

Supporting Information

Mössbauer spectroscopic and computational investigation of an iron cyclopentadienone complex.

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General procedure for the reaction of $[\text{LFe}(\text{CO})_3]$ with Me_3NO :

In glovebox, to toluene (3.93 mL) solution of $[\text{FeL}(\text{CO})_3]$ (0.022M) protected from light was added the desired quantity of Me_3NO under vigorous stirring and at room temperature. The solution turns from yellow to orange. Aliquots of the mixture were subjected to UV-Vis measurements along the time. UV-Vis spectra superimpose after 10 minutes indicating completion of the reaction. 400 μL of the solution were transferred in Delrin cup, frozen under argon and subjected to Mössbauer spectroscopy measurement. The remaining solution was quickly evaporated under vacuum at 305 K. The orange oily residue was dissolved in CDCl_3 and directly subjected to NMR spectroscopy.

Note that in the case of one or two equivalents of Me_3NO , the obtained solutions were found stable over hours (no significant UV-Vis evolution). With four equivalents of Me_3NO , a precipitate forms after 10 minutes indicating a poor stability of the species formed. Attempt to conduct the reaction with four equivalents of Me_3NO directly in deuterated solvent to analyze the species formed by NMR failed due to the poor stability of the sample (precipitation occurring in the NMR tube at the NMR time scale).

Mössbauer studies

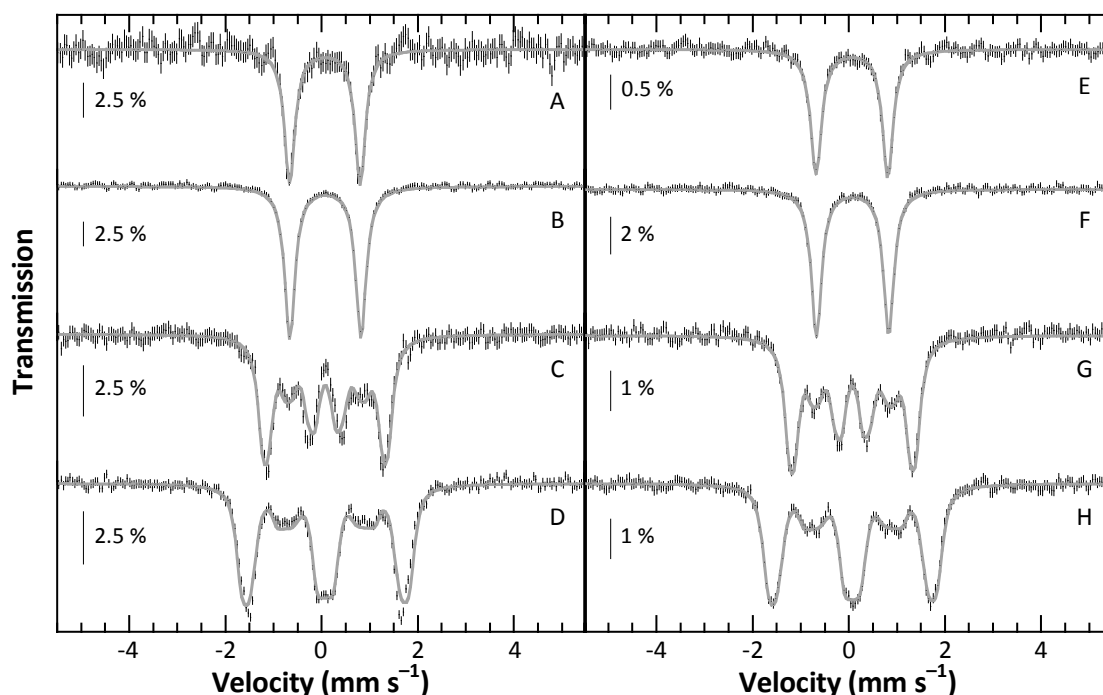


Figure S1. Experimental Mössbauer spectra of **1** (hatched bars) in powder (left column) and dissolved in toluene (right column). Spectra A and E were recorded in zero-field at 80 K. Spectra B-D and F-H were recorded at 4.5 K in zero-field (B and F) and with a 4 T (C and G) and 7 T (D and H) external magnetic field applied parallel to the γ -beam. Simulations are overlaid as solid grey lines with parameters listed in Table S1.

Table S1. Nuclear parameters of **1** used to simulate spectra of Figure S1. A $S=0$ electronic spin was assumed to reproduce magnetic spectra. Theoretical values obtained from DFT are listed in the last column.

State of 1	Experimental				DFT calculations
	Powder		Toluene solution		
T (K)	80	4.5	80	4.5	
δ (mm s^{-1})	0.06	0.07	0.06	0.07	0.06
ΔE_Q (mm s^{-1})	1.47	1.48	1.49	1.50	-1.49
η	–	0.96	–	0.95	0.97
Γ_{fwhm} (mm s^{-1})	0 T	0.26/0.27	0.26	0.28/0.27	0.26
	4 T		0.24		0.24
	7 T		0.22		0.24

UV/Vis studies

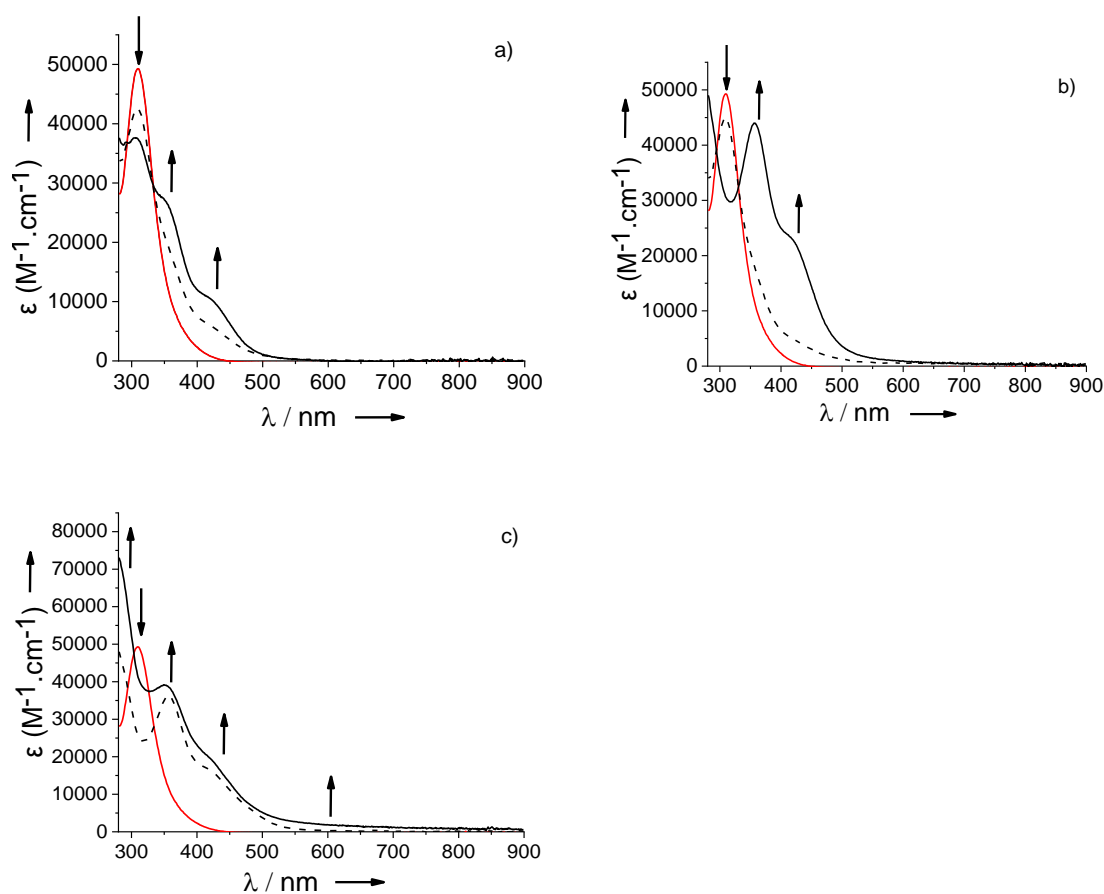


Figure S2. Evolution of UV/Vis spectra of a solution of $[\text{LFe}(\text{CO})_3]$ at 1.10^{-5}M in toluene at room temperature in the presence of different amount of Me_3NO : a) 1 equivalent, b) 2 equivalents, c) 4 equivalents. Solid red line: initial complex solution without Me_3NO , dashed black line: complex solution in the presence of Me_3NO after 10 seconds. Solid black line: complex solution in the presence of Me_3NO after 10 minutes. In each case, the reaction is completed after 10 minutes. With one and two equivalents of Me_3NO , no significant evolution of the spectra of the resulting mixture was observe over hours. In the case of four equivalents, a precipitate is formed.

Computational studies

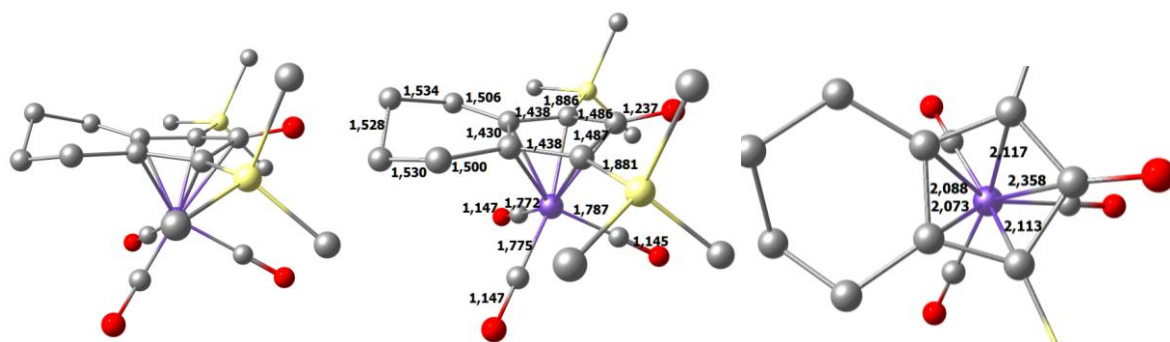


Figure S3. Geometry optimized structure of $[\text{LFe}(\text{CO})_3]$ (**1**) and selected bond distances. H atoms are omitted for clarity.

