SUPPORTING INFORMATION

2,2'-Pyridylpyrrolide ligand redistribution following Reduction

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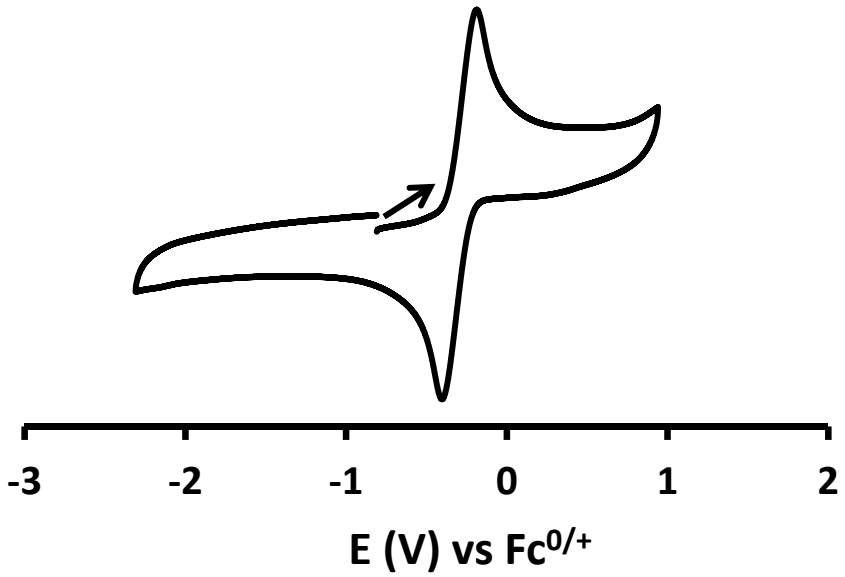


Figure 1. Cyclic voltammogram of $[KFe(L^2)_3]_2$ in THF/0.1M Bu_4NPF_6 100 mV/s scan rate at room temp.

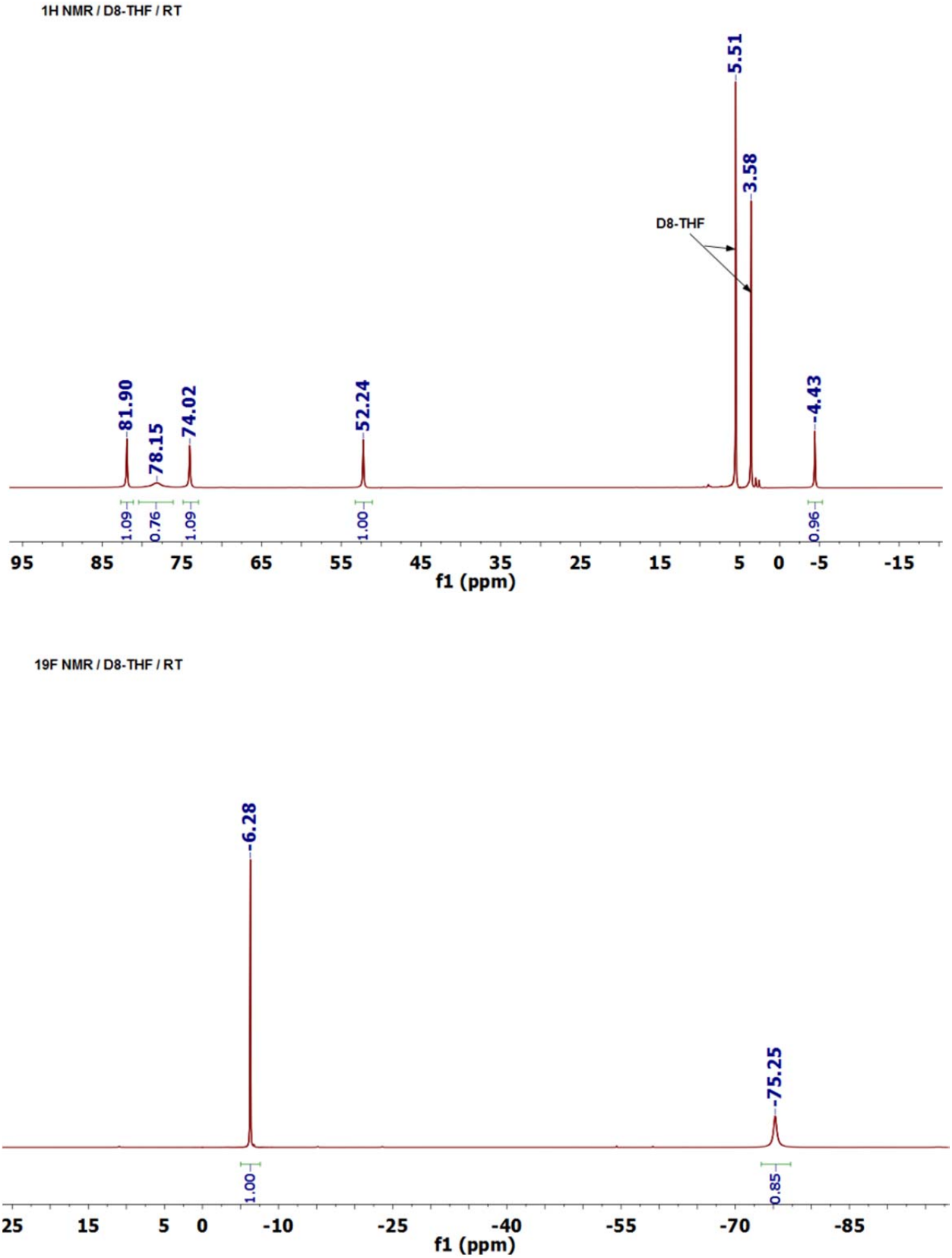


Figure 2. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of $Fe(L^2)_2(THF)$ in D8-THF.

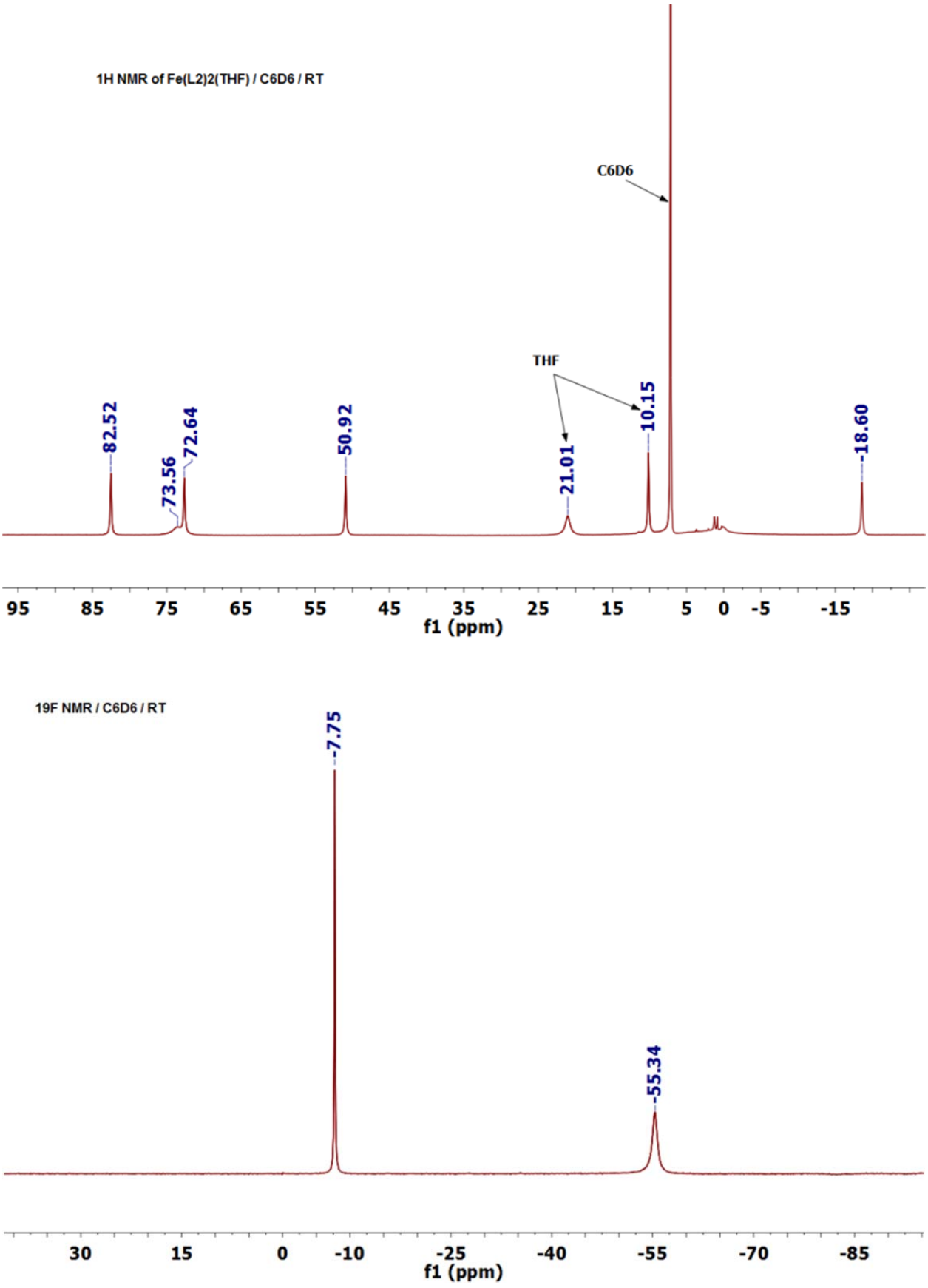


Figure 3. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of $Fe(L^2)_2(THF)$ in C_6D_6.

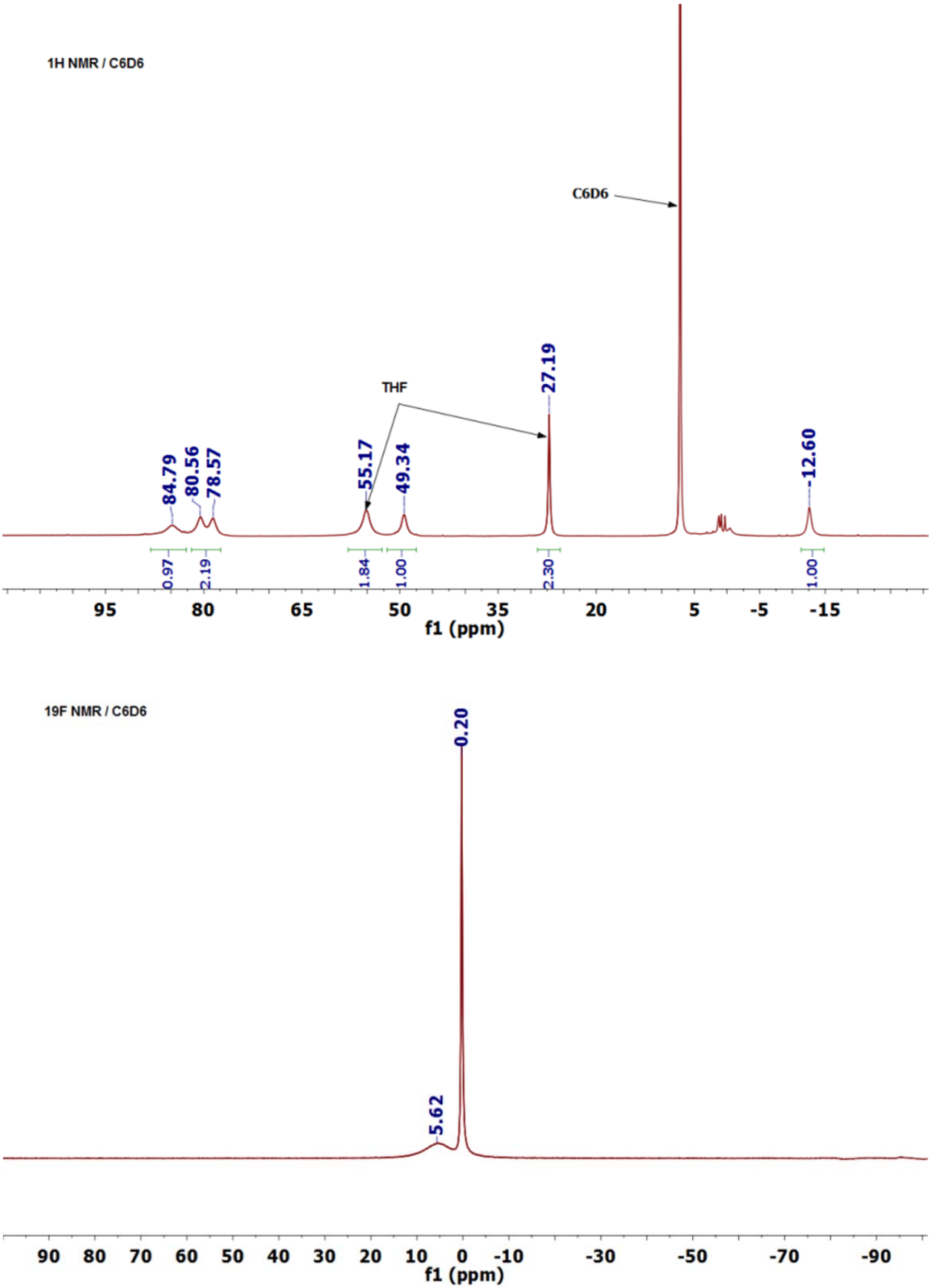


Figure 4. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of $[Fe(L^{2})_{2}]_{2}$THF in C_6D_6.

