85804
N	-0.35243	-1.90634	-0.54638
N	-0.20577	-0.21543	1.86743
N	-1.93157	0.36403	0.18596
N	0.44600	1.89246	-0.14155
C	0.45095	1.33281	-2.39599
C	0.87116	-0.48505	2.63068
C	0.31263	-3.47971	1.24420
C	-0.78206	-3.01050	0.31705
H	-1.14131	-3.83197	-0.31105
H	-1.62711	-2.64777	0.90552
C	0.07088	-0.97209	-2.63117
C	3.61511	0.71547	-2.37002
H	3.37730	-0.13516	-3.00031
C	2.99940	-0.68363	-0.37214
H	2.66760	-1.36464	-1.15788
H	3.80666	-1.17488	0.17995
C	-1.43215	-0.08751	2.40963
C	3.47235	0.61124	-0.98861
C	0.04333	-3.65963	2.59887
H	-0.94802	-3.44293	2.98260
C	2.04664	-0.63880	1.79760
H	3.01152	-0.92154	2.20866
C	-0.26232	-2.12223	-1.81594
H	-0.47184	-3.09501	-2.25145
C	-3.49038	-1.51111	-1.54523
H	-3.58766	-1.76690	-0.49584
C	3.80493	1.70146	-0.18351
H	3.72294	1.62470	0.89547
C	-3.10069	-0.22396	-1.91584
C	-2.39449	0.27341	1.38775
H	-3.42785	0.50869	1.62659
C	0.74868	-0.62702	4.00904
H	1.61865	-0.84402	4.61464
C	4.07016	1.89852	-2.94395
C	0.60858	2.32188	-1.34810
H	0.89532	3.34788	-1.56143
C	0.45609	0.35900	-4.58283
H	0.55647	0.45154	-5.65648
C	1.03325	-4.12464	3.45861
C	1.58280	-3.78505	0.75425
H	1.79795	-3.67406	-0.30309
C	0.20663	-0.88783	-4.01298
H	0.10137	-1.77253	-4.62671
C	4.38060	2.98897	-2.13761
H	4.74275	3.90794	-2.58199
C	-0.51599	-0.50822	4.58093
H	-0.63835	-0.62381	5.65011
C	-3.76451	-2.46939	-2.51362
C	0.65616	2.82614	0.96912
H	1.14112	3.72983	0.58772
H	1.34327	2.34683	1.66864
C	-1.62327	-0.24169	3.77930
H	-2.61157	-0.13618	4.20740
C	4.25218	2.88670	-0.75364
H	4.51839	3.72470	-0.12090
C	-2.82845	0.83368	-0.87396
H	-2.34251	1.69138	-1.34301
H	-3.75951	1.18807	-0.42035

C	0.57631	1.48580	-3.77355
H	0.78101	2.46007	-4.19754
C	2.30475	-4.40596	2.96866
H	3.07488	-4.77433	3.63518
C	2.57682	-4.24009	1.61210
H	3.55774	-4.48411	1.22226
C	-3.01435	0.09857	-3.26850
H	-2.73243	1.10349	-3.56426
H	4.19335	1.96498	-4.01824
C	-3.66415	-2.14401	-3.86474
H	-3.89280	-2.88624	-4.61974
C	-0.74158	3.00630	3.05289
H	0.11131	2.64684	3.61911
C	-0.63856	3.15579	1.67226
C	-3.29858	-0.85528	-4.24025
H	-3.24329	-0.59023	-5.28917
C	-1.92584	3.32540	3.70980
C	-3.01925	3.79086	2.98660
H	-3.93973	4.04643	3.49699
H	-4.07643	-3.46375	-2.21728
H	0.80962	-4.27593	4.50780
C	-1.73098	3.64554	0.95552
H	-1.65425	3.79509	-0.11636
H	-1.99118	3.22117	4.78615
C	-2.91783	3.95656	1.60662
H	-3.75776	4.34606	1.04398

$[Fe(L^1)_2]^{2+}$ (S=2)