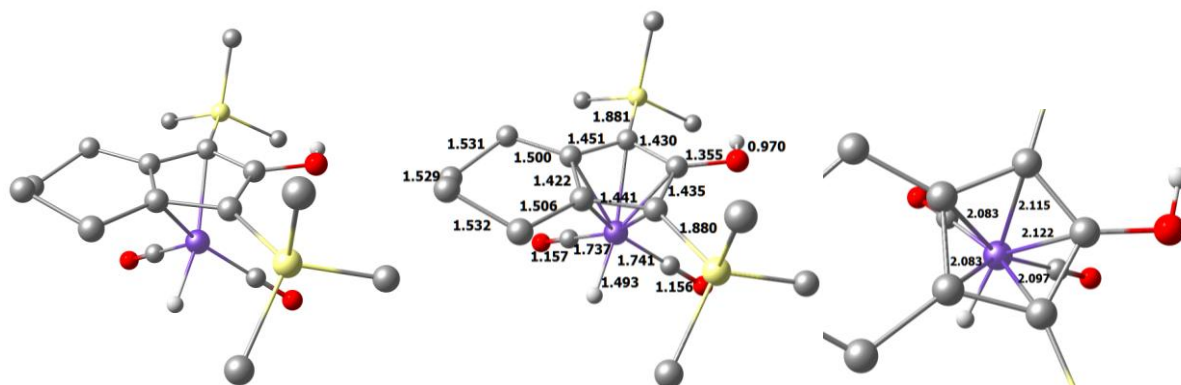


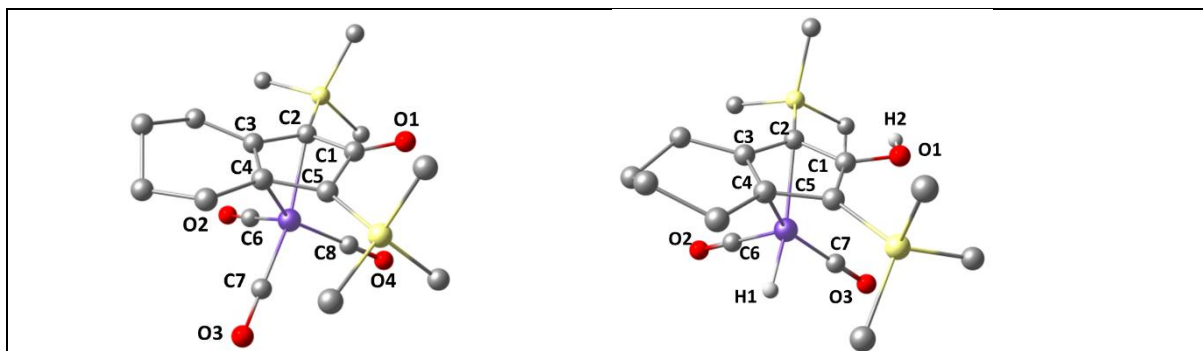
Figure S4. Geometry optimized structure of $[(\text{HL})\text{FeH}(\text{CO})_2]$ (**2**) and selected bond distances. H atoms are omitted except those of the hydride or hydroxyl group from the cyclopentadienyl ligand for clarity.

Table S2. Comparison of experimental and calculated first coordination sphere bond lengths (\AA) for $[\text{LFe}(\text{CO})_3]$ (**1**) and $[(\text{HL})\text{FeH}(\text{CO})_2]$ (**2**).^a

bond	$[\text{LFe}(\text{CO})_3]$ (exp)	$[\text{LFe}(\text{CO})_3]$ (calc)	$[(\text{HL})\text{FeH}(\text{CO})_2]$ (exp)	$[(\text{HL})\text{FeH}(\text{CO})_2]$ (calc)
Fe-C1	2.397(7)	2.358	2.1353(13)	2.122
Fe-C2	2.133(7)	2.117	2.1485(14)	2.115
Fe-C3	2.104(6)	2.088	2.0992(14)	2.083
Fe-C4	2.099(6)	2.073	2.0981(14)	2.083
Fe-C5	2.125(7)	2.113	2.1087(14)	2.097
Fe-C6	1.819(8)	1.772	1.741(2)	1.737
Fe-C7	1.777(8)	1.775	1.752(2)	1.741
Fe-C8	1.800(6)	1.787	-	
Fe-H1	-	-	1.38(2)	1.493

^a DFT: TPSSH/COSMO/ZORA/RIJCOSX/D3BJ/def2-TZVP/def2-TZVP/J

Atom numbering used:



The calculated Fe-H distance for $[(\text{HL})\text{FeH}(\text{CO})_2]$ is larger than the Fe-H distance from the X-ray experiment. The electron density map from X-ray crystallography with Fe(II) (24 electrons) can provide only an approximate position of the hydride (2 electrons). We assume that the position of the hydride from the DFT calculation of $[(\text{HL})\text{FeH}(\text{CO})_2]$ might provide a better determination of its location as it is additionally experimentally verified by the Mössbauer parameters.

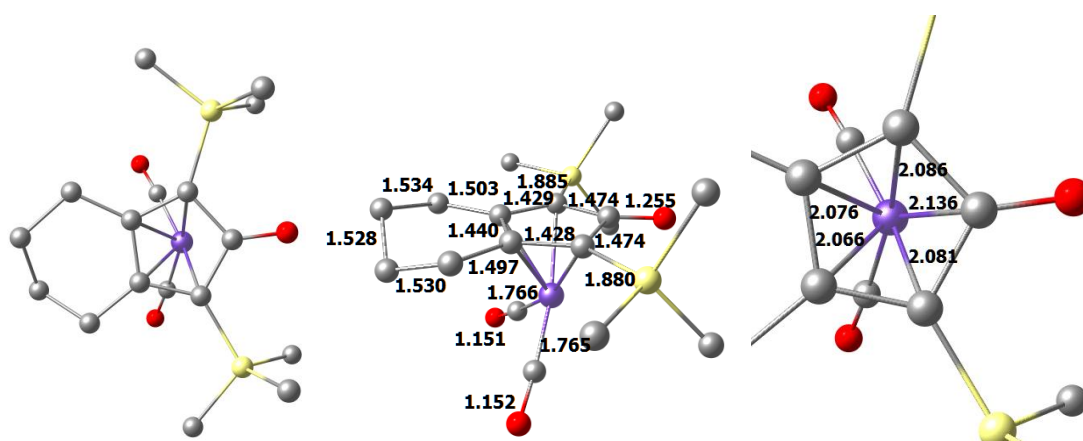


Figure S5. Geometry optimized structure of α - $[\text{LFe}(\text{CO})_2]$ and selected bond distances. H atoms are omitted for clarity.

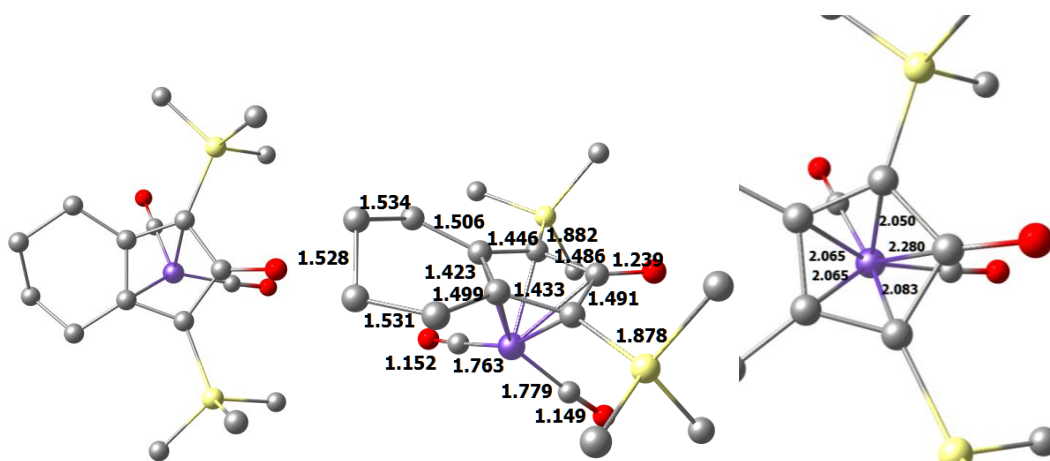


Figure S6. Geometry optimized structure of β - $[\text{LFe}(\text{CO})_2]$ and selected bond distances. H atoms are omitted for clarity.

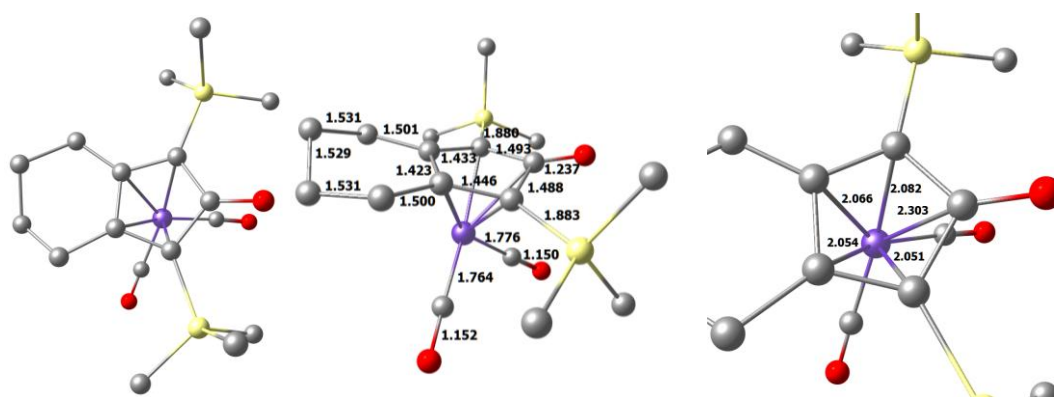


Figure S7. Geometry optimized structure of γ -[LFe(CO)₂] and selected bond distances. H atoms are omitted for clarity.

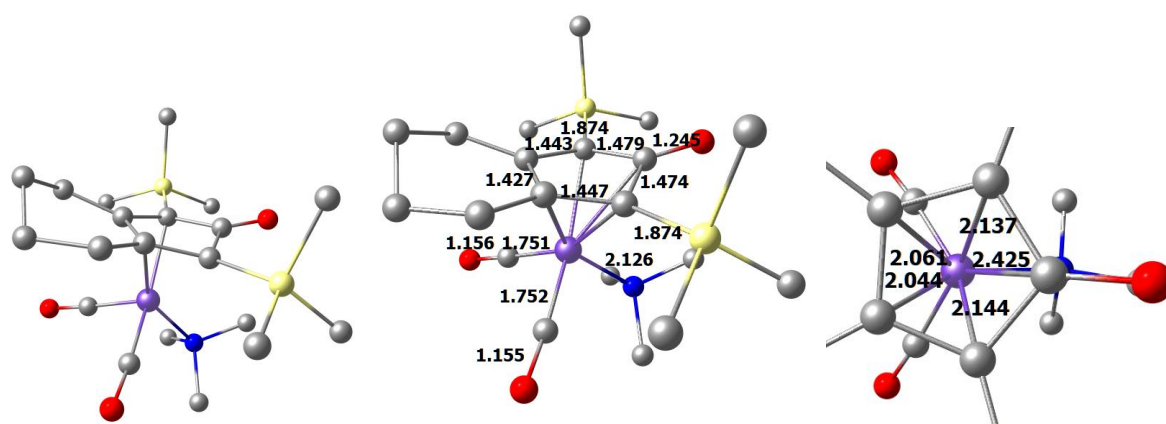


Figure S8. Geometry optimized structure of α -[LFe(CO)₂(NMe₃)] and selected bond distances. H atoms are omitted for clarity.