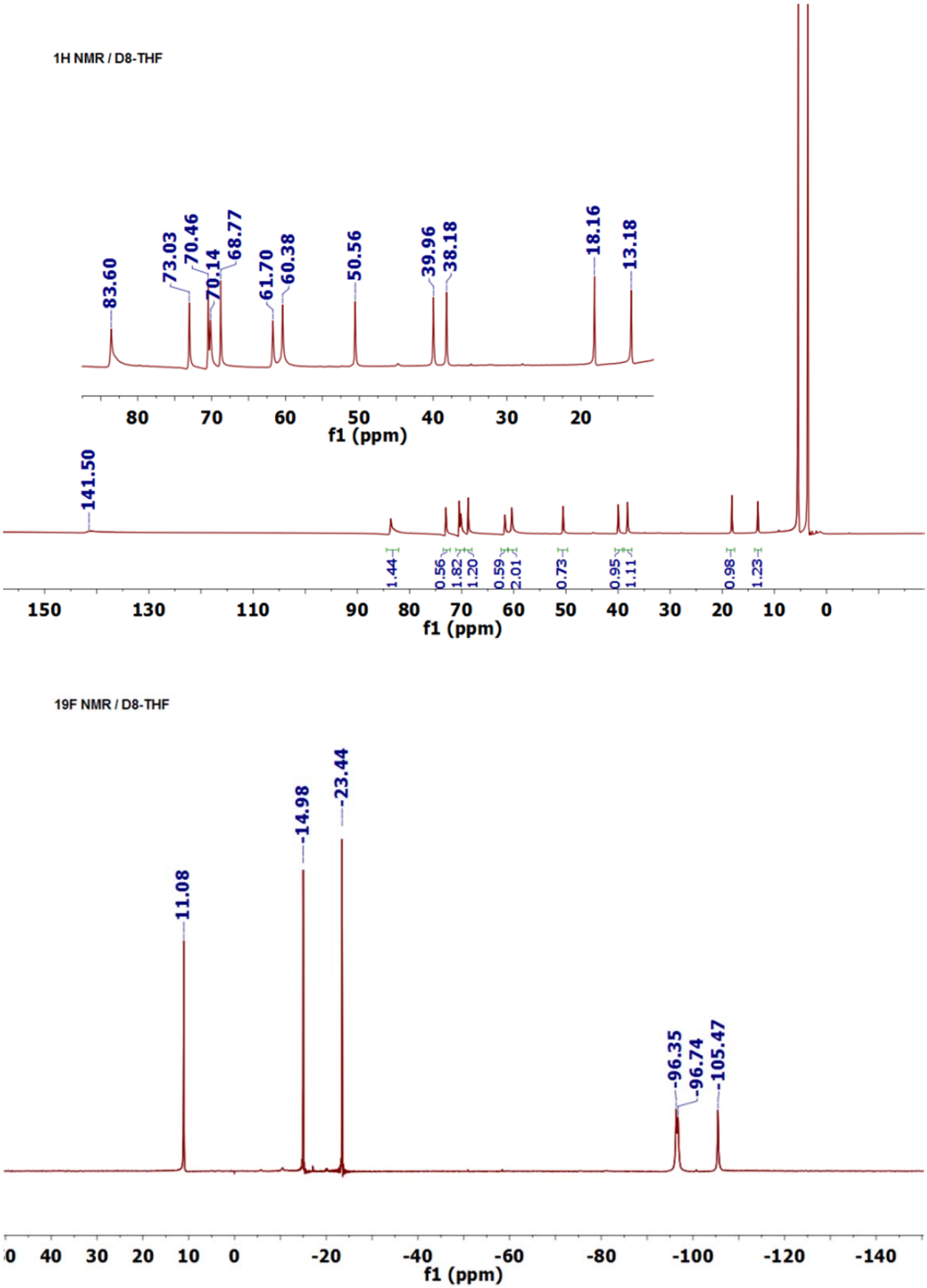


Figure 5. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of $KFe(L^2)_3$ in D8-THF.

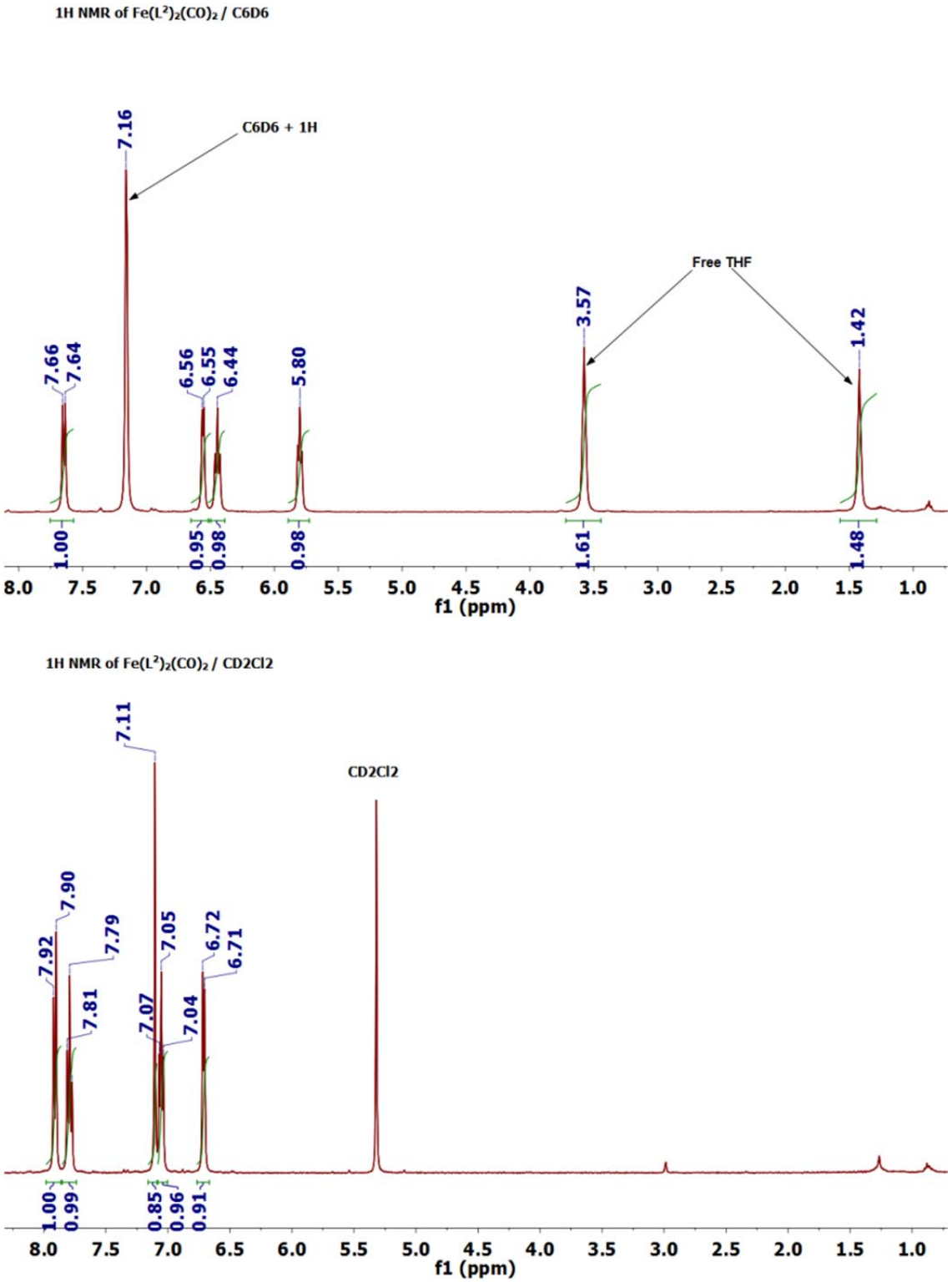


Figure 6. ^{1}H NMR spectra of $Fe(L^{2})_2(CO)_2$ in C_6D_6 (top, as formed, by displacement of THF) and CD_2Cl_2 (bottom).

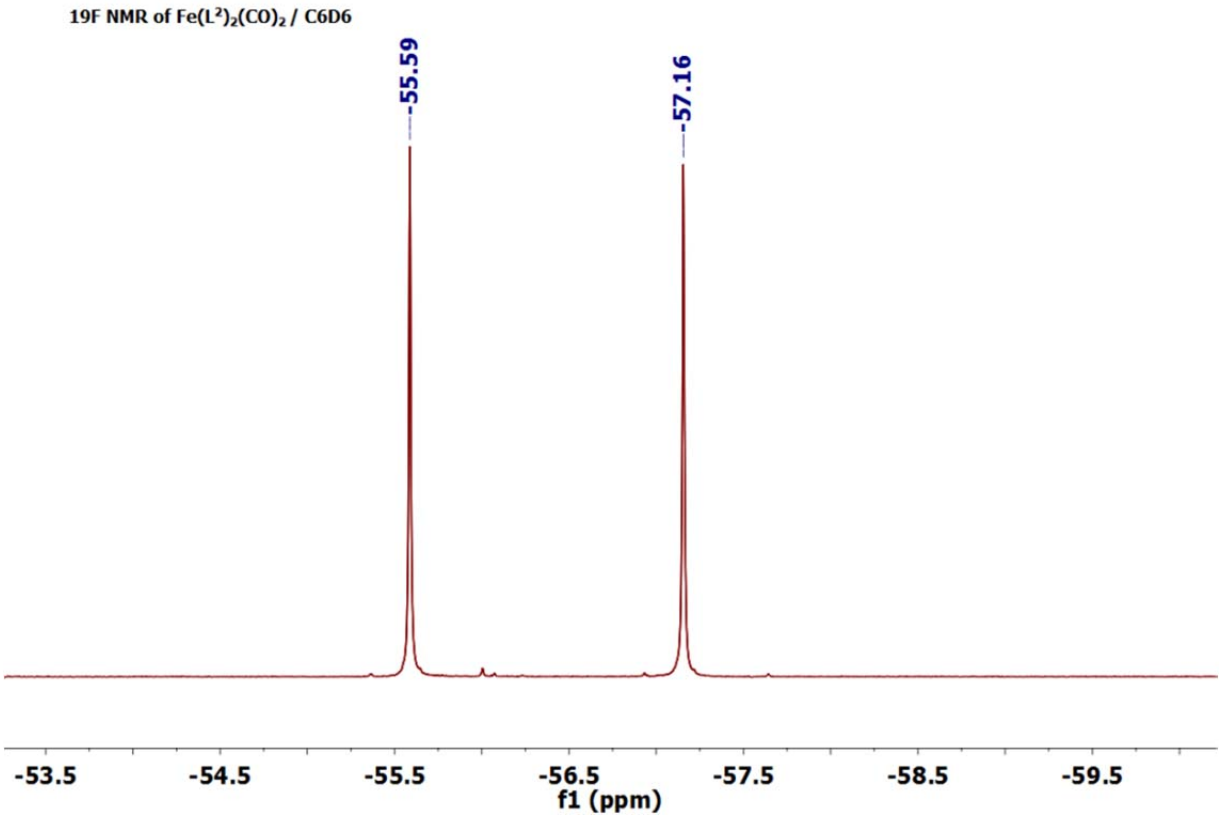


Figure 7. ^{19}F NMR spectra of $Fe(L^2)_2(CO)_2$ in C_6D_6.