87

Energy=-3216.252383354

Fe	-0.00970	-0.06241	-0.01394
N	1.97281	-0.63705	0.82259
N	0.26706	0.20750	-2.09036
N	-0.44364	-2.02128	-0.97164
N	-0.25791	-0.19131	2.08937
N	-2.12658	0.46844	0.40509
N	0.58914	2.03204	-0.28628
C	0.62531	1.40979	-2.54943
C	0.78249	-0.53285	2.85330
C	0.25123	-3.60525	0.74450
C	-0.82755	-3.23132	-0.24348
H	-1.02764	-4.04661	-0.94577
H	-1.75360	-3.00740	0.28875
C	0.08719	-0.82159	-2.92537
C	3.72061	0.53327	-2.00139
H	3.50420	-0.33775	-2.61114
C	3.19477	-0.84413	0.04356
H	2.97134	-1.59035	-0.72001
H	3.98776	-1.24165	0.68574
C	-1.46049	0.03845	2.62170
C	3.61792	0.44747	-0.61528
C	-0.01582	-3.62234	2.11105
H	-1.01122	-3.37856	2.46687
C	2.01532	-0.77400	2.09108
H	2.92142	-1.06786	2.61989
C	-0.32193	-2.05662	-2.24102
H	-0.51605	-2.95602	-2.82455
C	-3.78136	-1.51746	-1.14459
H	-4.00185	-1.66778	-0.09282
C	3.92620	1.56535	0.16199
H	3.87430	1.50241	1.24394
C	-3.32335	-0.27480	-1.58722
C	-2.47373	0.42985	1.63313
H	-3.47660	0.69044	1.96924
C	0.65410	-0.64727	4.23486
H	1.50641	-0.91601	4.84565
C	4.11545	1.72313	-2.60610
C	0.81194	2.40113	-1.49198
H	1.14851	3.40522	-1.74541
C	0.63166	0.57118	-4.79061
H	0.77366	0.71308	-5.85465
C	0.98094	-3.96841	3.01864
C	1.52700	-3.95120	0.29398
H	1.73724	-3.96909	-0.77040
C	0.27242	-0.68312	-4.29485
H	0.12779	-1.52659	-4.95748
C	4.40460	2.83880	-1.82623
H	4.72397	3.76177	-2.29485
C	-0.59780	-0.42469	4.80281
H	-0.73158	-0.51664	5.87350
C	-3.97362	-2.55929	-2.04263
C	0.76623	3.01005	0.78880

H	1.23433	3.91866	0.39624
H	1.44635	2.57018	1.52058
C	-1.67607	-0.08138	3.99238
H	-2.65614	0.10494	4.41245
C	4.31404	2.75620	-0.43798
H	4.56427	3.61445	0.17379
C	-3.11440	0.85216	-0.60388
H	-2.71886	1.72602	-1.12463
H	-4.05494	1.14009	-0.12276
C	0.80739	1.63493	-3.91521
H	1.09185	2.61559	-4.27421
C	2.25564	-4.29437	2.56401
H	3.02783	-4.57828	3.26874
C	2.52582	-4.29094	1.19692
H	3.50814	-4.57270	0.83756
C	-3.07904	-0.08428	-2.94489
H	-2.74530	0.88506	-3.29983
H	4.21235	1.77445	-3.68397
C	-3.71397	-2.36627	-3.39799
H	-3.87997	-3.17246	-4.10222
C	-0.71509	3.15728	2.82233
H	0.12165	2.81424	3.42224
C	-0.55714	3.31919	1.44839
C	-3.27505	-1.12455	-3.84854
H	-3.10186	-0.96131	-4.90569
C	-1.93320	3.44503	3.43131
C	-3.00553	3.89446	2.66668
H	-3.95090	4.12915	3.14056
H	-4.34320	-3.51547	-1.69226
H	0.75821	-4.00117	4.07850
C	-1.63078	3.78988	0.69089
H	-1.51216	3.94503	-0.37647
H	-2.04060	3.33289	4.50371
C	-2.84947	4.07324	1.29373
H	-3.67318	4.44939	0.69898

$[Fe(L^2)_2]^{2+}$ (S=0)