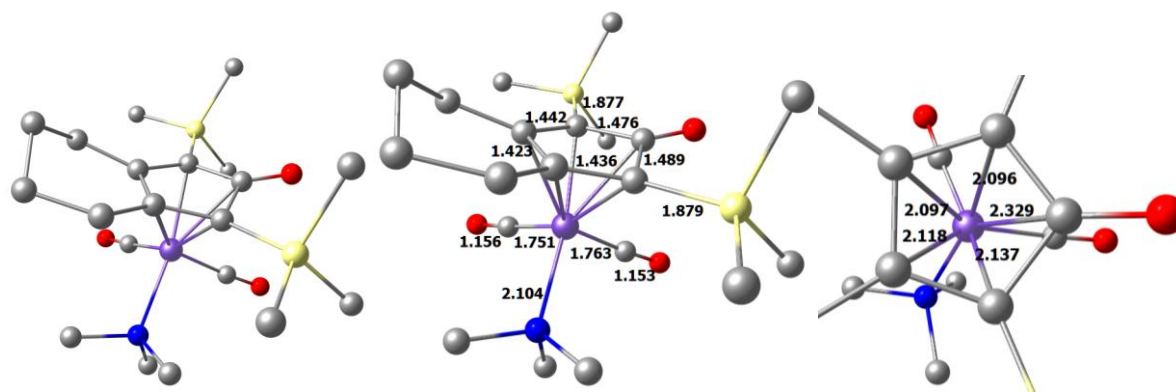


Figure S9. Geometry optimized structure of β -[LFe(CO)₂(NMe₃)] and selected bond distances. H atoms are omitted for clarity.

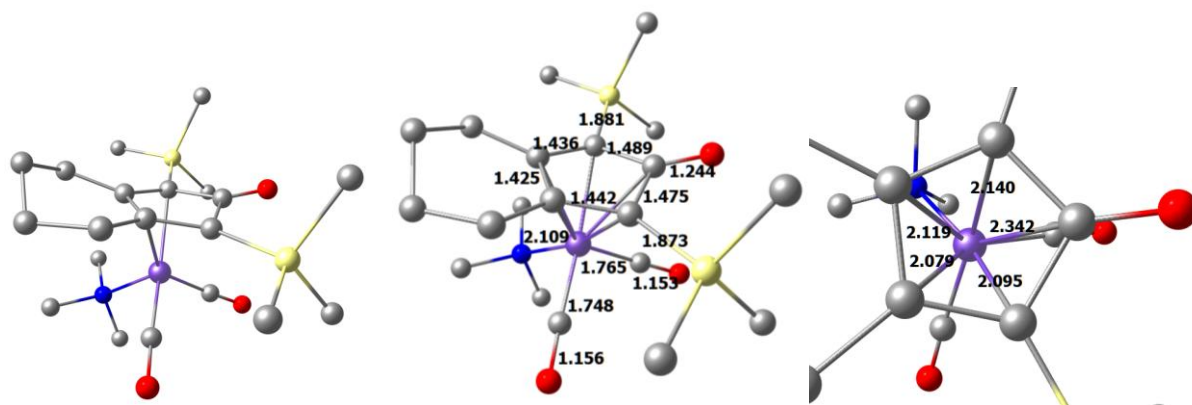


Figure S10. Geometry optimized structure of γ -[LFe(CO)₂(NMe₃)] and selected bond distances. H atoms are omitted for clarity.

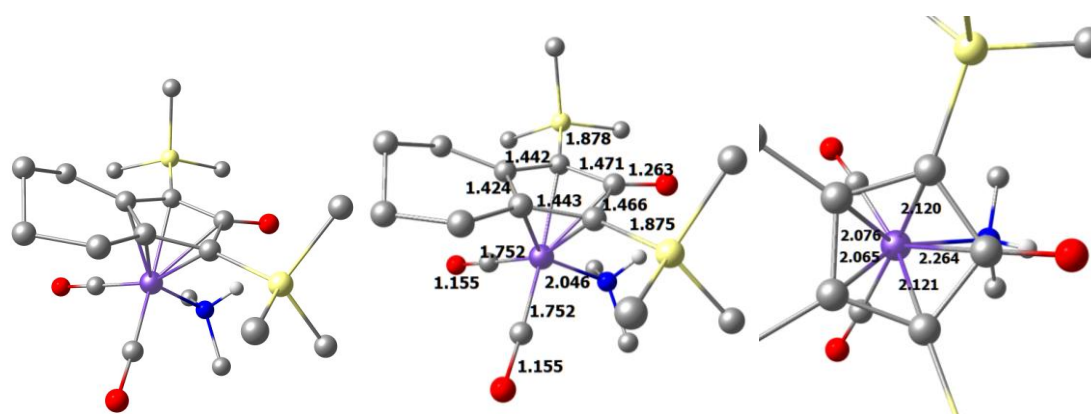


Figure S11. Geometry optimized structure of α -[LFe(CO)₂(NHMe₂)] and selected bond distances. H atoms are omitted for clarity except that bound to the nitrogen atom.

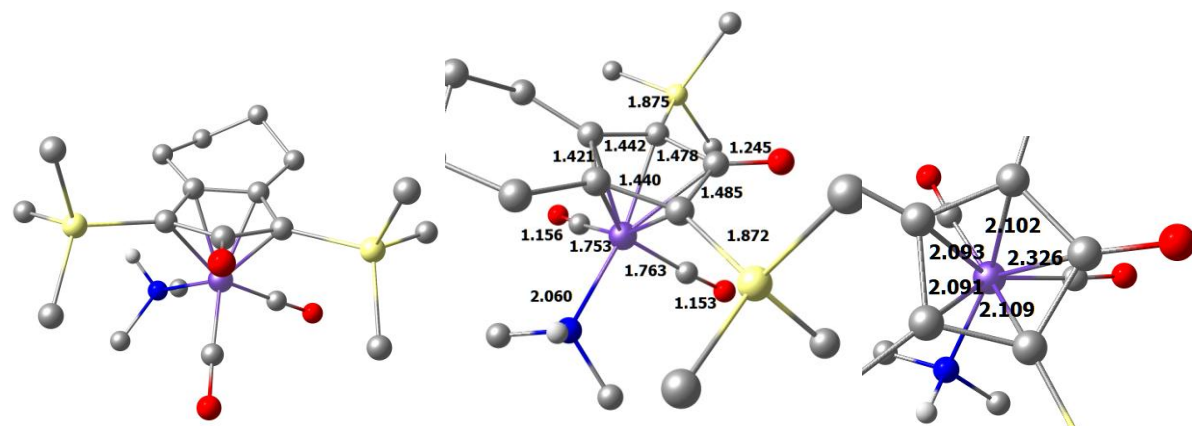


Figure S12. Geometry optimized structure of β -[LFe(CO)₂(NHMe₂)] and selected bond distances. H atoms are omitted for clarity except that bound to the nitrogen atom.

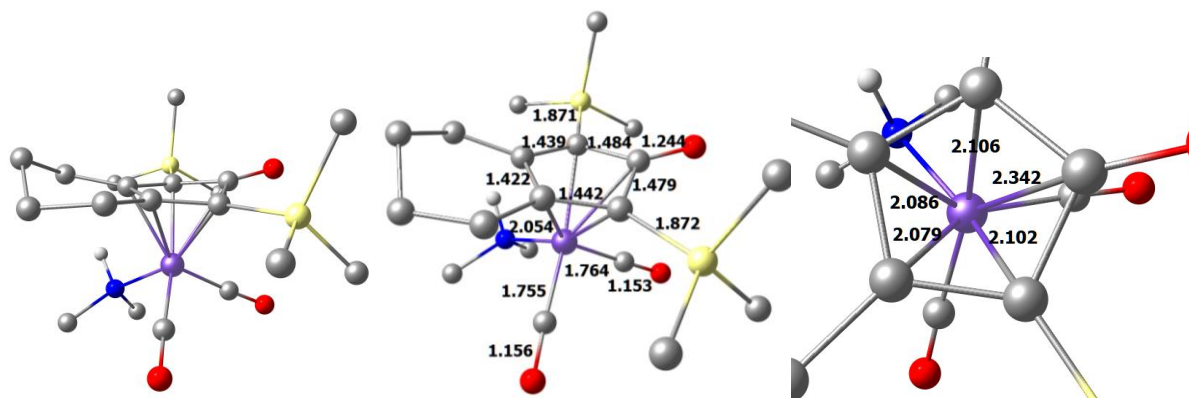


Figure S13. Geometry optimized structure of γ -[LFe(CO)₂(NHMe₂)] and selected bond distances. H atoms are omitted for clarity except that bound to the nitrogen atom.

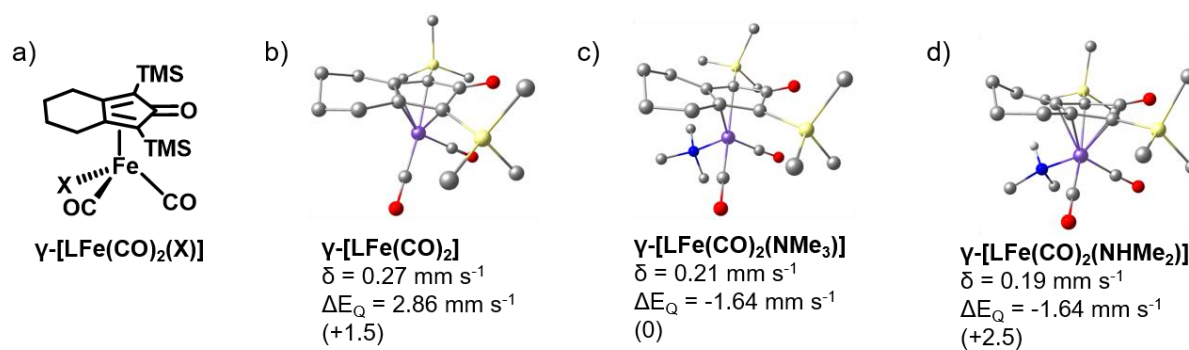


Figure S14. a) Scheme of the γ -isomer of [LFe(CO)₂(X)] (X=vacant, NMe₃, NHMe₂). (b-d) Geometry optimized structures and corresponding calculated Mössbauer nuclear parameters δ and ΔE_Q expressed in mm s⁻¹. H atoms omitted for clarity except that bound to the nitrogen atom. Energy are given in respect to their corresponding α -[LFe(CO)₂(X)] isomer (see main text).

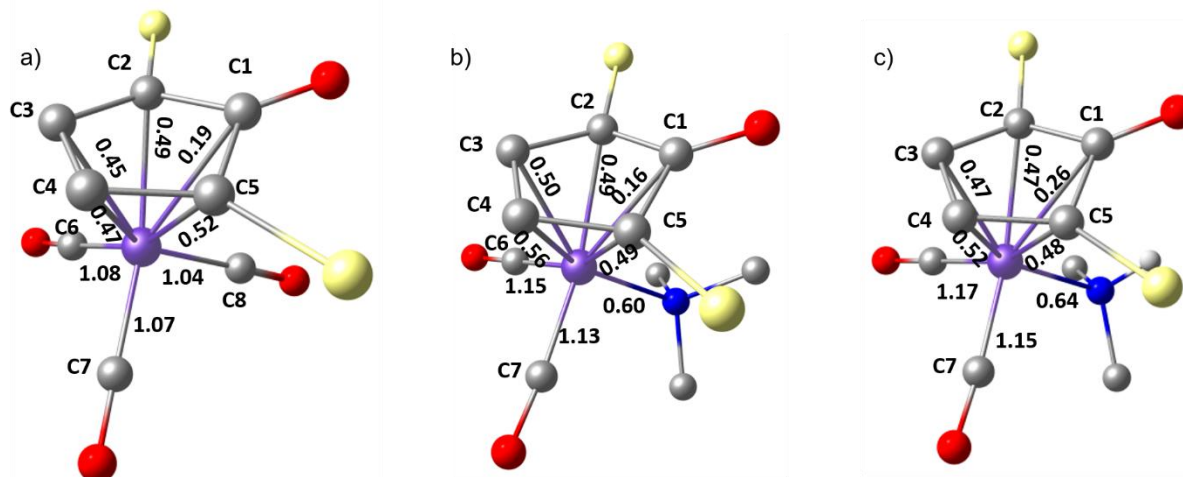


Figure S15. Analysis of the Mayer bond orders in a) [LFe(CO)₃], b) α -[LFe(CO)₂(NMe₃)] and c) α -[LFe(CO)₂(NHMe₂)]. Part of the ligand L and hydrogen atoms (except that bound to the nitrogen atom) are omitted for clarity.