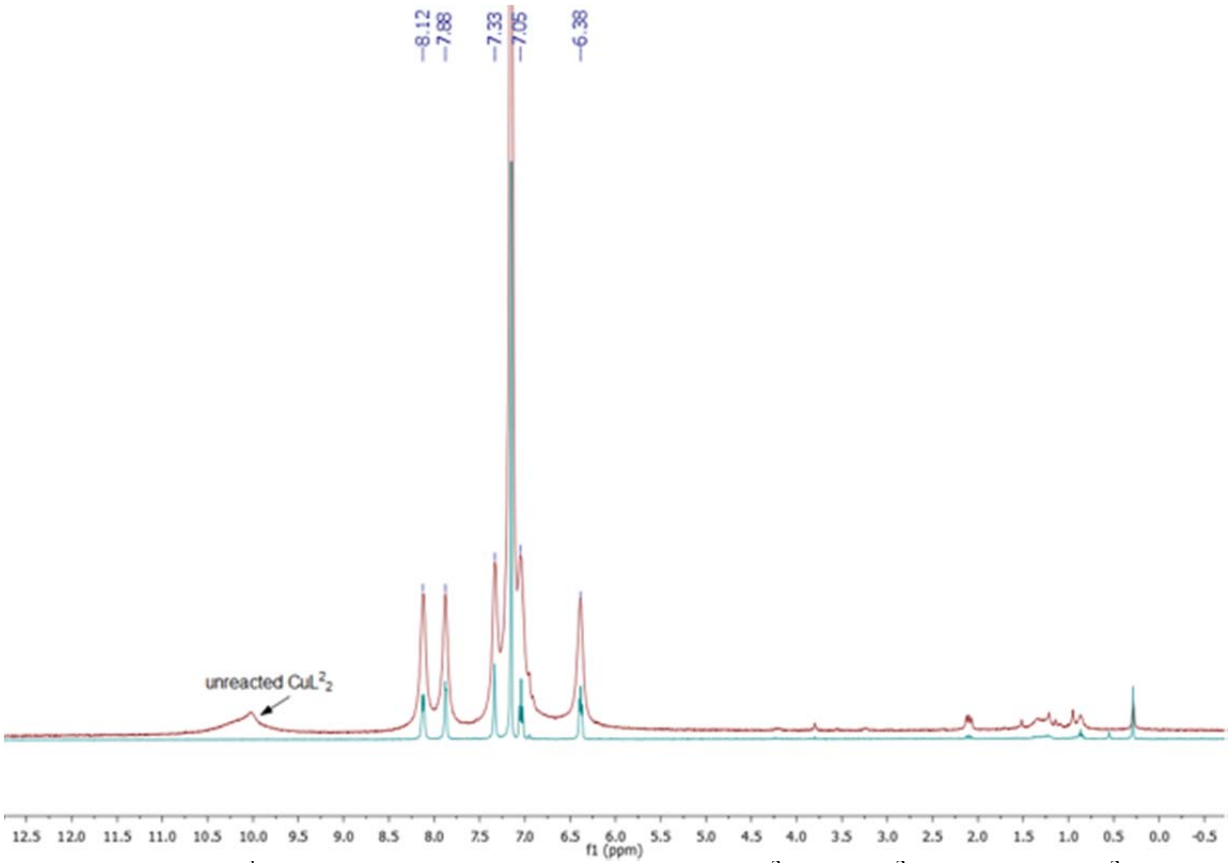
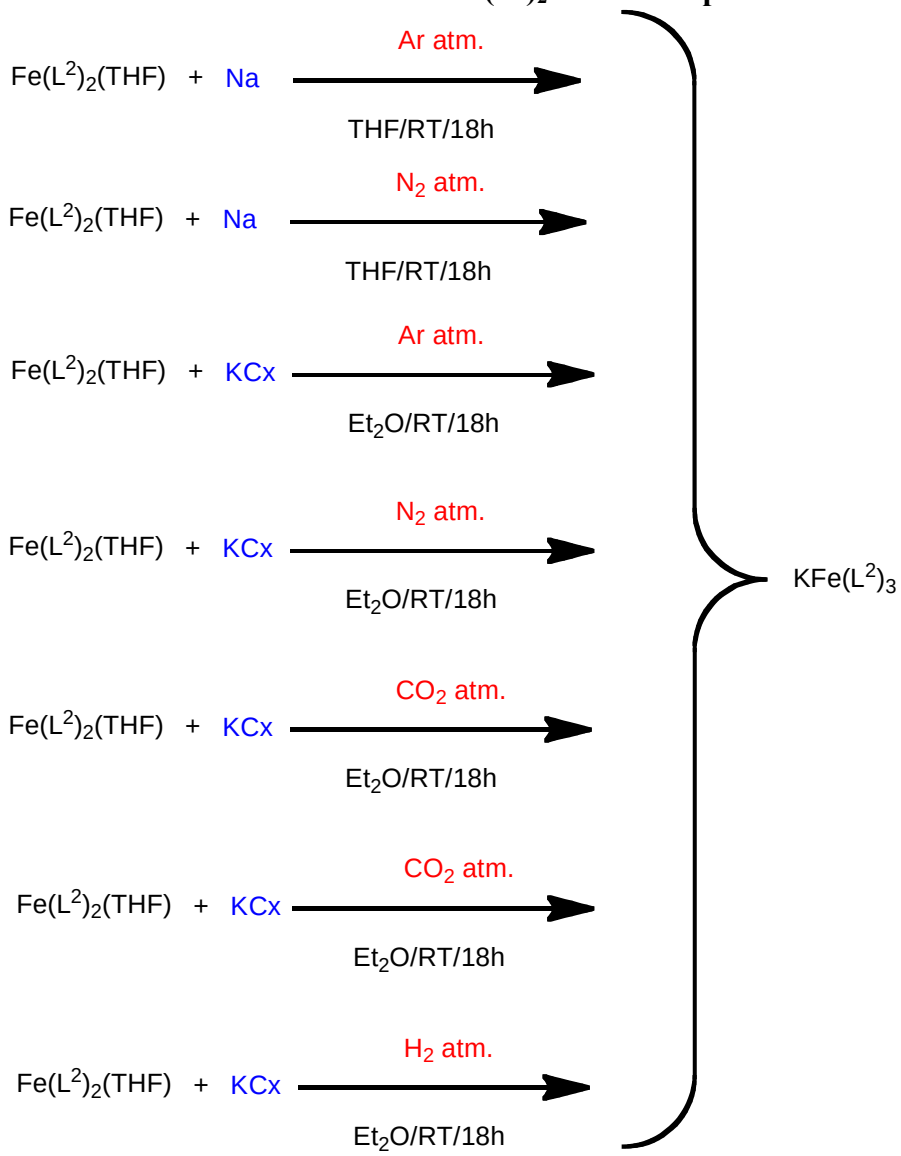
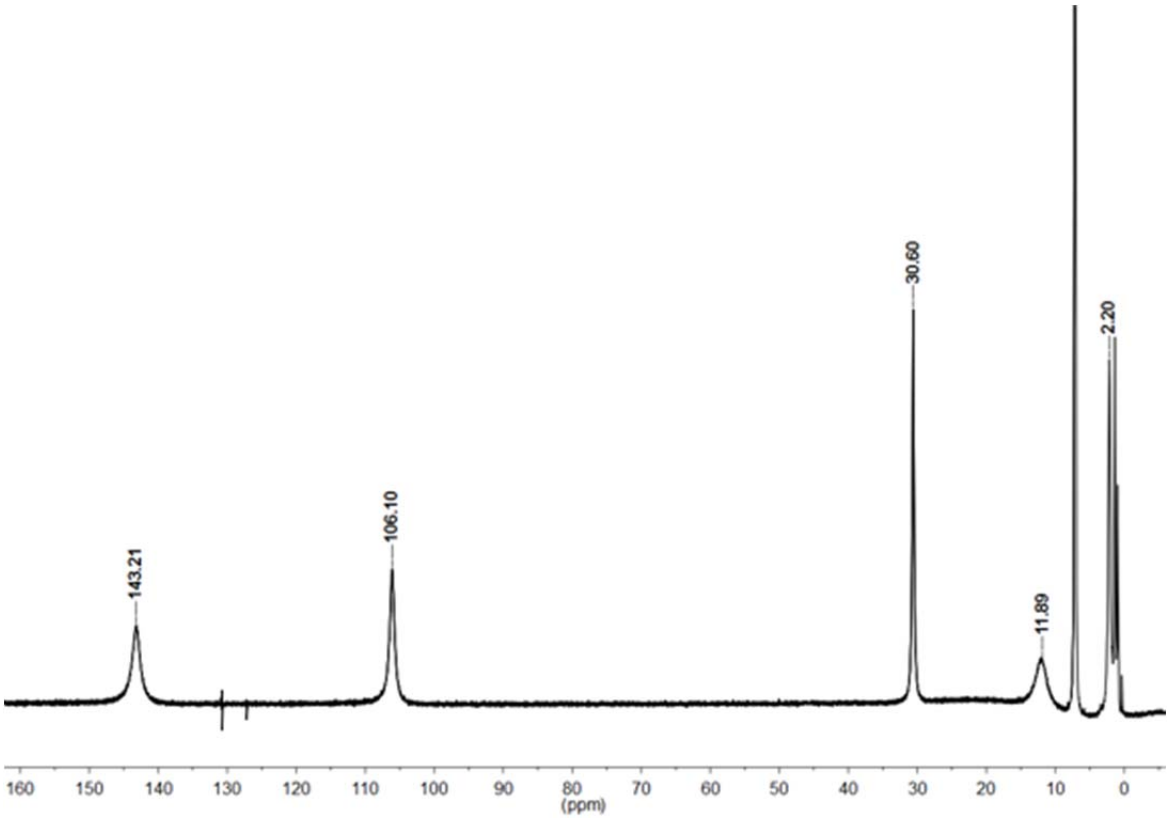


Figure 8 Overlaid ^1H NMR spectra of the products of $(CuL^2)_3 + 3KL^2$ (blue) and $CuL^2_2 + KC_8$ (red), both in C_6D_6. The broad peak at 10 ppm is from unreacted CuL^2_2.

Scheme: Reduction reactions of $Fe(L^2)_2$ with attempted reactive trapping





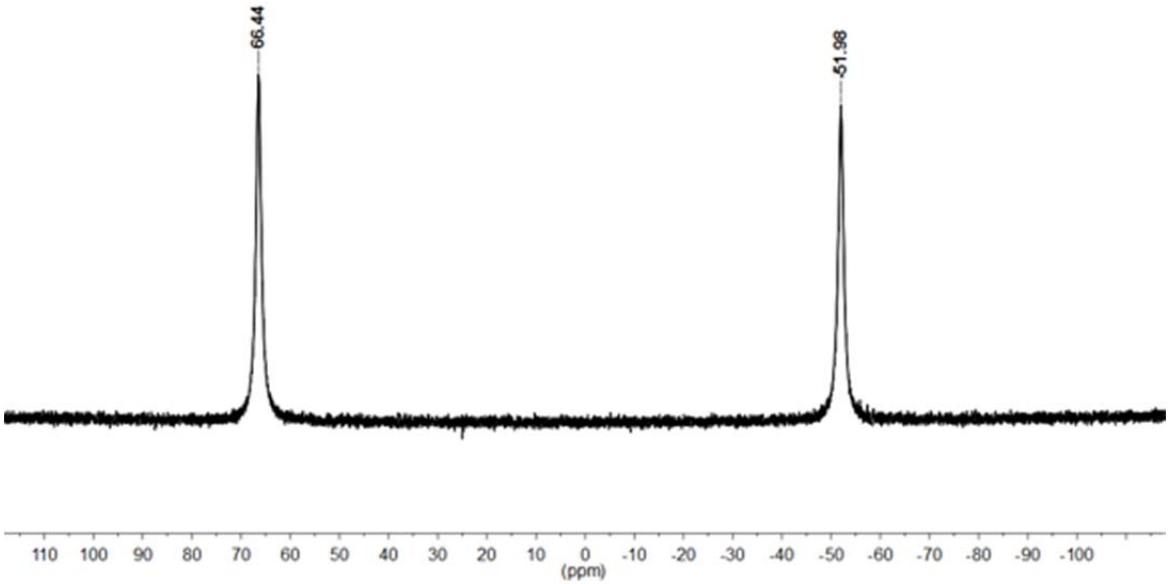


Figure 9. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of $[Co(L^{2})_2]$ in C_6D_6.