87

Energy=-5054.80772407

Fe	-0.03229	-0.06379	0.04053
N	1.81666	-0.52684	0.60946
N	0.15040	0.07141	-1.83013
N	-0.38465	-1.94935	-0.49066
N	-0.27218	-0.21292	1.90364
N	-1.96646	0.38428	0.19037
N	0.44617	1.85771	-0.13832
C	0.40552	1.27158	-2.38654
C	0.78822	-0.47402	2.69211
C	0.40753	-3.52166	1.22960
C	-0.75821	-3.06803	0.38431
H	-1.14280	-3.88773	-0.22938
H	-1.56773	-2.72348	1.02961
C	-0.00758	-1.02880	-2.59142
C	3.47111	0.62151	-2.29852
H	3.18354	-0.21715	-2.92091
C	2.97027	-0.76095	-0.26634
H	2.65730	-1.46952	-1.03383
H	3.77345	-1.22401	0.31441
C	-1.50643	-0.06680	2.42491
C	3.43538	0.52229	-0.91161
C	0.27801	-3.55780	2.61366
H	-0.65448	-3.27918	3.08880
C	1.97626	-0.66019	1.88308
H	2.93039	-0.94411	2.31834
C	-0.31942	-2.17335	-1.76024
H	-0.52469	-3.15309	-2.18301
C	-3.29622	-1.43092	-1.68805
H	-3.30052	-1.78379	-0.66510
C	3.83517	1.60702	-0.13082
H	3.83416	1.52999	0.95068
C	-3.07392	-0.08832	-1.98027
C	-2.44687	0.30280	1.38678
H	-3.47878	0.55838	1.61159
C	0.64319	-0.58173	4.07223
H	1.50031	-0.78993	4.69846
C	3.88196	1.81053	-2.89316
C	0.59476	2.26954	-1.35324
H	0.88915	3.28952	-1.58469
C	0.34893	0.28001	-4.56384
H	0.43340	0.36197	-5.63946
C	1.35734	-3.95515	3.39661
C	1.60884	-3.91297	0.63825

H	1.71127	-3.91285	-0.44116
C	0.09475	-0.95779	-3.97710
H	-0.03226	-1.84729	-4.57966
C	4.26640	2.90286	-2.12284
H	4.59330	3.81624	-2.60219
C	-0.63060	-0.45154	4.61983
H	-0.77162	-0.54438	5.68843
C	-3.49550	-2.33640	-2.72267
C	0.67617	2.80809	0.95499
H	1.17241	3.69836	0.55798
H	1.35477	2.33145	1.66373
C	-1.72322	-0.19959	3.79334
H	-2.71694	-0.08104	4.20444
C	4.24869	2.78749	-0.73544
H	4.57329	3.62413	-0.12887
C	-2.83608	0.90422	-0.86940
H	-2.34256	1.78970	-1.27546
H	-3.78271	1.23130	-0.42718
C	0.50086	1.41209	-3.76786
H	0.71388	2.37757	-4.20671
C	2.56489	-4.32966	2.81702
H	3.39080	-4.64579	3.44054
C	2.67777	-4.31532	1.42949
H	3.60556	-4.63259	0.96911
C	-3.10585	0.34199	-3.30540
H	-2.94889	1.38902	-3.53846
Cl	3.89829	1.92615	-4.62161
C	-3.53071	-1.91756	-4.04919
H	-3.70770	-2.63422	-4.84036
C	-0.75209	2.94738	3.01301
H	0.06461	2.52975	3.58875
C	-0.61697	3.16895	1.64668
C	-3.34957	-0.56750	-4.32926
H	-3.39225	-0.22750	-5.35660
C	-1.94712	3.26979	3.64844
C	-3.01175	3.81599	2.93997
H	-3.93123	4.06827	3.45165
Cl	-3.67411	-4.01921	-2.34069
Cl	1.18794	-3.96224	5.12056
C	-1.67260	3.73536	0.93202
H	-1.56584	3.94055	-0.12748
Cl	-2.10617	2.96992	5.34698
C	-2.86069	4.05528	1.57693
H	-3.67483	4.50759	1.02380

$[Fe(L^2)_2]^{2+}$ (S=2)