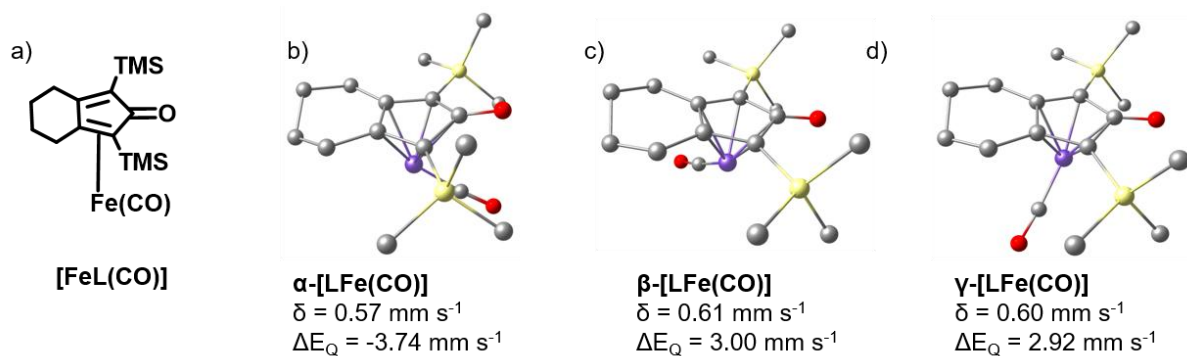


Figure S16. a) Scheme of the complex **[LFe(CO)]**. (b-d) Geometry optimized structures and corresponding calculated Mössbauer nuclear parameters δ and ΔE_Q expressed in mm s^{-1} . H atoms omitted for clarity.

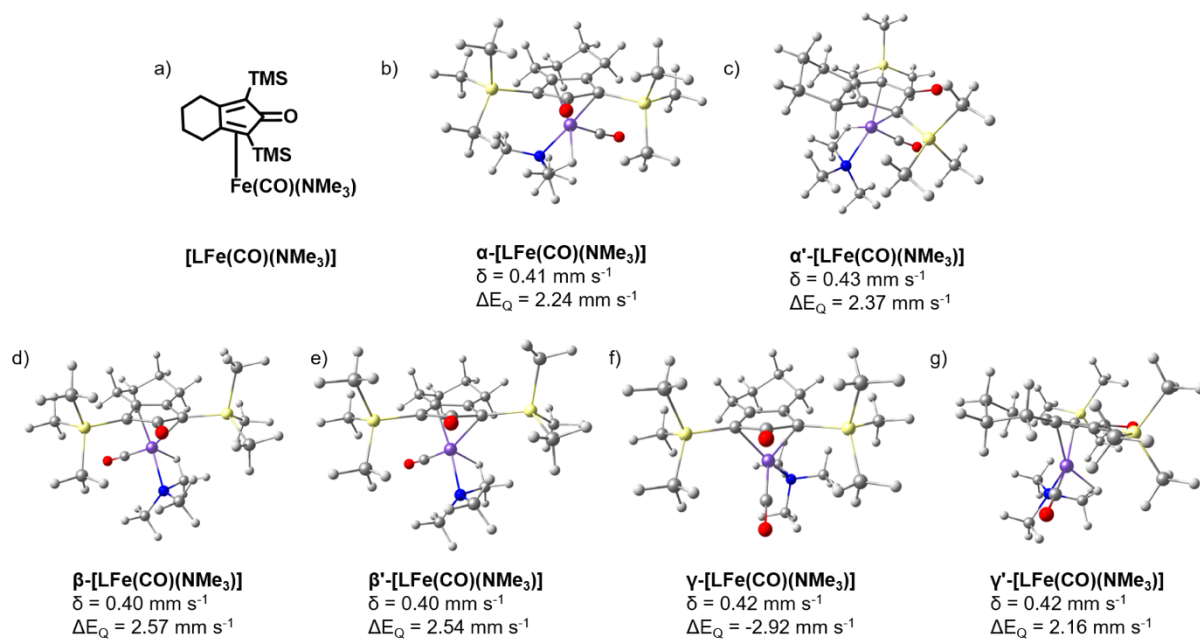


Figure S17. a) Scheme of the complex **[LFe(CO)(NMe₃)]**. (b-g) Geometry optimized structures and corresponding calculated Mössbauer nuclear parameters δ and ΔE_Q expressed in mm s^{-1} .

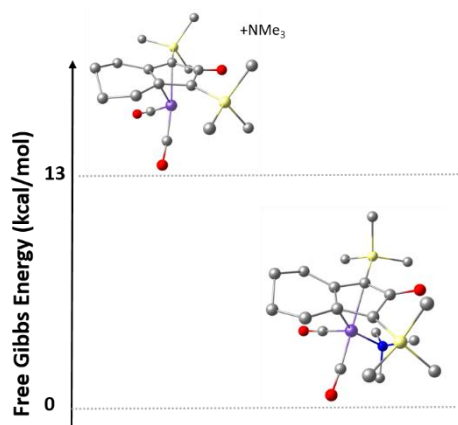


Figure S18. Gibbs free energy NMe₃ coordination pathway calculated for **α -[LFe(CO)₂]**.

We calculated the chemical shift for carbon atoms relative to the σ (^{13}C) of tetramethylsilane (TMS) as $\delta = \sigma_{\text{TMS}} - \sigma$. The results obtained for $[\text{LFe}(\text{CO})_3]$ and $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$ are represented in Figure S19. The computed chemical shifts are overestimated in both cases but the general trend when comparing $[\text{LFe}(\text{CO})_3]$ to $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$ is well reproduced by calculations. Indeed, the computed ^{13}C values for the coordinated CO ligands are uphill shifted by 9 ppm in α - $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$ as compared to $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$ which reproduces the observed experimental shift ($\delta = 209.2$ ppm and 214.8 ppm for $[\text{LFe}(\text{CO})_3]$ and $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$, respectively). Moreover, the ^{13}C chemical shift of the coordinated NMe_3 are predicted to be 59, 64 and 65 ppm for α - $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$ which compares well to the experimental value of 58 ppm. Note that the difference between theoretical and experimental results can be related to the use of a single conformer/rotamer in the theoretical methodology. However, these results further support the formation of $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$.

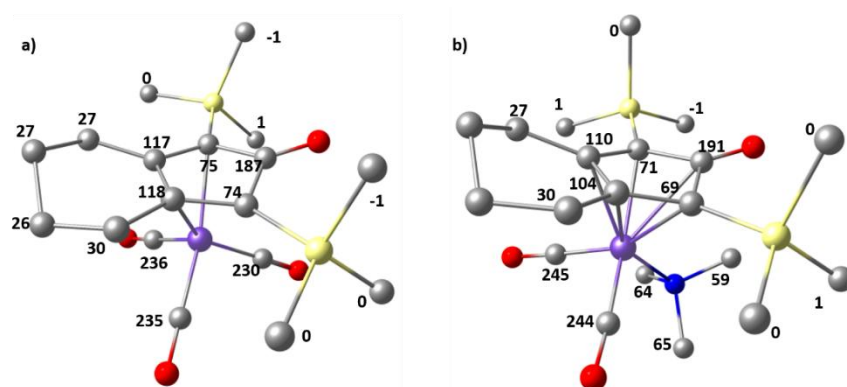


Figure S19. Computed ^{13}C chemical shift of complexes a) $[\text{LFe}(\text{CO})_3]$ and b) α - $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$.

NMR measurements

NMR spectra were recorded at 400 MHz on a Varian Avance III 400 spectrometer. An inverse gated decoupled methodology in which proton decoupling is only applied during the acquisition period was used to perform quantitative ^{13}C NMR. Applying a long relaxation delay ($D1 = 40$ s) allows quantitative measurement for all carbon atoms of $[\text{LFe}(\text{CO})_3]$ (Figure S18). However, it results in long acquisition time to achieve sufficient signal-to-noise ratio. In order to decrease the acquisition time, a 12 s relaxation delay was set up (with $P1 = 7$ μs) which allows quantitative measurement for the carbon atoms of the coordinated carbonyl ligands (at 209.2 ppm) and TMS groups (at -0.13 ppm) (Figure S19). The same methodology was applied for the sample of $[\text{LFe}(\text{CO})_3]$ reacted with 2 equivalents of Me_3NO in order to investigate the replacement of CO ligands by Me_3N (Figure S20).

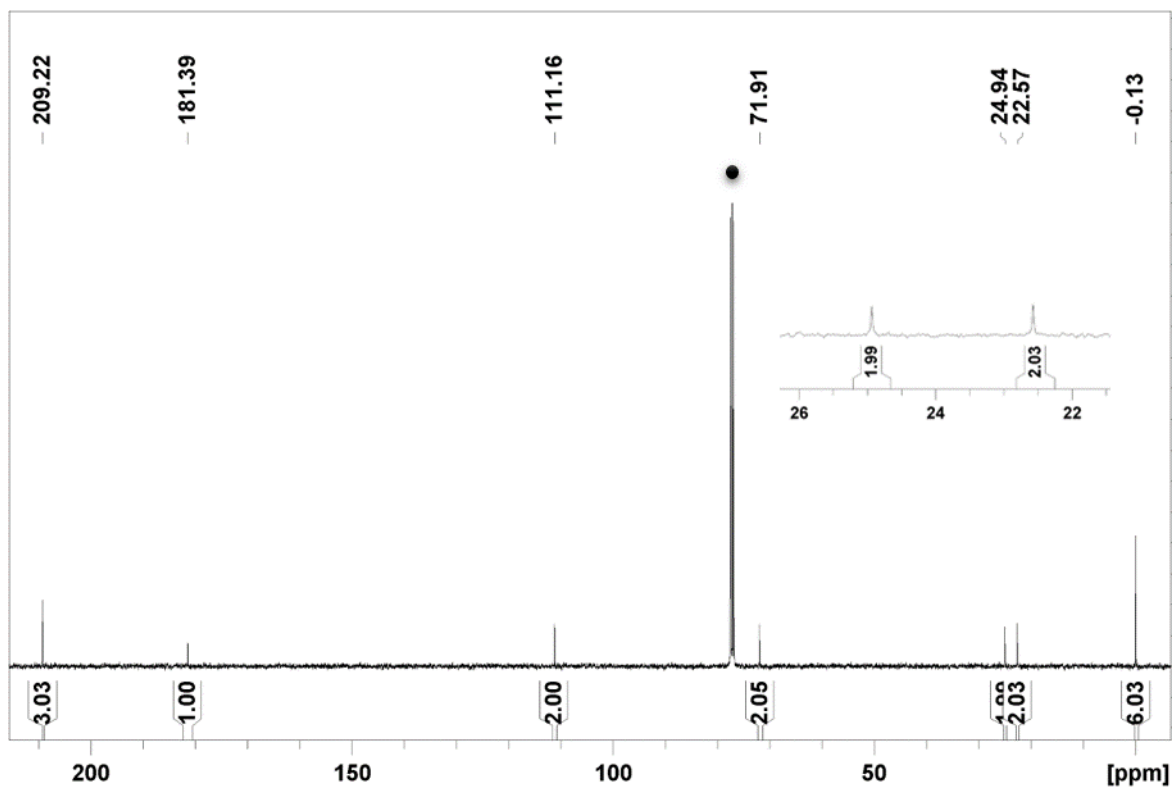


Figure S20. Inverse gated proton decoupled ^{13}C NMR spectra recorded in CDCl_3 of complex $[\text{LFe}(\text{CO})_3]$. Measurement parameters: $D1 = 40$ s, $P1 = 5$ μs , $T = 298$ K. Black dot denotes chloroform solvent resonances.