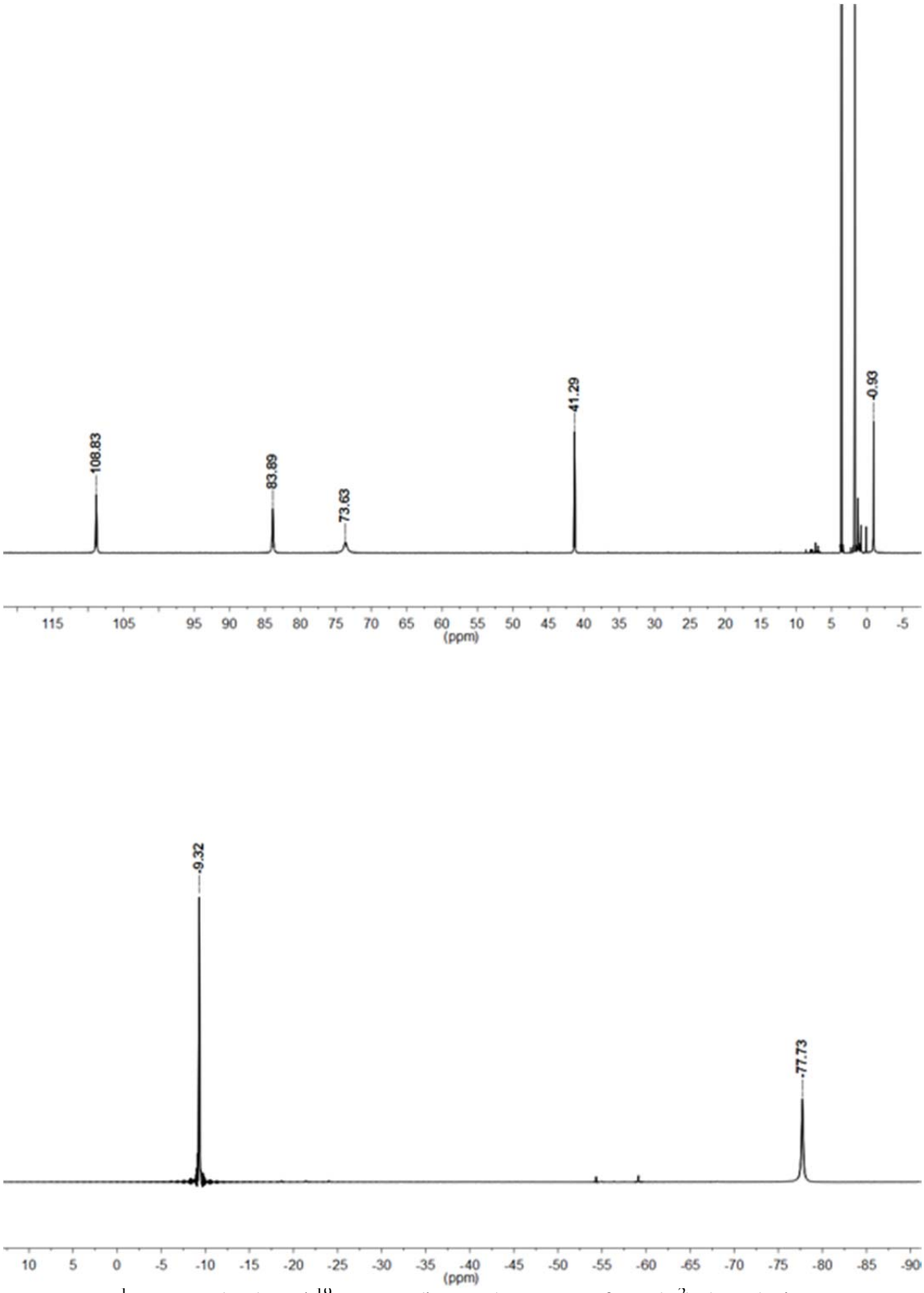
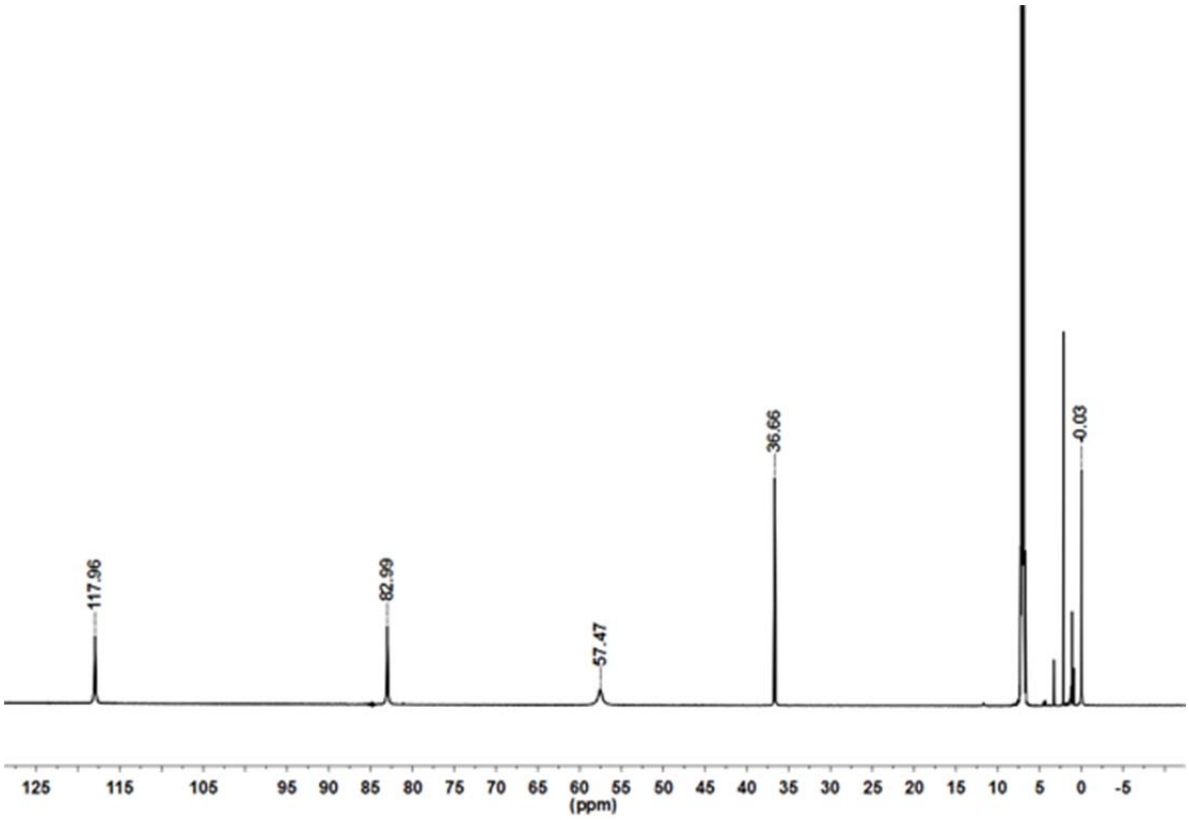


Figure 10. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of [Co(L^2)$_2$(THF)] in D8-THF.



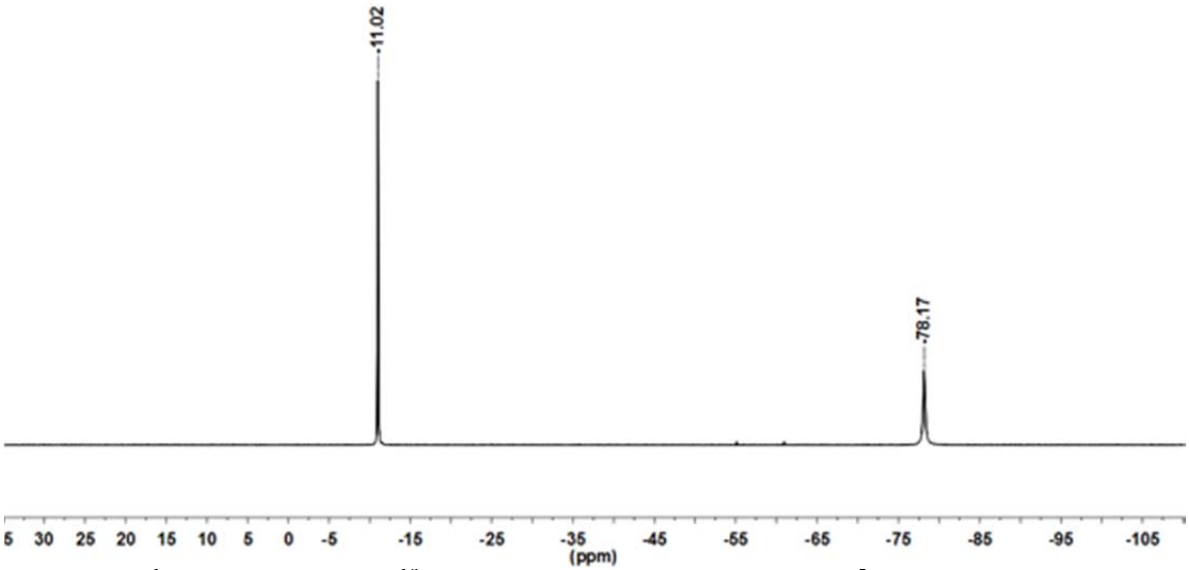


Figure 11. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of [Co(L^2)$_2$(Benzonitrile)] in C_6D_6 .