87

Energy=-5054.772987622

Fe	0.00207	-0.04870	-0.02106
N	1.97871	-0.62672	0.83588
N	0.25548	0.20537	-2.09984
N	-0.42170	-2.02930	-0.96390
N	-0.27465	-0.19063	2.07138
N	-2.11769	0.50913	0.37310
N	0.59928	2.04407	-0.31045
C	0.60635	1.40721	-2.57113
C	0.75452	-0.53934	2.84907
C	0.27685	-3.61072	0.75586
C	-0.80106	-3.24025	-0.23477
H	-0.99699	-4.05959	-0.93281
H	-1.73006	-3.02330	0.29506
C	0.07151	-0.82765	-2.92789
C	3.68922	0.52399	-1.99079
H	3.46214	-0.34447	-2.59711
C	3.21288	-0.82749	0.07494
H	3.01164	-1.59091	-0.67751
H	4.00727	-1.19737	0.73152
C	-1.48299	0.04006	2.59192
C	3.62374	0.45891	-0.60221
C	-0.00454	-3.62434	2.11861
H	-0.99686	-3.38576	2.48108
C	1.99911	-0.77229	2.10452
H	2.89764	-1.06508	2.64725
C	-0.32048	-2.06340	-2.23522
H	-0.51967	-2.96412	-2.81543
C	-3.67834	-1.47710	-1.16504
H	-3.83434	-1.65553	-0.10809
C	3.95005	1.58318	0.15697
H	3.92636	1.53184	1.23980
C	-3.30529	-0.21594	-1.62892
C	-2.48098	0.44947	1.59650
H	-3.48837	0.70484	1.92380

C	0.60858	-0.65998	4.22822
H	1.45085	-0.93329	4.84964
C	4.07094	1.71269	-2.60582
C	0.80082	2.40585	-1.52280
H	1.12422	3.41124	-1.78893
C	0.59511	0.55492	-4.80698
H	0.73412	0.69081	-5.87195
C	0.99500	-3.97226	3.02245
C	1.55437	-3.95492	0.31141
H	1.77088	-3.97513	-0.75090
C	0.24322	-0.69591	-4.30080
H	0.09745	-1.54445	-4.95675
C	4.38249	2.84275	-1.85669
H	4.69023	3.75399	-2.35262
C	-0.65110	-0.44169	4.78074
H	-0.79909	-0.54084	5.84840
C	-3.85348	-2.51906	-2.06570
C	0.78246	3.03206	0.75481
H	1.23268	3.94431	0.35051
H	1.47660	2.60564	1.48081
C	-1.71797	-0.09304	3.95884
H	-2.70180	0.09208	4.36888
C	4.32486	2.76560	-0.46801
H	4.59277	3.63243	0.12366
C	-3.09195	0.90806	-0.64193
H	-2.68414	1.77698	-1.16101
H	-4.03495	1.20458	-0.17048
C	0.77405	1.62539	-3.93930
H	1.05648	2.60234	-4.30831
C	2.27650	-4.29848	2.58872
H	3.03585	-4.57994	3.30649
C	2.54570	-4.29439	1.22313
H	3.53160	-4.57749	0.87513
C	-3.13905	-0.00677	-2.99513
H	-2.86306	0.97548	-3.36155
Cl	4.16775	1.77788	-4.33561
C	-3.68718	-2.31955	-3.43435
H	-3.84718	-3.13815	-4.12381
C	-0.68312	3.11359	2.79484
H	0.14313	2.73997	3.38772
C	-0.53584	3.33323	1.42898
C	-3.33954	-1.05312	-3.89104
H	-3.23164	-0.88305	-4.95555
C	-1.90111	3.38991	3.40914
C	-2.97955	3.88033	2.68003
H	-3.91540	4.09966	3.17711
Cl	-4.27045	-4.09179	-1.47053
Cl	0.62928	-4.01218	4.71615
C	-1.60691	3.84256	0.69433
H	-1.49215	4.04052	-0.36568
Cl	-2.06944	3.11847	5.11262
C	-2.81859	4.11269	1.31722
H	-3.64409	4.52140	0.74719