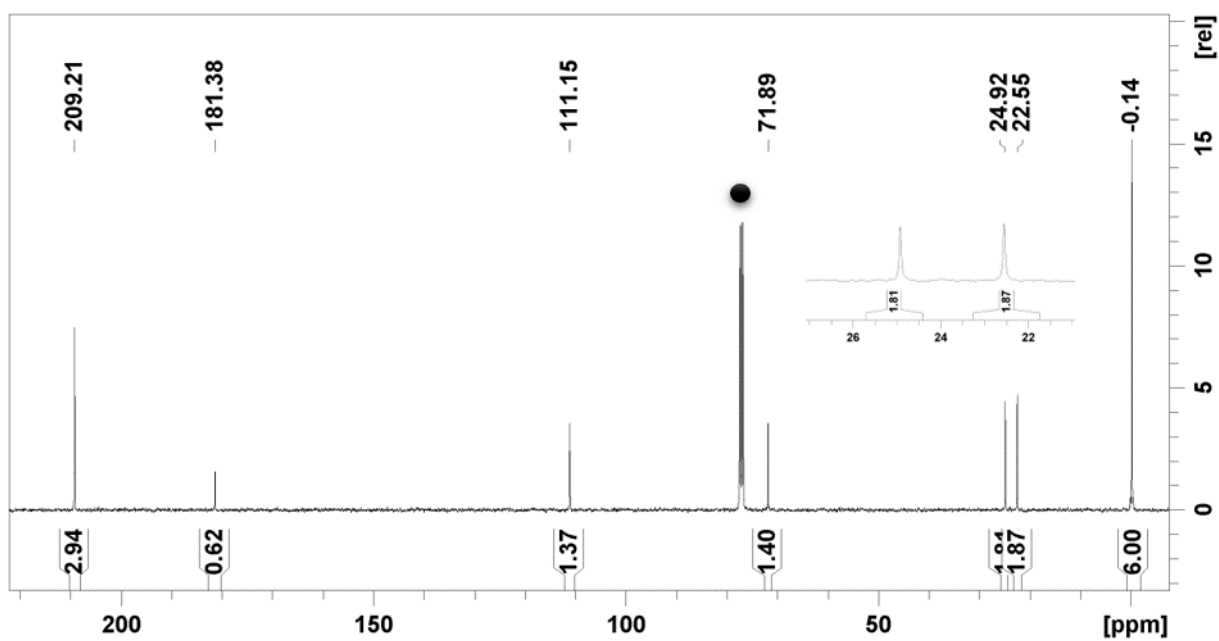


Figure S21. Inverse gated proton decoupled ^{13}C NMR spectra recorded in CDCl_3 of complex $[\text{LFe}(\text{CO})_3]$. Measurement parameters: $D1 = 12$ s, $P1 = 7$ μs , $T = 298$ K. Black dot denotes chloroform solvent resonances.

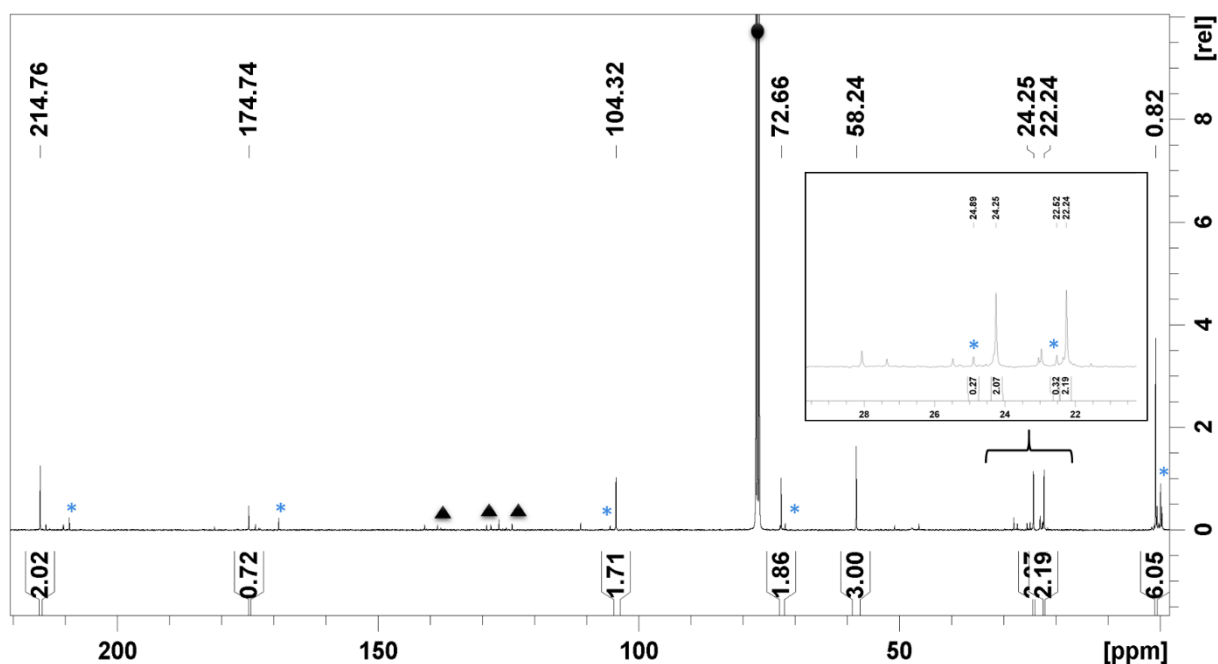


Figure S22. Inverse gated proton decoupled ^{13}C NMR spectra recorded in CDCl_3 of complex $[\text{LFe}(\text{CO})_3]$ reacted with 2 equivalents of Me_3NO ; including signal assignment. Measurement parameters: $D1 = 12 \text{ s}$, $P1 = 7 \mu\text{s}$, $T = 298 \text{ K}$. Blue stars denote $[\text{LFe}(\text{CO})_3]$ resonances, black triangles and dot denote toluene and chloroform solvent resonances, respectively. In addition to the resonances attributed to $[\text{LFe}(\text{CO})_2(\text{NMe}_3)]$ and $[\text{LFe}(\text{CO})_3]$ other set of signals with minor contribution are observed. These resonances might be due to the fast degradation of the species labeled **4** formed at the NMR time scale and therefore we refrain in attributing them.

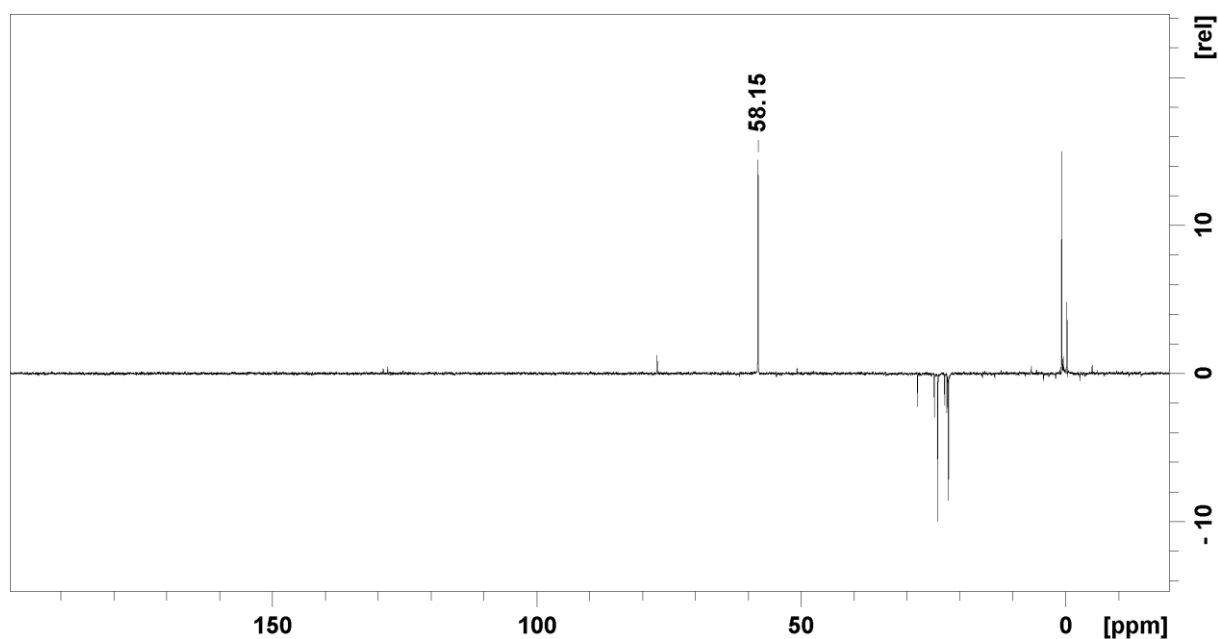


Figure S23. DEPT 135 NMR spectra recorded in CDCl_3 of complex $[\text{LFe}(\text{CO})_3]$ reacted with 2 equivalents of Me_3NO . $T = 298 \text{ K}$.