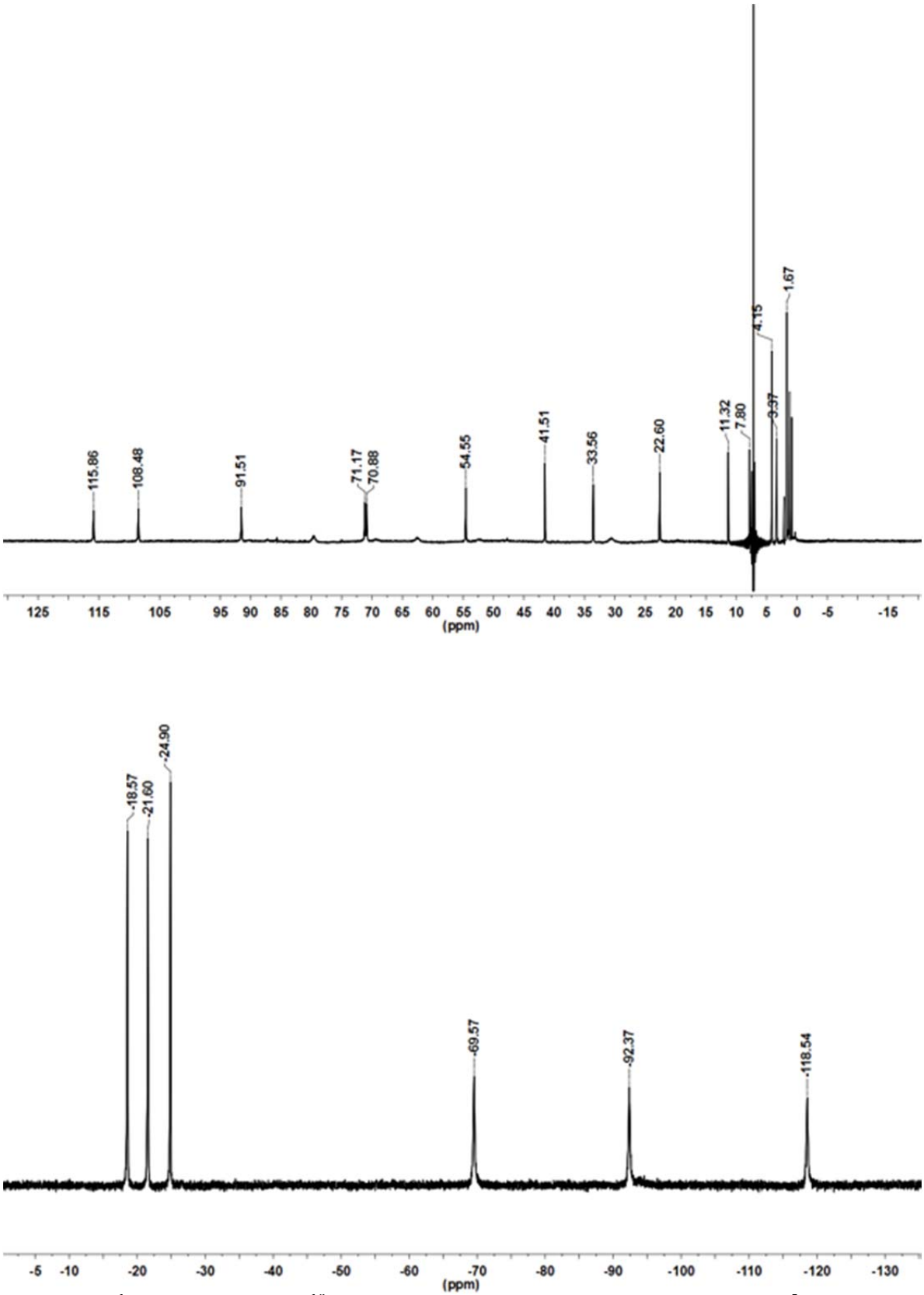


Figure 12. ^{1}H NMR (top) and ^{19}F NMR (bottom) spectra of [K(toluene)][Co(L^2)$_3$] in C_6D_6 .

MSC11060 $KCo(L^2)_3$(toluene)

A colorless plate (approximate dimensions 0.25 × 0.12 × 0.03 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker APEX II Kappa Duo diffractometer equipped with an APEX II detector at 150(2) K.

Data collection

The data collection was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 60 seconds and a detector distance of 5.00 cm. A collection strategy was calculated and complete data to a resolution of 0.80 Å with a redundancy of 4 were collected. Four major sections of frames were collected with 0.50º omega and phi scans. Data to a resolution of 0.80 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 2616 strong reflections from the actual data collection after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2]

Structure solution and refinement

The space group P-1 was determined based on intensity statistics and the lack of systematic absences. The structure was solved using SIR-2004[3] and refined with SHELXL-97.[4] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to R1 = 0.0641 and wR2 = 0.1818 (F^2, all data). The remaining electron density is minuscule and located on bonds. The structure was found as proposed with one half toluene molecule per formula unit. The solvent is disordered over an inversion center and one of the CF3 groups of the ligand is disordered over two sites (ratio 82:18).

MSC 11051 $KFe(L^2)_3$(toluene)

An orange block (approximate dimensions 0.07 × 0.05 × 0.04 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker APEX II Kappa Duo diffractometer equipped with an APEX II detector at 150(2) K.

Data collection

The data collection was carried out using Cu Kα radiation (graphite monochromator) with a frame time of 30 seconds and a detector distance of 4.00 cm. A collection strategy was calculated and complete data to a resolution of 0.70 Å with a redundancy of 4 were collected. Twenty-eight major sections of frames were collected with 0.50º omega and phi scans. Data to a resolution of 0.84 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 5609 strong reflections from the actual data collection after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2]

Structure solution and refinement

The space group C2/c was determined based on intensity statistics and systematic absences. The structure was solved using SIR-2004[3] and refined with SHELXL-97.[4] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to R1 = 0.0457 and wR2 = 0.1238 (F^2, all data). The remaining electron density is minuscule and located on bonds. The structure was found as a dimer with solvent toluene completing the coordination of K. Toluene is disordered over two sites.

MSC11034 $Fe(L^2)_2$(THF)

A yellow crystal (approximate dimensions 0.673 x 0.290 x 0.154 mm^3) was placed onto the tip of a glass capillary and mounted on an Apex Kappa Duo diffractometer and measured at 150 K.

Data collection

A preliminary set of cell constants was calculated from reflections harvested from three sets of 12 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 299 reflections. The data collection was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 10 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to achieve complete data with a redundancy of 4. Sections of frames were collected with 0.50º steps in ω and ϕ scans. Data to a resolution of 0.71 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 7171 strong reflections from the actual data collection after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2]

Structure solution and refinement

The space group $P2_1/n$ was determined based on intensity statistics and systematic absences. The structure was solved using SIR-92[3] and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* system.[4] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms. The final full matrix least squares refinement converged to R1 = 0.0355 and wR2 = 0.0819 (F^2, all data).

MSC11038 $Co(L^2)_2$*toluene

A red prism (approximate dimensions 0.23 × 0.21 × 0.17 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker APEX II Kappa Duo diffractometer equipped with an APEX II detector at 250(2) K. Previous attempts to collect data for this compound had shown that this material is not amiable to flash-freezing, and the increased mosaicity (and possibly twinning) of the crystal gave rise to very poor diffraction patterns.

Data collection

The data collection was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 5 seconds and a detector distance of 5.00 cm. A collection strategy was calculated and complete data to a resolution of 0.74 Å with a redundancy of 4 were collected. Four major sections of frames were collected with 0.50º ω and ϕ scans. Data to a resolution of 0.80 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 6309 strong reflections from the actual data collection after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2]

Structure solution and refinement

The space group Fddd was determined based on intensity statistics and systematic absences. The structure was solved using SIR-2004[3] and refined with SHELXL-97.[4] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. A whole molecule disorder was refined for the Co complex using a strong set of restraints. The final full matrix least squares refinement converged to R1 = 0.0488 and wR2 = 0.1525 (F^2, all data). The remaining electron density is minuscule and located on bonds.

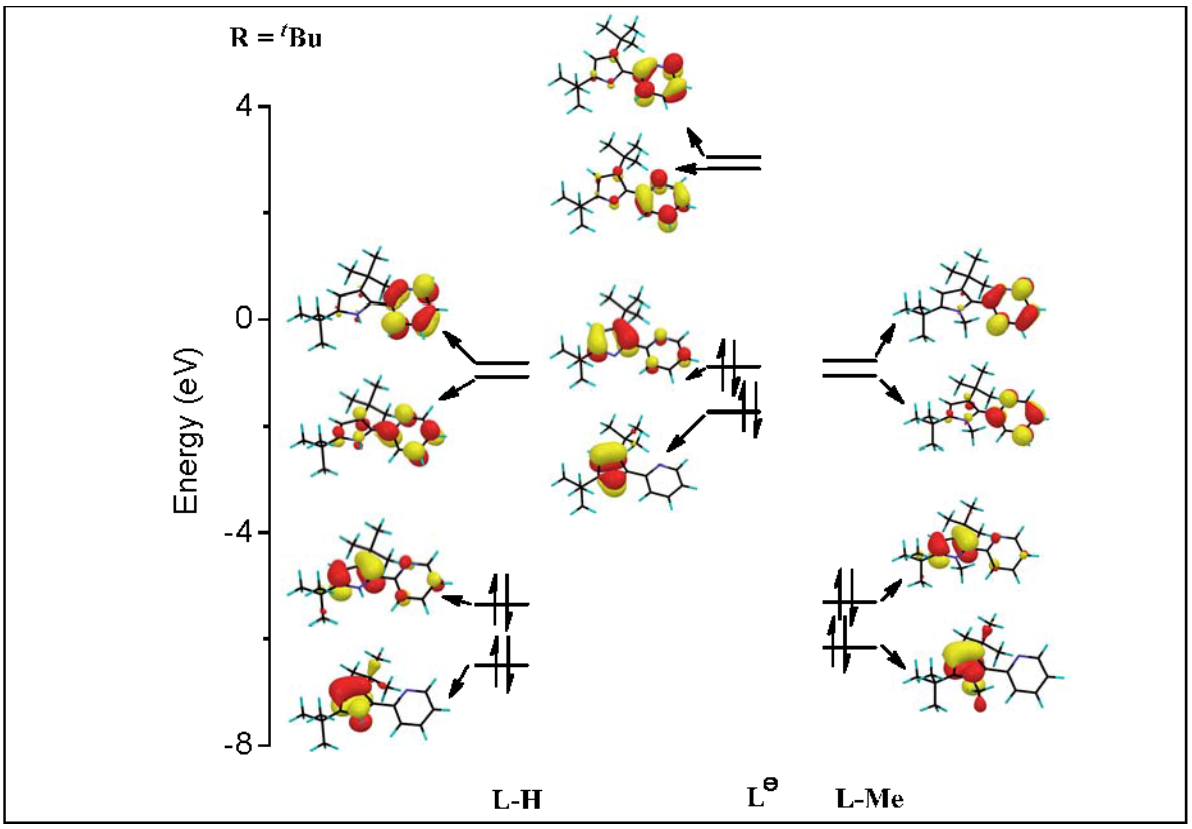
Structure description

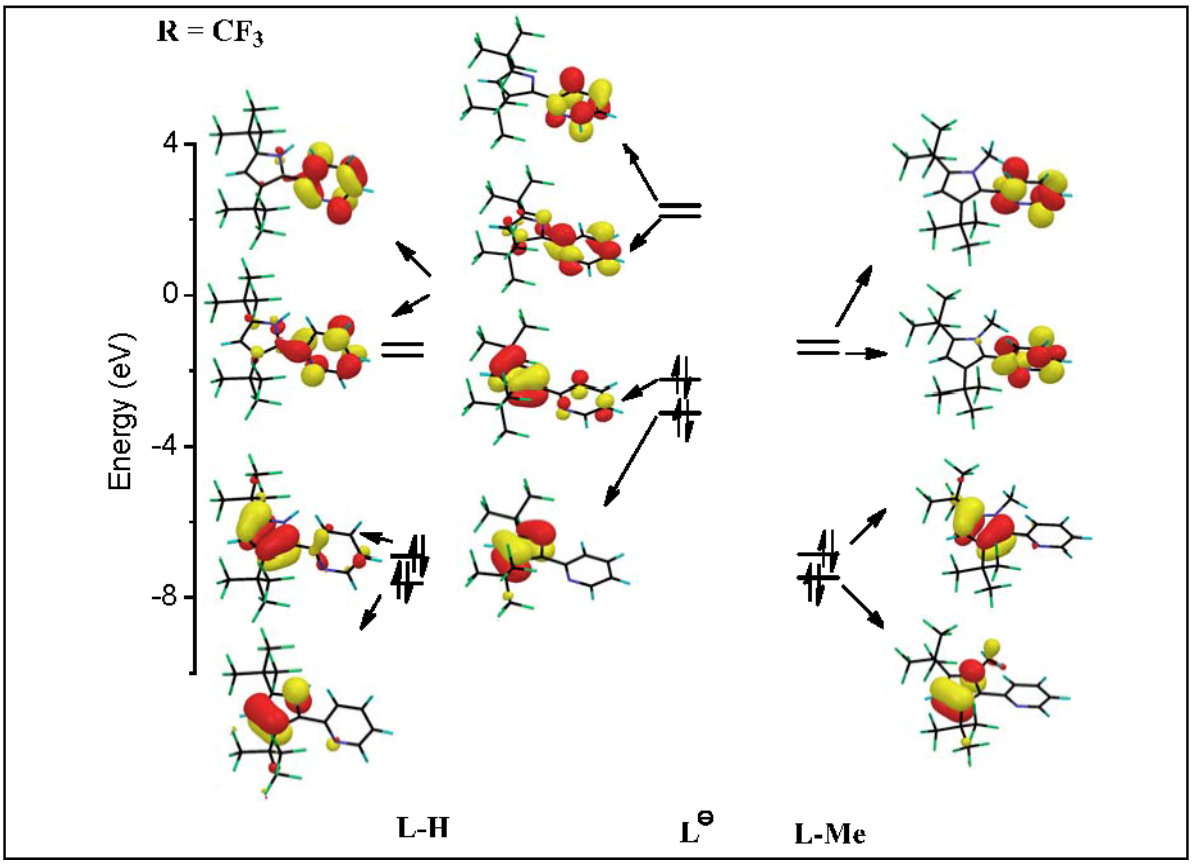
Half of the cobalt complex and included solvent molecule (toluene) are crystallographically

unique. Both the cobalt complex and toluene are disordered; toluene is disordered over a two-fold axis. Short F..F distances (2.84 Å) and F…H distances (2.37 Å) are observed.

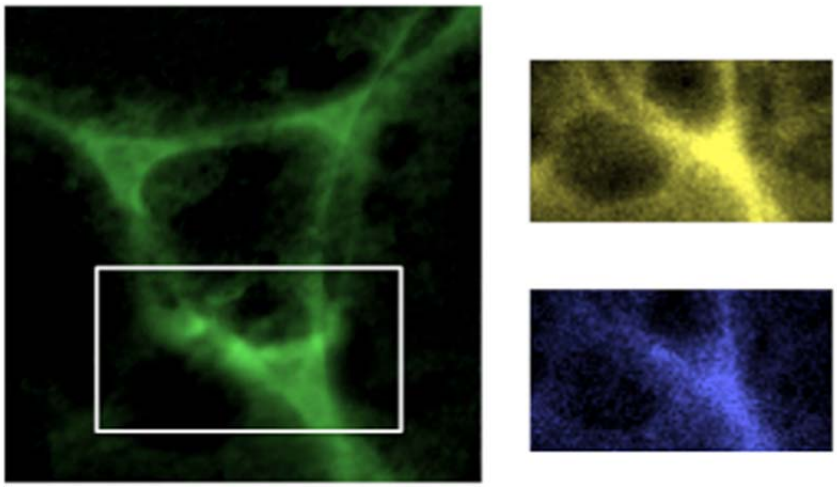
1. SAINT, Bruker Analytical X-Ray Systems, Madison, WI, current version.
2. An empirical correction for absorption anisotropy. R. Blessing, *Acta Cryst*. A51, 33 - 38 (1995).
3. Sir2004, A Program for Automatic Solution and Refinement of Crystal Structures. M. C. Burla, R. Caliandro, M. Carnalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, R. Sagna. Vers. 1.0 (2004).
4. A short history of *SHELX*. G. M. Sheldrick, *Acta Cryst*. A64, 112 - 122 (2008).

Frontier MO's for LH, L^- and L-Me (^{t}Bu substituted). Only HOMO-1 to LUMO+1 has been plotted to understand those MO's involved in oxidation and reduction process. For all of these three cases, HOMOs are mainly populated by the pyrrolide ring pi orbital and the oxidation by one or two electron can takes place from pyrrolide ring. The reduction is possible at the pyridine ring as the LUMOs are mostly populated by pyridine pi orbital. Second figure shows similarities when pyrrolide substituents are tBu.





Control experiments were done to detect whether molecular species chemisorbed to graphite gave (misleading) EDX response. First $RuCl_2(PPh_3)_3$ was adsorbed onto graphite at loading levels comparable to those used here for iron and cobalt, then this sample was slurried in CH_2Cl_2 as were the other samples, and coated on a grid, then visualized by STEM/EDX. No Ru EDX signals were detected from this, which involves loading comparable to the Fe and Co examples.



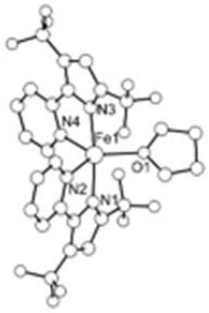
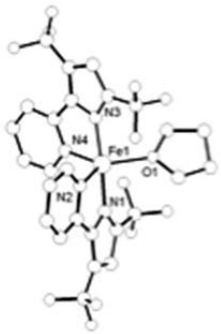
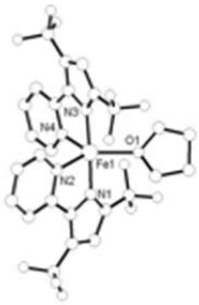
Energy Dispersive Spectroscopy map of insoluble residue from KC_8 reduction of $Co(L^2)_2$ (left in green). Carbon (bottom right in purple) and cobalt (top right in yellow) have both been identified in the same area of the insoluble residue.

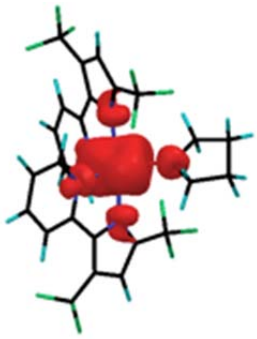
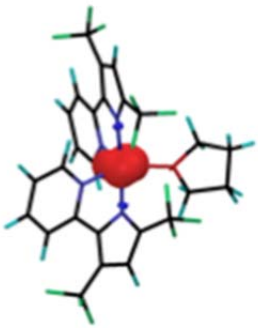
Computational Details

All calculations were carried out using DFT as implemented in the Jaguar 7.7[1] suite of *ab initio* quantum chemistry programs. Geometry optimizations were performed with B3LYP[2-5] functional and the 6-31G** basis set. Fe were represented using the Los Alamos LACVP basis[6,7] that includes relativistic effective core potentials. The energies of the optimized structures were reevaluated by additional single point calculations on each optimized geometry using Dunning's correlation consistent triple-□□□basis set[8] cc-pVTZ(-f) that includes a double set of polarization functions. For Fe, we used a modified version of LACVP, designated as LACV3P, in which the exponents were deconstructed to match the effective core potential with triple-ζ quality. The energy values were presented in this manuscript as E(SCF) only. The optimized geometry minima were confirmed by frequency calculation where minima have no imaginary frequency. The assignment of the type of each molecular orbital was made on the basis of its composition and by visual inspection of its localized orbital. The coordinate frame was assigned by a visual inspection of the d*z2* and d*xy* orbitals

(1) Jaguar 7.7, Schrödinger, LLC, New York, NY, 2007.
(2) Becke, A. D. *Phys. Rev. A,* **1988,** *38*, 3098-3100.
(3) Becke, A. D. *J. Chem. Phys.,* **1993,** *98*, 5648-5652.
(4) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.,* **1980,** *58*, 1200-1211.
(5) Lee, C.; Yang, W.; Parr, R. G. *Physical Review B: Condensed Matter and Materials Physics,* **1988,** *37*, 785-789.
(6) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.,* **1985,** *82*, 270-283.
(7) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.,* **1985,** *82*, 284-298.
(8) Noodleman, L. *J. Chem. Phys.* **1981**, *74*, 5737–5743.
(9) Noodleman, L.; Lovell, T.; Han, W.-G.; Li, J.; Himo, F. *Chem. Rev*. **2004**, *104*, 459–508.

Electronic structure of [FeL_2(THF)]

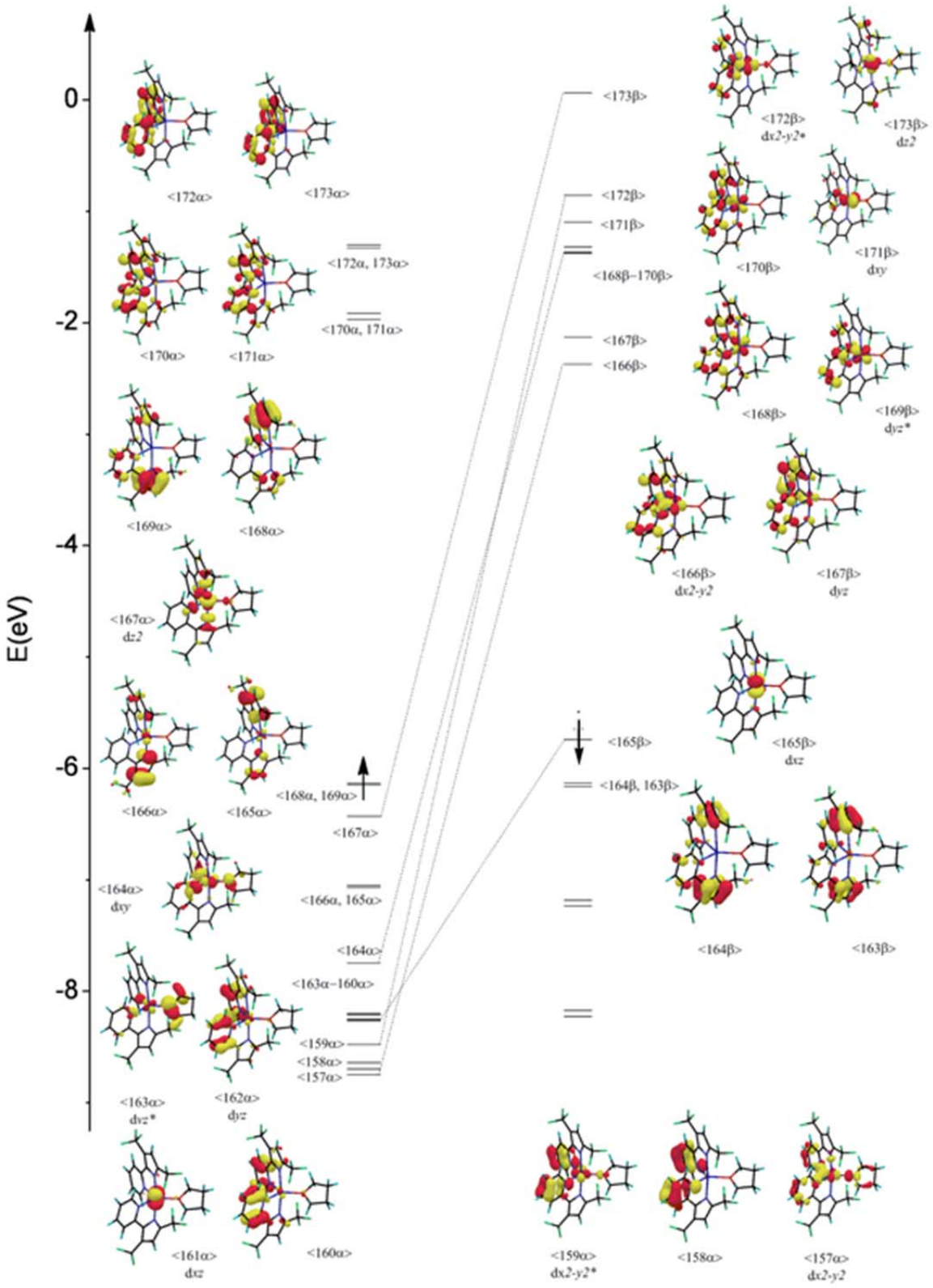
[FeL_2(THF)] **Ircp030: S=2**	**[FeL_2(THF)]** **Ircp031: S=1**	**[FeL_2(THF)]** **Ircp032: S=0**
ΔE_{ele}(Kcal/mol) **0.0**	**10.9**	**23.5**
		