XYZ Coordinates of optimized structures:

[LFe(CO)₃] denoted 1:

Fe	0.37883463735411	3.49672626504899	-0.16977288766741
O	0.26034304573418	6.85682580709619	-0.10924010689449
O	-1.53562993445603	1.42635405220758	0.59651795965650
O	2.70542501772397	1.73996508571791	-0.31310805102866
Si	-2.68323471581282	5.46245393707207	-0.09136081723441
Si	3.02876168267338	5.66645164010319	-1.34838284169614
C	0.16439422118180	5.78085179096176	-0.71260400794764
C	1.26027932918694	5.01115523437718	-1.35692117947607
C	0.63535967751629	4.00931324756954	-2.17737093630521
C	1.24290754068045	3.21978960121589	-3.30672920848684
H	1.82720139735983	3.90790585106896	-3.92199783926619
H	1.94751369735692	2.47661406826762	-2.92785325602000
C	0.16934449515175	2.54007878165521	-4.16622438679369
H	-0.27691593939087	3.28094936225862	-4.83847985601320
H	0.64090351190151	1.78054031821741	-4.79326853498067
C	-0.94009776489678	1.92804866946674	-3.31243653426615
H	-0.50872977349272	1.22411140596321	-2.59207078249127
H	-1.63734364174281	1.36684826846112	-3.93825472319781
C	-1.69973149063571	3.02672710398862	-2.56720131234207
H	-2.26046637743975	3.63396521203419	-3.28846636418204
H	-2.43453310620729	2.60406430396153	-1.88182233362661
C	-0.75484835504286	3.94314034406737	-1.84748618469762
C	-1.04055874113216	4.91663343611259	-0.82867370036867
C	-2.44801962804324	5.78040384789028	1.73997997214932
H	-3.34387485222665	6.24564384784592	2.16261103640687
H	-1.59871726088838	6.44441823251777	1.91505765178712
H	-2.27023878546482	4.84556773840798	2.27921185760571
C	-4.03135090059902	4.17661759944345	-0.31449452890568
H	-4.93277796147274	4.52965681900310	0.19765768079466
H	-3.76132872233475	3.21243974676843	0.12410560973249
H	-4.28636989214655	4.01784000238854	-1.36480368981594
C	-3.16025931781372	7.04708594642917	-0.97943322891731
H	-4.08516070855459	7.45763592686287	-0.56218477913810
H	-3.31991977107980	6.87041231371198	-2.04719333829282
H	-2.37150954739418	7.79549508608659	-0.86961221934884
C	4.21110640444907	4.55664502761648	-2.29210531786315
H	5.22365633121217	4.95758981345638	-2.17689662625129
H	3.98519179577605	4.53163390310829	-3.36076806700105
H	4.21643820479225	3.53042122472104	-1.91757936672691
C	3.58871174529728	5.81494557512765	0.43493204966052
H	4.54821111999614	6.33727499093750	0.49777132868120
H	3.71270933592296	4.82938868227958	0.89247223685316
H	2.85454995226445	6.37517579002681	1.01889475698018
C	2.97364210463865	7.35678877016869	-2.16135914439617
H	3.96977618923001	7.80960365936280	-2.17792025451799
H	2.30148580200175	8.01903811509808	-1.61043549643442
H	2.61413696106850	7.28829306081159	-3.19259305640552
C	-0.77412486547377	2.23023812682359	0.29691364170440

C	1.77993052860049	2.41409740249424	-0.24330806472784
C	0.67449156717499	4.13001773421273	1.47435333259153
O	0.86208675749611	4.51865922950501	2.53504290912224

[(HL)FeH(CO)₂] denoted 2:

Fe	2.63640135224687	1.21289378576395	3.19704413311531
C	0.61856240933722	0.95950700325212	2.59118819495071
O	0.13466519727642	0.76478152887368	1.34064000613786
H	0.22388112442011	-0.17000606107164	1.09727035228559
C	0.97687210165464	-0.05435813603293	3.53426066893652
C	1.33484131552374	0.67919217374449	4.73335275803000
C	1.68337991235379	0.13685581109111	6.08757141873386
H	2.33442394413239	-0.73402113221047	6.00541174434824
H	0.75612016888065	-0.20803801919157	6.56118325490124
C	2.32624831645693	1.21725405115568	6.96178152776469
H	2.41755523420539	0.84578632376990	7.98503028989637
H	3.33805326842390	1.42820112697850	6.59880273290503
C	1.49775035281921	2.50179049725227	6.93442849130232
H	1.89553965237163	3.22934671716177	7.64571898325891
H	0.47447944652127	2.26816733942570	7.24930649578377
C	1.46953882976599	3.12497990800910	5.53507083103374
H	0.67079496319161	3.86998531844309	5.47700757826146
H	2.40464958235957	3.65231350682136	5.33974561543864
C	1.24012976700610	2.07523063390643	4.47924249210456
C	0.83242750306000	2.27930540750903	3.11176970766878
Si	0.83089135196098	-1.90499082092544	3.22859365577904
C	1.24483562120466	-2.25211172201687	1.42148743364227
H	0.44926349574343	-1.97278978670502	0.72018423172196
H	1.38094530452204	-3.33109777876990	1.29554986190744
H	2.17101309312918	-1.76195930408480	1.11040237701772
C	-0.95749781173840	-2.38332005352555	3.54039756362419
H	-1.62670875566687	-1.77907985386153	2.92010436245220
H	-1.23508490484970	-2.22159812059255	4.58611811859815
H	-1.13248863061426	-3.43576932263090	3.29663744314522
C	1.98763509964569	-2.89836942662274	4.31302233459794
H	1.71810821194545	-2.83498484383140	5.36953272078157
H	3.02613494431102	-2.57775066126145	4.19856388576774
H	1.92504255737343	-3.94996676397043	4.01557617913963
Si	0.46773083936855	3.92347832960317	2.27535205953379
C	-1.21924827331911	4.48955796225939	2.88431331424623
H	-1.49086860242180	5.44719049382217	2.42891643885408
H	-1.23992339082717	4.61540387447247	3.97069296817749
H	-1.98840641434380	3.75934380471310	2.61526763445250
C	1.77856822488983	5.19115889791859	2.70817404304758
H	1.58402283819335	6.11301012674686	2.15023213097796
H	2.77195965962471	4.82716325703597	2.43308966235369
H	1.78769439767814	5.43778328878832	3.77193106122824
C	0.40588292861997	3.71702771677502	0.41341763756738
H	0.19172074836260	4.68647640159419	-0.04836323906990
H	-0.37467712291880	3.01563395330630	0.11385076378349

H	1.35674861337862	3.35268041210490	0.01593449836494
C	3.23399658758389	1.20178190290988	1.56143842103285
O	3.61662404052457	1.21290977348483	0.47044157385196
C	3.98659791016139	0.37402226897128	3.89807131226234
O	4.88543691128497	-0.16489696599512	4.38853029424099
H	3.45533808518597	2.44329517563576	3.41031098006175

α -[LFe(CO)₂]:

Fe	0.35037112620657	3.68458444688890	-0.22208978288899
O	0.31976257330879	6.62539794797921	0.08994638635395
O	-1.50231754220391	1.69552186457423	0.82906918540363
O	2.69146227797088	1.95798223274799	-0.03885925867091
Si	-2.69883710067983	5.51788582439502	-0.18993684654367
Si	3.00213929992914	5.71468318529763	-1.43909201978812
C	0.15604000639891	5.73683102343482	-0.78137923578243
C	1.23669989212402	5.05766066688751	-1.51781561498078
C	0.62385610297255	3.99860062160904	-2.25588333649376
C	1.25132216797864	3.08455685015870	-3.27100690071887
H	1.84924506953061	3.69096474075858	-3.95531027776771
H	1.94974433614478	2.40282641748610	-2.77947185176133
C	0.20384097071868	2.28508938089760	-4.05573605581231
H	-0.24003073955661	2.92756979576124	-4.82397005474041
H	0.69780536447969	1.45978143373644	-4.57291838115133
C	-0.91208124625341	1.76885155368940	-3.14865344689923
H	-0.48558402810192	1.16848960476185	-2.33750489627225
H	-1.59287625793660	1.12395283541675	-3.70835440659501
C	-1.69592360314806	2.94296903224727	-2.55961472197532
H	-2.24426964585590	3.45244790032329	-3.36208325076016
H	-2.44219630018341	2.60173542214041	-1.84217819679193
C	-0.77821634741559	3.94511024250349	-1.93239410845650
C	-1.08788638680286	4.97586511164337	-0.99426113511118
C	-2.45488028057122	5.61849333380960	1.66751316095984
H	-3.35552001544744	6.01635705466612	2.14599365954246
H	-1.61601417707612	6.27524877606379	1.90721484703542
H	-2.25176515357863	4.63423032260769	2.09914347513291
C	-4.09769411686141	4.32449370219419	-0.55894056408393
H	-5.00834474005059	4.69903536916662	-0.07923337790170
H	-3.90059875125611	3.32738064789369	-0.15564909100367
H	-4.29842821061145	4.23027695467245	-1.62884805017911
C	-3.10335437442188	7.22238881046965	-0.86887134244061
H	-4.00497670193775	7.61983797302794	-0.39240194757188
H	-3.27529108634025	7.19587483078902	-1.94888502898699
H	-2.27981002836128	7.91363197033783	-0.67063573989749
C	4.15358774219100	4.74899304750556	-2.56114644522013
H	5.16834841201543	5.14401347024502	-2.44710986785606
H	3.87590535475911	4.84302937051309	-3.61406246056804
H	4.17912030552802	3.68623904437626	-2.30626001995426
C	3.61593124859067	5.62150691341928	0.33269561745716
H	4.55650076589642	6.17230938376769	0.43501812933723
H	3.79648854906563	4.59160522774675	0.65082926362216
H	2.88268439680064	6.06726967644255	1.00905374830267
C	2.92530990006749	7.51321444325055	-1.96991156667987

H	3.91426372186952	7.97674645490782	-1.90256517897148
H	2.24298234610175	8.06338622095543	-1.31706000615672
H	2.56788156317082	7.61427583658997	-2.99904906580082
C	-0.75788234442713	2.49708210899259	0.46804083492992
C	1.76997468525962	2.64820192025002	-0.05466877484240

β -[LFe(CO)₂]:

Fe	0.41812812996151	3.59427816544398	-0.23605008670068
O	0.28585119270338	6.85510315744781	-0.10066752705421
O	2.78093132443333	1.89280364617381	-0.34451714716824
Si	-2.67714670710983	5.50156183436718	-0.12703170168553
Si	3.03696826551538	5.66188142370588	-1.35844763447889
C	0.17331611199286	5.80281022460824	-0.74532179417260
C	1.26020798672040	5.04287848720315	-1.41640960997369
C	0.62245628806515	4.04092195643203	-2.24203775133933
C	1.21156152940085	3.24053952912217	-3.37293434200039
H	1.72915393132203	3.92988598988884	-4.04509816416074
H	1.96942105831696	2.54520768160730	-3.00490473497062
C	0.12692807682831	2.47856815461230	-4.14523571244221
H	-0.38848029957494	3.16871298078619	-4.82224165109396
H	0.59603427672113	1.71081960323664	-4.76433481536598
C	-0.90295722301671	1.85983829191164	-3.20165347445898
H	-0.39689880302888	1.21381212507796	-2.47543992612436
H	-1.60429612091968	1.23261616637916	-3.75652423133514
C	-1.67773620470450	2.95516423634132	-2.46323013402304
H	-2.36065280316355	3.46003970681516	-3.15797601860180
H	-2.30313958521722	2.52884347347365	-1.67542154050482
C	-0.75527094999685	3.98762536345204	-1.88926541771251
C	-1.04042261141839	4.94430906402418	-0.86100646861933
C	-2.46778141341029	5.85028214343350	1.70241905096868
H	-3.36761139990740	6.33201469874840	2.09809154928790
H	-1.61579047482020	6.50963250341819	1.88102944842768
H	-2.30898066604174	4.92439496831209	2.26220764025695
C	-4.02518320981166	4.21225287082544	-0.33538953921534
H	-4.93488584368499	4.57828481634099	0.15271455078131
H	-3.75506398794057	3.26334277677986	0.13674303715176
H	-4.26413191701482	4.01855990508589	-1.38373624530811
C	-3.15689976752531	7.07719916826240	-1.03227128938994
H	-4.07843965168696	7.49675226878478	-0.61622532652182
H	-3.32108813518098	6.88836589602421	-2.09733234182151
H	-2.36624000950826	7.82592948336806	-0.93561802699842
C	4.18621163932134	4.60549664559981	-2.39941189185304
H	5.20648244562910	4.98740584531158	-2.28887698214202
H	3.92785999822315	4.64873000747873	-3.46029482615914
H	4.18731890283124	3.55823021027071	-2.08864906801763
C	3.60612078590183	5.66649954089567	0.42896965728519
H	4.57466923419174	6.16780591288285	0.52109038195840
H	3.71253222529113	4.65217553241059	0.82210688176305
H	2.88390948467871	6.20006773148025	1.05184931894507
C	3.01590975150695	7.41990125543076	-2.01432050924008
H	4.01746942185540	7.85874727406765	-1.97183527333385
H	2.34262193210373	8.03139986153274	-1.40900882627961