Spin Density Plot Fe1=3.8	Spin Density Plot Fe1=2.0	
		

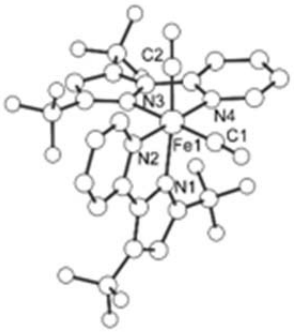
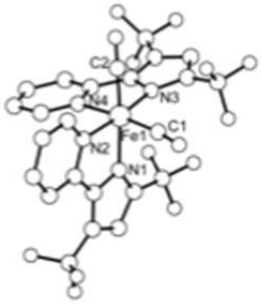
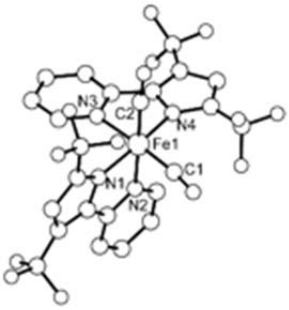
Selected calculated bond distances and angles for different spin states of [FeL_2(THF)]

distances (Å), angles (°) and twist angles (°)	**[FeL_2(THF)] Ircp030: S=2**	**[FeL_2(THF)] Ircp031: S=1**	**[FeL_2(THF)] Ircp032: S=0**	**[FeL_2(THF)] X-ray**
Fe1-N1	2.114	1.978	1.974	2.102
Fe1-N2	2.168	2.091	1.971	2.118
Fe1-N3	2.112	1.979	1.974	2.112
Fe1-N4	2.171	2.092	1.971	2.116
Fe1-O1	2.118	2.113	2.177	2.077
N3-Fe1-N1	173.3	175.5	177.1	177.7
N3-Fe1-O1	93.2	92.2	91.1	91.2
N3-Fe1-N2	98.9	97.0	96.2	101.0
N4-Fe1-N2	104.4	108.3	93.2	106.1
N2-Fe1-O1	128.1	125.6	134.3	127.7
N1/N2 ring torsion angle	-5.6	-2.3	1.5	-6.1
N3/N4 ring torsion angle	-4.6	-2.2	2.1	-9.1

MO Diagram of [FeL_2(THF)] : S = 2



Electronic structure of $[Fe(L)_2(CO)_2]$ with different isomeric structure

Compound L: CF_3	**Ircp203** **$[Fe(L)_2(CO)_2]$** **(N,N trans)** **Singlet** 	**Ircp204** **$[Fe(L)_2(CO)_2]$** **(N,N' trans)** **Singlet** 	**Ircp205** **$[Fe(L)_2(CO)_2]$** **(N',N' trans)** **Singlet** 
ΔE(SCF) (Kcal/mol)	12.7	9.8	0.0
Fe1-N1	2.036	2.035	1.999
Fe1-N2	2.024	2.024	2.032
Fe1-N3	2.033	1.999	2.036
Fe1-N4	2.025	2.029	2.000
Fe1-C1	1.823	1.835	1.831
Fe1-C2	1.821	1.823	1.833
C1-O	1.143	1.143	1.140
C2-O	1.143	1.140	1.140

Optimized coordinate

[FeL_2(THF)] Ircp030: S=2				FeL_2(THF)] Ircp031: S=1			
Fe	2.192963698	9.859338246	12.396283593	Fe	2.304135204	9.737412231	12.404451303
F	0.730470751	5.825754970	8.107727669	F	0.611243527	6.222517884	8.000856884
F	1.663165421	4.651985587	9.675201352	F	1.372203182	4.768122558	9.416520267
F	-0.502559366	4.634912406	9.448988765	F	-0.776248168	5.043431978	9.195708476
F	-1.878068863	9.721231019	12.356426777	F	-1.784266914	9.725634075	12.652287840
F	-0.583535973	9.081391132	13.976396039	F	-0.319100869	9.102338306	14.128442870
F	-2.240543095	7.809675781	13.327609179	F	-1.981993811	7.784848901	13.602755986
F	6.002868955	11.283660156	16.904312159	F	5.575427191	11.433898258	16.983376306
F	7.148993346	10.023836281	15.560808560	F	7.050403431	10.367042323	15.806639476
F	7.461156872	12.178844185	15.559899626	F	7.032556718	12.544301386	15.805155185
F	4.851464155	13.886593065	11.254205543	F	4.892516035	13.609704955	11.033427724
F	2.843584536	13.872052510	12.088520349	F	2.870474316	13.755986169	11.804361962
F	3.422397598	12.341380856	10.662369584	F	3.414610971	12.080874922	10.534163168
O	0.791180407	11.440466975	12.255617499	O	0.910659888	11.319158884	12.251259668
N	3.346303551	8.947285882	10.802290934	N	3.410995908	8.930557531	10.822519192
N	0.853014588	8.429888317	11.601044046	N	0.998570735	8.418597538	11.716487133
N	2.794172727	8.783551338	14.183612720	N	2.809597572	8.707148083	14.152708877
N	3.691582562	11.103153237	13.213986136	N	3.707845494	10.939447648	13.109193358
C	4.588353882	9.315046984	10.450477038	C	4.672945214	9.246873229	10.490518031
C	5.293983575	8.685779025	9.433899947	C	5.371482835	8.582622528	9.491435240
C	4.667223564	7.637007199	8.756159427	C	4.723494583	7.546259532	8.814444553
C	3.381175265	7.251448216	9.110511187	C	3.421937771	7.203758280	9.155347400
C	2.724984665	7.921974768	10.156961124	C	2.771782545	7.911252475	10.179555935
C	1.378786721	7.612896573	10.638268248	C	1.423406775	7.652083597	10.664779398
C	0.455769666	6.581573697	10.343229428	C	0.401795261	6.742074528	10.306317796
C	-0.664680885	6.797530047	11.164706928	C	-0.668492299	6.975012876	11.183701465
C	-0.373229457	7.932756888	11.916365953	C	-0.260706835	8.006575909	12.029728150
C	0.582900368	5.435201737	9.406716291	C	0.397840992	5.705735811	9.242226842
C	-1.261384751	8.622958277	12.884536291	C	-1.075516490	8.646392302	13.094179721
C	2.237338407	7.641272212	14.615438273	C	2.303399398	7.532177445	14.559917812
C	2.668090943	6.986472752	15.761475896	C	2.775380688	6.863542912	15.681377282
C	3.716230113	7.559334720	16.486044464	C	3.818731564	7.447940827	16.403709602
C	4.296721392	8.742613413	16.048804272	C	4.355506456	8.658784947	15.987521807
C	3.823188573	9.348806820	14.872856378	C	3.837003107	9.282577521	14.841289216
C	4.349541825	10.585924805	14.295573658	C	4.311878603	10.534889335	14.269261386
C	5.472833863	11.394113405	14.590908160	C	5.311866375	11.468794257	14.626242353
C	5.479192798	12.436122816	13.645915934	C	5.303105232	12.464081114	13.636552900
C	4.377590804	12.211501007	12.824659829	C	4.308977099	12.100174668	12.727612373
C	6.511674126	11.223640395	15.639495106	C	6.233050848	11.458032607	15.791515584
C	3.885514423	13.070589472	11.719181372	C	3.877746435	12.875578777	11.536033892
C	0.401532243	12.304199567	13.365004966	C	0.578127573	12.238048312	13.331093058
C	-0.355424906	13.459523399	12.713727994	C	-0.227229697	13.355311380	12.669819346
C	-1.000841401	12.786242753	11.490506109	C	-0.926076022	12.622539619	11.511527062
C	0.087161419	11.816462182	11.033646555	C	0.140870939	11.628766391	11.054232862
H	5.012822610	10.139944524	11.013021111	H	5.119330060	10.058232912	11.052912904
H	6.298006442	9.009118013	9.182309294	H	6.388653115	8.871580383	9.253044071

H	5.179536671	7.120407123	7.949303326	H	5.233816807	7.001667619	8.025626892
H	2.887121418	6.450417075	8.580314155	H	2.917312888	6.395375297	8.646656209
H	-1.561793715	6.198400067	11.205198988	H	-1.614407148	6.455902034	11.201598328
H	1.424134352	7.255443121	14.009906416	H	1.496271275	7.132738803	13.957613521
H	2.195296372	6.062310032	16.075019950	H	2.337023303	5.917134769	15.976556078
H	4.079938091	7.086184159	17.393914045	H	4.217424598	6.958432645	17.287280396
H	5.096931363	9.197788711	16.613436466	H	5.170791590	9.111507781	16.532310752
H	6.198772203	13.237936211	13.571866716	H	5.940163480	13.334228952	13.589129976
H	1.313981760	12.605317034	13.882216747	H	1.512457337	12.574364689	13.782268819
H	-0.233219503	11.715481195	14.035062220	H	-0.011149036	11.685172940	14.068917458
H	-1.086591269	13.904241726	13.394329958	H	-0.928979874	13.820254434	13.366994742
H	0.346716913	14.237195875	12.399364265	H	0.445493032	14.126653612	12.286524180
H	-1.271963238	13.495572045	10.703788189	H	-1.231883243	13.292879362	10.704198642
H	-1.897177873	12.232345176	11.784482064	H	-1.808065910	12.087104152	11.872206379
H	0.814759197	12.290425921	10.367263185	H	0.826938866	12.064785049	10.322017104
H	-0.295966426	10.901040256	10.579978728	H	-0.265619877	10.693450115	10.667512219
$[FeL_2(THF)]$				**$[Fe(L)_2(CO)_2]$ (N,N trans)**			
Ircp032: S=0				**Ircp 302: Singlet**			
Fe	2.253171125	9.786008350	12.417843113	Fe	1.117077497	-1.093141708	1.141076438
F	0.746221945	6.091538794	8.137722694	F	-3.548937560	2.472953352	0.465757171
F	1.437606399	4.726240595	9.672700553	F	-1.881719717	3.859088297	0.451789257
F	-0.698111258	4.965777183	9.318258175	F	-2.874464733	3.336582824	-1.415337861
F	-1.846417926	9.830531415	12.604497664	F	-0.011586832	-2.037140918	-2.372806693
F	-0.406105524	9.198836425	14.102460435	F	1.638044255	-0.653950798	-2.680938259
F	-2.086404083	7.902021455	13.570368452	F	-0.226006523	-0.369150305	-3.755396978
F	5.781014615	11.255801232	16.857539808	F	6.620196671	-0.757180617	-1.006758459
F	7.137560657	10.229622126	15.513935805	F	5.418232641	0.022811460	-2.634632412
F	7.180012228	12.403574375	15.644028225	F	6.559642919	1.386752095	-1.377469106
F	4.783382970	13.720128723	11.055467646	F	3.517342280	3.309323146	2.254866878
F	2.762214454	13.814446500	11.836685721	F	2.613390824	1.652993082	3.338650978
F	3.335829115	12.161298385	10.549024930	F	1.473148271	2.721221920	1.824937118
O	0.813180871	11.409213672	12.238062979	N	0.165220591	0.085249265	2.484664665
N	3.405767068	8.875891123	11.102627734	N	-0.024502573	-0.009335204	-0.145727806
N	0.930189336	8.487177144	11.739408839	N	2.072966477	-2.281900583	-0.190017398
N	2.895013260	8.674843635	13.913583824	N	2.726380368	0.093603907	0.758250146
N	3.644656016	11.010071540	13.098236285	C	0.282038536	0.004897925	3.825020016
C	4.698867030	9.162601877	10.870405709	C	-0.468217780	0.776198927	4.694234010
C	5.448403157	8.500582087	9.907956347	C	-1.390040016	1.675308893	4.148387282
C	4.828510496	7.502489458	9.152823659	C	-1.525277196	1.764614080	2.774330064
C	3.494210524	7.197468731	9.383746431	C	-0.732280620	0.954687857	1.940422665
C	2.788694531	7.894207598	10.376543193	C	-0.790442441	0.933063750	0.497496200
C	1.404024122	7.669764838	10.753175379	C	-1.501387055	1.698545923	-0.451272947
C	0.405321808	6.735033798	10.395026858	C	-1.157512955	1.186203972	-1.707071800
C	-0.703348328	7.004040324	11.214487310	C	-0.260616191	0.143141181	-1.480324751
C	-0.335758267	8.080376197	12.024131407	C	-2.439041629	2.832748687	-0.243544079
C	0.467029310	5.640851917	9.393047252	C	0.289892051	-0.721360022	-2.559152815
C	-1.161440544	8.744186089	13.064163306	C	1.685930106	-3.520082665	-0.555501681
C	2.424126529	7.458085456	14.235790019	C	2.443771745	-4.333368392	-1.378637782
C	2.899954975	6.735337405	15.320893331	C	3.668217121	-3.842170256	-1.843166253
C	3.903906054	7.303382720	16.107798009	C	4.079323328	-2.573262567	-1.475284182
C	4.397047595	8.560328592	15.786195171	C	3.261524533	-1.789896941	-0.639643373