H	2.66943911104774	7.45641782369297	-3.05155384912283
C	1.82954665279169	2.53813586902690	-0.27447288034083
C	0.56202938492598	4.09733120897691	1.46413253757926
O	0.72442364240270	4.47337851944742	2.53806870532599

ν -[LFe(CO)₂]:

Fe	0.07682933781670	-0.00870766508028	-0.02894974111466
O	3.38229250899536	0.02330074859951	-0.01439345416139
O	-1.73504237744132	2.27318332255775	-0.07883259272983
Si	2.00422198352711	2.68470374531444	-1.23299144064437
Si	1.96246693043841	-3.03230786225161	0.17055446649865
C	2.30457903645095	-0.15508463848601	-0.59432486430873
C	1.49129293619779	-1.40608073433551	-0.64549427332923
C	0.50785181408298	-1.19281197271261	-1.66586958857697
C	-0.47304895746417	-2.19243596017467	-2.20577940152495
H	0.03840597836172	-3.14284207587539	-2.37932648496179
H	-1.23545059282226	-2.39695893553595	-1.44249710003909
C	-1.14441552961879	-1.69495550123124	-3.48901577934809
H	-0.43123736297643	-1.76555448449633	-4.31731454733524
H	-1.98561321613129	-2.34719757209133	-3.73299256382640
C	-1.61096271433347	-0.24590479948078	-3.34850017083287
H	-2.30069079803877	-0.16714875172292	-2.49964420103955
H	-2.16010421629399	0.06544411260020	-4.23978966147818
C	-0.42474290003880	0.69544595288745	-3.12315600268855
H	0.17030471460091	0.76231118941685	-4.04235458544644
H	-0.76965922207026	1.70542407501674	-2.89947683033710
C	0.47050719688378	0.18072367462528	-2.03577090204538
C	1.46241518863450	0.88164669834272	-1.25086552908189
C	2.16845844997034	3.21924059593624	0.55804832076440
H	2.63800314302095	4.20515283191015	0.62892287575757
H	2.78333337778471	2.50421296774931	1.10967035092381
H	1.19053556502685	3.27605906023054	1.04367937961653
C	0.79760250705401	3.81353031220449	-2.12312098563093
H	1.16755508030381	4.84145246834591	-2.04651864929567
H	-0.20171039229474	3.78813626810561	-1.68303881159799
H	0.71315702525177	3.56981998896771	-3.18516454048623
C	3.67097336241435	2.74686227581551	-2.09423103366263
H	4.06603588076615	3.76726509181507	-2.10195279677943
H	3.59163522529760	2.40365144337218	-3.13029451482450
H	4.38473474266902	2.10197816372467	-1.57599089183814
C	0.41894628990137	-4.03177815637162	0.56322359417124
H	0.69779040635328	-4.91100221080400	1.15307077141866
H	-0.09584077499975	-4.38445979841550	-0.33312831613343
H	-0.29100695860552	-3.44619604429373	1.15510745935747
C	2.88926712686522	-2.70601475565307	1.76652198529749
H	3.25522617974196	-3.65204903121988	2.17834931092032
H	2.24054589674971	-2.24302136042500	2.51446474753147
H	3.74002010724612	-2.04383916385698	1.59726367265197
C	3.05053002995503	-3.98090119456605	-1.03077248466420
H	3.36392086610697	-4.93675760781933	-0.59924629413205
H	3.94947204955407	-3.40870422001739	-1.27775716209176
H	2.51717375095543	-4.18988891464334	-1.96300858362687

C	-1.04590606830940	1.35114591005169	-0.04334180649868
C	0.61030216118397	0.17329080205375	1.65550194978742
O	1.00717058575621	0.36163963058635	2.71859013477224

α -[LFe(CO)₂(NMe₃):

26	0.000000000	0.000000000	0.000000000
8	3.475713000	0.000000000	0.000000000
8	-1.878209000	2.215100000	0.000000000
8	-2.172088000	-1.926125000	-0.012674000
14	2.243079000	2.869456000	-0.838327000
14	2.101203000	-2.985669000	-0.555194000
6	2.361182000	-0.028927000	-0.553060000
6	1.537197000	-1.222038000	-0.843714000
6	0.558387000	-0.799900000	-1.815665000
6	-0.225180000	-1.659279000	-2.776208000
1	0.440652000	-2.434253000	-3.165416000
1	-1.036069000	-2.185247000	-2.269646000
6	-0.791956000	-0.829970000	-3.934692000
1	0.009569000	-0.602973000	-4.646446000
1	-1.539411000	-1.421236000	-4.468748000
6	-1.390211000	0.486157000	-3.438899000
1	-2.143372000	0.283428000	-2.669089000
1	-1.892604000	1.010324000	-4.255310000
6	-0.291174000	1.378981000	-2.860073000
1	0.369375000	1.708226000	-3.672244000
1	-0.712628000	2.282477000	-2.418609000
6	0.546370000	0.625963000	-1.867838000
6	1.548553000	1.132696000	-0.955945000
6	2.880981000	3.257653000	0.884870000
1	3.382190000	4.231396000	0.874165000
1	3.602084000	2.507501000	1.216508000
1	2.070662000	3.312648000	1.617428000
6	0.993739000	4.196599000	-1.294563000
1	1.457164000	5.175691000	-1.131068000
1	0.094376000	4.147904000	-0.675473000
1	0.691325000	4.143848000	-2.342908000
6	3.679969000	2.936126000	-2.049890000
1	4.179581000	3.909749000	-2.021164000
1	3.335476000	2.760586000	-3.073683000
1	4.415491000	2.165792000	-1.801794000
6	0.643393000	-4.163952000	-0.428915000
1	1.018905000	-5.183003000	-0.288132000
1	0.019512000	-4.158104000	-1.325335000
1	0.005388000	-3.923229000	0.425611000
6	3.135072000	-3.151166000	1.003718000
1	3.594753000	-4.145014000	1.023825000
1	2.540985000	-3.047818000	1.914947000
1	3.927835000	-2.400885000	1.024566000
6	3.173327000	-3.451411000	-2.031224000
1	3.514947000	-4.488938000	-1.960238000
1	4.056187000	-2.806056000	-2.072641000
1	2.631769000	-3.336521000	-2.974466000

6	-1.124541000	1.342213000	0.063171000
6	-1.295986000	-1.175854000	0.056247000
7	0.409666000	-0.078882000	2.084665000
6	-0.029295000	-1.380697000	2.647247000
1	0.453828000	-2.187466000	2.101701000
1	0.249806000	-1.437195000	3.705555000
1	-1.109656000	-1.475171000	2.558268000
6	1.841014000	0.074260000	2.424166000
1	2.203149000	1.024898000	2.047419000
1	1.959074000	0.033631000	3.513296000
1	2.414897000	-0.721442000	1.962322000
6	-0.328767000	0.988237000	2.805714000
1	-1.396870000	0.878265000	2.626969000
1	-0.132899000	0.908170000	3.880870000
1	0.006830000	1.960927000	2.450474000

β -[LFe(CO)₂(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.324580000	0.000000000	0.000000000
8	1.255436000	2.631012000	0.000000000
8	-1.653497000	0.302432000	2.370700000
14	2.282780000	-0.674253000	-2.917260000
14	2.029307000	-0.753362000	2.851765000
6	2.244768000	-0.617910000	-0.044227000
6	1.429501000	-1.065836000	1.101185000
6	0.433599000	-1.968609000	0.578880000
6	-0.355823000	-3.013495000	1.326844000
1	0.228186000	-3.345355000	2.186609000
1	-1.288900000	-2.603571000	1.722773000
6	-0.665955000	-4.201554000	0.410801000
1	0.261127000	-4.744187000	0.193401000
1	-1.335059000	-4.895308000	0.925671000
6	-1.293317000	-3.729241000	-0.899499000
1	-2.206224000	-3.171635000	-0.669605000
1	-1.590624000	-4.582724000	-1.513340000
6	-0.316752000	-2.859199000	-1.700267000
1	0.428548000	-3.512302000	-2.170771000
1	-0.828453000	-2.361054000	-2.527246000
6	0.446909000	-1.890890000	-0.841875000
6	1.445748000	-0.946429000	-1.257390000
6	2.739277000	1.134989000	-3.124097000
1	3.389003000	1.264827000	-3.995569000
1	3.269365000	1.488832000	-2.237363000
1	1.857404000	1.764561000	-3.268756000
6	1.321540000	-1.230383000	-4.437791000
1	2.011825000	-1.177127000	-5.287538000
1	0.467588000	-0.595132000	-4.678365000
1	0.972670000	-2.263288000	-4.362880000
6	3.848593000	-1.720036000	-2.861109000
1	4.467778000	-1.537150000	-3.745227000
1	3.603778000	-2.786771000	-2.837142000
1	4.433783000	-1.481524000	-1.969963000

6	0.880363000	-1.443602000	4.170109000
1	1.239380000	-1.108372000	5.149248000
1	0.874262000	-2.536496000	4.178623000
1	-0.148358000	-1.095416000	4.054826000
6	2.212148000	1.098146000	3.104353000
1	2.709617000	1.316959000	4.054530000
1	1.237296000	1.593622000	3.111765000
1	2.806328000	1.528697000	2.295006000
6	3.705395000	-1.587015000	3.014955000
1	4.139526000	-1.408869000	4.003849000
1	4.389799000	-1.194991000	2.258488000
1	3.623153000	-2.668805000	2.869791000
6	0.726070000	1.606525000	-0.022799000
6	-1.028640000	0.195430000	1.403946000
7	-1.570490000	0.550576000	-1.287132000
6	-1.134239000	0.580095000	-2.698366000
1	-0.834931000	-0.418115000	-2.998403000
1	-1.957336000	0.918611000	-3.337132000
1	-0.291454000	1.260000000	-2.799090000
6	-2.728175000	-0.370207000	-1.183508000
1	-3.086486000	-0.391972000	-0.156482000
1	-3.532540000	-0.026335000	-1.842959000
1	-2.423601000	-1.366651000	-1.484740000
6	-2.066052000	1.911687000	-0.956085000
1	-1.272018000	2.637680000	-1.114866000
1	-2.910267000	2.157290000	-1.608788000
1	-2.391930000	1.945627000	0.081463000

y-[LFe(CO)₂(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.344961000	0.000000000	0.000000000
8	-1.682794000	2.365123000	0.000000000
8	1.258206000	0.420682000	2.596221000
14	2.057941000	2.743456000	-1.077746000
14	2.286574000	-2.958120000	-0.256045000
6	2.260770000	-0.112139000	-0.599845000
6	1.460071000	-1.353738000	-0.785376000
6	0.469562000	-1.049740000	-1.780013000
6	-0.303223000	-2.010399000	-2.642991000
1	0.381199000	-2.798026000	-2.969077000
1	-1.086026000	-2.522918000	-2.079315000
6	-0.910507000	-1.318800000	-3.873585000
1	-0.127278000	-1.183981000	-4.627374000
1	-1.668942000	-1.970136000	-4.314210000
6	-1.500298000	0.053395000	-3.544383000
1	-2.270431000	-0.039259000	-2.773385000
1	-1.984133000	0.476259000	-4.428010000
6	-0.404365000	1.001148000	-3.057957000
1	0.252715000	1.258571000	-3.898205000
1	-0.830050000	1.940377000	-2.702027000
6	0.441929000	0.357575000	-1.999493000
6	1.441456000	0.976720000	-1.164741000