C	3.883831759	9.239636532	14.670964386
C	4.316520275	10.540158577	14.190921672
C	5.351578421	11.440342172	14.532020511
C	5.299605947	12.481084347	13.590151365
C	4.244284865	12.173812520	12.729264522
C	6.353181448	11.338412528	15.623442093
C	3.787443870	12.960022157	11.555569714
C	0.470537439	12.336084228	13.308113848
C	-0.337018346	13.446415624	12.637575461
C	-1.025110404	12.705067101	11.478550483
C	0.048320815	11.711409344	11.035802110
H	5.125325196	9.949462093	11.479260966
H	6.489161252	8.765914264	9.758853191
H	5.381969685	6.964600803	8.388582178
H	2.996083090	6.429863837	8.808345987
H	-1.645206430	6.475867982	11.222627790
H	1.641891644	7.070138241	13.595666329
H	2.489532850	5.755320880	15.537587202
H	4.300089943	6.770055639	16.967022324
H	5.170877796	9.017978410	16.385664089
H	5.953567834	13.338711271	13.537095433
H	1.400445411	12.679863861	13.763778467
H	-0.121853411	11.785211909	14.046218216
H	-1.045587032	13.910461838	13.329201842
H	0.333842875	14.220572570	12.255337406
H	-1.326330129	13.370085354	10.664482138
H	-1.909230402	12.169525380	11.835111837
H	0.738376769	12.147600201	10.306144767
H	-0.352337654	10.773044904	10.648989614
C	3.582115590	-0.465522723	-0.160964901
C	4.643882180	0.424633984	-0.428584200
C	4.421037558	1.551941149	0.368868598
C	3.247925221	1.311963019	1.082235477
C	5.796984408	0.275800964	-1.354272190
C	2.706591067	2.239861564	2.111806709
H	1.006612053	-0.701889500	4.209852940
H	-0.328950983	0.675398172	5.764499876
H	-2.001139482	2.298993670	4.793916035
H	-2.241435329	2.444837145	2.339109028
H	-1.519599547	1.522410574	-2.665999827
H	0.731547215	-3.863833965	-0.176422510
H	2.081982403	-5.319473675	-1.646471416
H	4.298434791	-4.449887675	-2.485532071
H	5.028839913	-2.186853689	-1.813852242
H	5.037127066	2.435126632	0.429092448
C	2.169028134	-1.898828252	2.393497979
O	2.877721655	-2.392852879	3.141468473
C	-0.321968739	-2.197708155	1.300528666
O	-1.261687823	-2.840684899	1.398309685

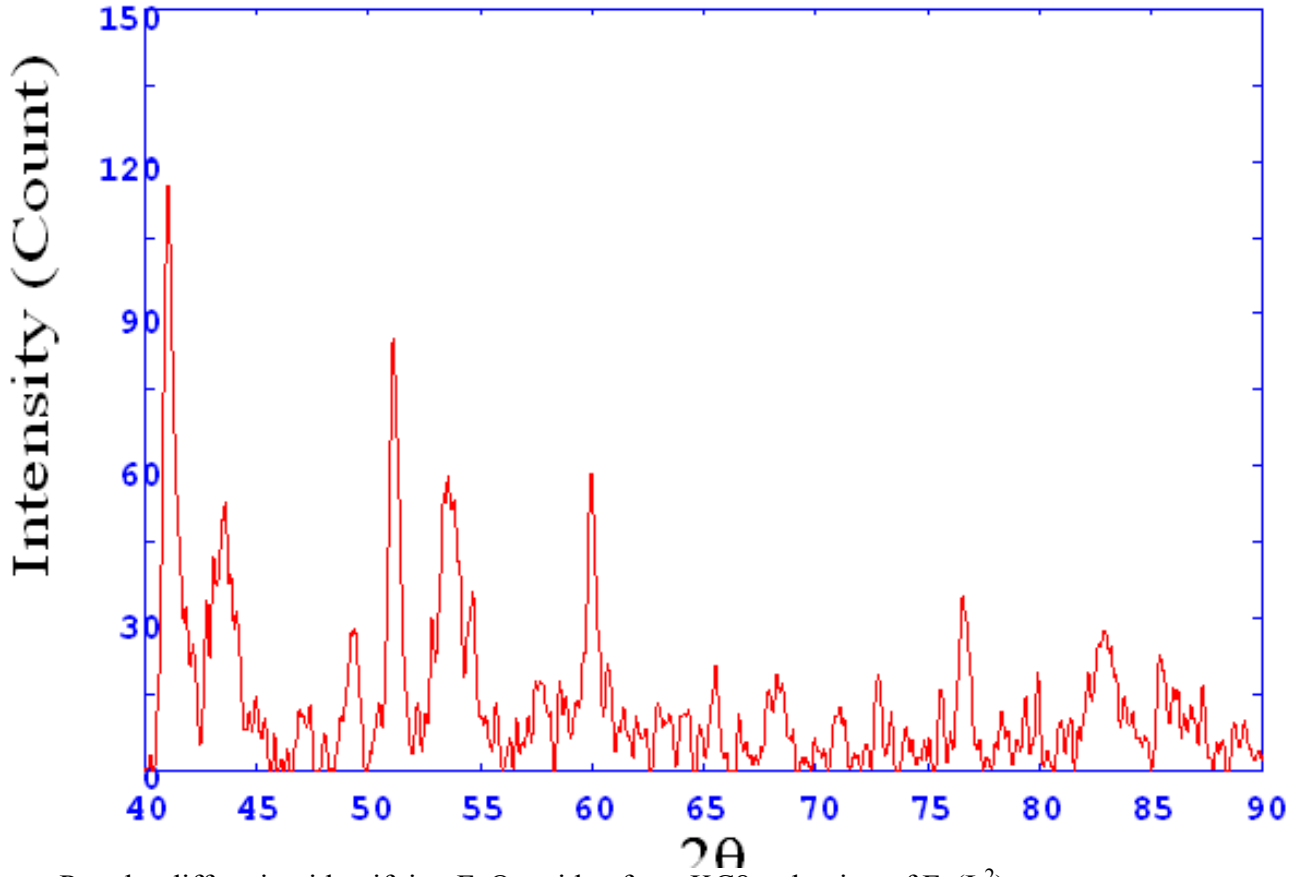
$[Fe(L)_2(CO)_2]$ (N,N' trans)
Ircp204: Singlet

Fe	2.085594289	9.936889843	12.298327303
F	0.673450112	5.746702009	8.344814338
F	1.259129526	4.611426498	10.097625928
F	-0.849232867	4.818258984	9.591694795
F	-1.631595374	10.401977276	12.276082543
F	-1.374005708	9.010654853	13.929658307
F	-2.858410830	8.608543124	12.398764898
F	-0.654152801	9.895860133	17.538475844
F	1.266183359	10.801059425	17.977799500
F	-0.512196249	12.050135450	17.824118574
F	-0.219200911	14.291094778	13.133304286
F	-0.445947479	12.723503971	11.644701347
F	1.537154038	13.426396700	12.166019972
N	3.256622929	8.824051798	11.077805445
N	0.688317337	8.610816548	11.642110370
N	2.371659618	8.703089579	13.883895070
N	1.022668582	10.932688657	13.668513403
C	4.559605509	9.051670727	10.814026609
C	5.307294519	8.252958473	9.966313427
C	4.668552109	7.170595458	9.348806386

$[Fe(L)_2(CO)_2]$ (N',N' trans)
Ircp205: Singlet

Fe	1.164298150	-1.286364020	1.357488463
F	-1.825400896	3.714637853	0.794660337
F	-3.469455867	2.304365253	0.891355781
F	-2.979760616	3.518469153	2.632242701
F	1.672328641	0.126518903	4.743194458
F	0.144327643	-1.415963967	4.835165090
F	-0.177486254	0.493291645	5.840149316
F	5.393552483	-1.200279874	-2.677250169
F	6.543448043	-1.832312712	-0.951043300
F	5.980266440	-3.288556805	-2.469973940
F	1.812071971	-5.842948773	-0.607071395
F	0.245135587	-4.325904826	-0.573094939
F	1.240991372	-4.893556085	1.273050171
N	0.247284385	-0.510208201	-0.286647360
N	-0.002544546	0.072749223	2.247522428
N	2.639985604	0.082881864	1.082290779
N	2.402465730	-2.368653803	0.219540437
C	0.434427843	-0.922831174	-1.552309924
C	-0.176053347	-0.303692330	-2.634012840
C	-1.015308345	0.785263005	-2.388522248

C	3.329267684	6.929871406	9.600037771	C	-1.227924691	1.207730694	-1.084631121
C	2.619775268	7.773309656	10.479471879	C	-0.588883643	0.535269432	-0.029947582
C	1.225213233	7.643054806	10.823019827	C	-0.735082440	0.841782947	1.379889608
C	0.223177044	6.710490216	10.469644597	C	-1.505812287	1.770441625	2.111764889
C	-0.951793450	7.143830456	11.089759260	C	-1.225798588	1.540930332	3.467201717
C	-0.629320337	8.309626447	11.787535918	C	-0.309119434	0.492998193	3.507523131
C	0.320052429	5.484362312	9.635186107	C	-2.438942117	2.816415803	1.616669786
C	-1.609867285	9.090267526	12.598699188	C	0.321927982	-0.072454239	4.726796114
C	3.065433597	7.551868185	13.873560919	C	2.670711317	1.314092648	1.618263452
C	3.134855716	6.707270260	14.970347459	C	3.662416341	2.235429545	1.312385871
C	2.440938263	7.069483211	16.128815171	C	4.661371564	1.859583534	0.412047417
C	1.721249854	8.252792843	16.152573698	C	4.649112202	0.583529378	-0.131713428
C	1.700857221	9.075453253	15.012644351	C	3.625811214	-0.308946340	0.226796525
C	1.017178184	10.344818776	14.906563386	C	3.497929711	-1.678213510	-0.231583504
C	0.357700804	11.190251213	15.823571398	C	4.275277255	-2.518695700	-1.056278759
C	-0.021771525	12.334121232	15.106586972	C	3.622802216	-3.760740771	-1.088095522
C	0.406034483	12.140314368	13.795058270	C	2.486474149	-3.628032634	-0.293414704
C	0.114285678	10.990412794	17.275919357	C	5.537686078	-2.217967936	-1.781005551
C	0.306849978	13.133551630	12.692488386	C	1.457984068	-4.670846679	-0.050156991
H	5.010746976	9.904315439	11.308211582	H	1.090763418	-1.772867173	-1.682996738
H	6.353161199	8.477503701	9.791056342	H	0.005562464	-0.669569114	-3.638177382
H	5.215238590	6.522870330	8.669961413	H	-1.505945341	1.299723318	-3.209559376
H	2.822421163	6.107406261	9.117524013	H	-1.878308504	2.045096496	-0.877191225
H	-1.922776067	6.676413536	11.040389050	H	-1.633523619	2.073541830	4.312671371
H	3.577952364	7.309641756	12.951474076	H	1.875501520	1.549577846	2.312972772
H	3.710408359	5.790380559	14.911766453	H	3.645364111	3.217933199	1.770277107
H	2.458821026	6.428904505	17.005538946	H	5.449364038	2.555424724	0.139354139
H	1.164955069	8.541970374	17.032092236	H	5.417163766	0.275577748	-0.825959834
H	-0.541574749	13.197763500	15.491967613	H	3.937344684	-4.645232861	-1.620549271
C	1.669774757	10.938480753	10.817904609	C	-0.245865747	-2.439940806	1.555531201
O	1.449669615	11.439176815	9.817442379	O	-1.200376787	-3.039958681	1.726972793
C	3.429542681	11.025338707	12.874431323	C	2.081481201	-1.969131492	2.787610224
O	4.253756529	11.705697698	13.281155117	O	2.743115923	-2.453700113	3.580050673



X-ray Powder diffraction identifying FeO residue from KC8 reduction of Fe(L^2) .