6	2.303741000	3.226621000	0.719259000
1	2.801436000	4.198859000	0.791657000
1	2.916967000	2.484279000	1.235087000
1	1.345888000	3.298210000	1.242234000
6	0.886870000	3.978471000	-1.872667000
1	1.307500000	4.981993000	-1.745053000
1	-0.102277000	3.973139000	-1.409078000
1	0.765112000	3.802582000	-2.944320000
6	3.705060000	2.815220000	-1.984964000
1	4.169179000	3.799503000	-1.865195000
1	3.577045000	2.631360000	-3.056107000
1	4.386969000	2.060014000	-1.586115000
6	1.320565000	-4.542100000	-0.578373000
1	2.027288000	-5.376025000	-0.505662000
1	0.874215000	-4.576796000	-1.575320000
1	0.532306000	-4.720367000	0.155187000
6	2.708586000	-2.866363000	1.571786000
1	3.316588000	-3.726281000	1.871140000
1	1.810842000	-2.859586000	2.195755000
1	3.270532000	-1.952382000	1.773986000
6	3.867949000	-3.045669000	-1.273212000
1	4.457112000	-3.928968000	-1.007067000
1	4.473407000	-2.153507000	-1.098287000
1	3.639702000	-3.099890000	-2.342626000
6	-1.049975000	1.397575000	0.013917000
6	0.722256000	0.215239000	1.595765000
7	-1.568559000	-1.232983000	0.682076000
6	-2.011051000	-0.797147000	2.032421000
1	-2.308321000	0.249132000	2.003416000
1	-2.862466000	-1.407649000	2.351627000
1	-1.196114000	-0.927159000	2.740999000
6	-2.762096000	-1.176373000	-0.197115000
1	-2.498683000	-1.504289000	-1.197436000
1	-3.543204000	-1.832499000	0.201654000
1	-3.136020000	-0.155276000	-0.235425000
6	-1.151013000	-2.645644000	0.797526000
1	-0.287265000	-2.708608000	1.454837000
1	-1.969600000	-3.245294000	1.210446000
1	-0.891703000	-3.026585000	-0.184266000

α -[LFe(CO)₂(NHMe₂):

Fe	0.275563	3.366885	-0.112377
O	0.186657	6.484015	0.546271
O	-1.753963	1.369729	0.462667
O	2.334178	1.351436	-0.483990
Si	-2.791855	5.481500	-0.092200
Si	2.925928	5.699762	-1.275456
C	0.089108	5.609388	-0.359880
C	1.192781	4.994894	-1.113682
C	0.595017	4.065478	-2.040782
C	1.250545	3.370989	-3.207463
H	1.903013	4.083154	-3.718923

H	1.896986	2.559985	-2.865695
C	0.207129	2.821921	-4.186722
H	-0.210384	3.647292	-4.774369
H	0.694334	2.140773	-4.888188
C	-0.932961	2.121573	-3.447564
H	-0.524487	1.343094	-2.793352
H	-1.606133	1.632679	-4.155636
C	-1.719636	3.133117	-2.611897
H	-2.264158	3.808193	-3.283693
H	-2.471048	2.635225	-1.997695
C	-0.799242	3.967120	-1.770076
C	-1.125880	4.854119	-0.680102
C	-2.912001	5.518755	1.779669
H	-3.781983	6.111035	2.081550
H	-2.022137	5.973921	2.219970
H	-3.037234	4.515782	2.196650
C	-4.229075	4.471488	-0.754213
H	-5.157465	4.892754	-0.353461
H	-4.178809	3.424851	-0.441289
H	-4.290737	4.502688	-1.844639
C	-2.922415	7.240163	-0.747732
H	-3.859801	7.707304	-0.429517
H	-2.885945	7.260449	-1.841097
H	-2.091418	7.840550	-0.368215
C	4.207915	4.341205	-1.471054
H	5.192372	4.793648	-1.630349
H	3.997177	3.690912	-2.323004
H	4.268319	3.714164	-0.577425
C	3.402140	6.798510	0.167508
H	4.340434	7.309960	-0.072962
H	3.554837	6.243748	1.095696
H	2.629518	7.547988	0.348112
C	2.884745	6.778000	-2.819682
H	3.872553	7.203140	-3.023886
H	2.184600	7.607105	-2.676651
H	2.565815	6.222054	-3.705151
C	-0.941091	2.168304	0.276629
C	1.534163	2.162362	-0.295596
N	0.752198	3.972652	1.782470
C	2.181087	3.809587	2.133826
H	2.798846	4.207444	1.334382
H	2.405835	4.331868	3.068464
H	2.397580	2.748861	2.258925
C	-0.076292	3.430238	2.880866
H	0.093675	2.356347	2.955374
H	0.197645	3.901810	3.829386
H	-1.124969	3.618473	2.672069
H	0.567598	4.983986	1.711461

β -[LFe(CO)₂(NHMe₂):

26	0.000000000	0.000000000	0.000000000
8	3.328525000	0.000000000	0.000000000

8	1.142826000	2.681134000	0.000000000
8	-1.744296000	0.441800000	2.283285000
14	2.100159000	-0.610293000	-2.926156000
14	2.037819000	-0.662777000	2.884349000
6	2.244431000	-0.611807000	-0.019804000
6	1.434668000	-1.023772000	1.145765000
6	0.433505000	-1.939237000	0.656820000
6	-0.383146000	-2.936793000	1.438531000
1	0.229524000	-3.325017000	2.254556000
1	-1.252405000	-2.462634000	1.901361000
6	-0.839146000	-4.088077000	0.536085000
1	0.022831000	-4.718059000	0.288547000
1	-1.553240000	-4.714360000	1.076136000
6	-1.457274000	-3.560927000	-0.756993000
1	-2.287596000	-2.892410000	-0.509872000
1	-1.873123000	-4.379653000	-1.348855000
6	-0.411843000	-2.817727000	-1.593859000
1	0.265261000	-3.546786000	-2.056280000
1	-0.887694000	-2.301917000	-2.433959000
6	0.435016000	-1.897056000	-0.764043000
6	1.432188000	-0.960934000	-1.212961000
6	2.623155000	1.186894000	-3.062576000
1	3.185845000	1.345067000	-3.988276000
1	3.258767000	1.456024000	-2.216482000
1	1.767747000	1.866798000	-3.074764000
6	0.853815000	-0.989460000	-4.283181000
1	1.296440000	-0.716257000	-5.247159000
1	-0.075099000	-0.420090000	-4.185532000
1	0.599215000	-2.051192000	-4.325649000
6	3.605367000	-1.710314000	-3.165440000
1	4.081303000	-1.519557000	-4.132615000
1	3.330290000	-2.768723000	-3.125115000
1	4.339926000	-1.518320000	-2.378552000
6	0.870437000	-1.307403000	4.208477000
1	1.220591000	-0.953141000	5.183944000
1	0.846508000	-2.399518000	4.242477000
1	-0.151923000	-0.947583000	4.070604000
6	2.217311000	1.195573000	3.083637000
1	2.710148000	1.444283000	4.028785000
1	1.239628000	1.685681000	3.073606000
1	2.811445000	1.606013000	2.263891000
6	3.711802000	-1.496071000	3.081033000
1	4.128982000	-1.313258000	4.076283000
1	4.410477000	-1.109137000	2.334979000
1	3.629952000	-2.578451000	2.940235000
6	0.664003000	1.632370000	-0.029807000
6	-1.091230000	0.270684000	1.345229000
7	-1.415231000	0.263935000	-1.472789000
6	-1.319522000	1.533961000	-2.228682000
1	-0.310088000	1.650104000	-2.613983000
1	-2.031891000	1.537113000	-3.058609000
1	-1.548323000	2.359779000	-1.556696000

6	-2.822938000	0.052447000	-1.057824000
1	-3.111263000	0.855497000	-0.381538000
1	-3.481705000	0.065438000	-1.930519000
1	-2.911790000	-0.900310000	-0.542015000
1	-1.189693000	-0.480429000	-2.128691000

γ -[LFe(CO)₂(NHMe₂):

26	0.000000000	0.000000000	0.000000000
8	3.353251000	0.000000000	0.000000000
8	1.136849000	2.684889000	0.000000000
8	-1.878927000	0.412612000	-2.183268000
14	2.073523000	-0.557938000	-2.903880000
14	2.070184000	-0.688056000	2.909773000
6	2.263555000	-0.599125000	-0.004183000
6	1.445334000	-0.986431000	1.171214000
6	0.457242000	-1.915453000	0.689065000
6	-0.373151000	-2.883067000	1.487956000
1	0.244837000	-3.298196000	2.288149000
1	-1.212500000	-2.386422000	1.988138000
6	-0.909718000	-4.014398000	0.603356000
1	-0.090777000	-4.703713000	0.369933000
1	-1.661237000	-4.581503000	1.157402000
6	-1.489072000	-3.477336000	-0.704647000
1	-2.273468000	-2.745011000	-0.486155000
1	-1.956401000	-4.284256000	-1.273923000
6	-0.396062000	-2.822828000	-1.551287000
1	0.265558000	-3.601350000	-1.952020000
1	-0.824919000	-2.309751000	-2.412974000
6	0.450023000	-1.893094000	-0.732963000
6	1.448637000	-0.957000000	-1.185405000
6	2.365515000	1.290660000	-3.045074000
1	2.878528000	1.529852000	-3.981930000
1	2.977473000	1.646484000	-2.213170000
1	1.418546000	1.837623000	-3.029028000
6	0.871590000	-1.079293000	-4.250123000
1	1.271794000	-0.761844000	-5.219095000
1	-0.109707000	-0.613647000	-4.128189000
1	0.734373000	-2.162907000	-4.284925000
6	3.694744000	-1.482780000	-3.134485000
1	4.151140000	-1.240819000	-4.099683000
1	3.538856000	-2.565331000	-3.095657000
1	4.397319000	-1.210180000	-2.342825000
6	0.736388000	-0.931501000	4.216221000
1	1.207490000	-0.842499000	5.201315000
1	0.262673000	-1.914708000	4.167668000
1	-0.046846000	-0.169222000	4.173869000
6	2.744633000	1.056300000	3.047504000
1	3.207734000	1.214013000	4.026764000
1	1.954949000	1.802417000	2.925726000
1	3.491486000	1.226306000	2.269917000
6	3.440651000	-1.942646000	3.194416000
1	3.879267000	-1.842473000	4.192038000

1	4.235035000	-1.803731000	2.455290000
1	3.058179000	-2.962944000	3.090130000
6	0.656908000	1.636502000	0.029594000
6	-1.165117000	0.255545000	-1.287835000
7	-1.340024000	0.225535000	1.540899000
6	-2.737392000	-0.155317000	1.231512000
1	-2.753151000	-1.143615000	0.778621000
1	-3.342011000	-0.159491000	2.142372000
1	-3.149718000	0.568074000	0.530173000
6	-1.328543000	1.543298000	2.216244000
1	-1.670946000	2.301243000	1.513608000
1	-1.992541000	1.529239000	3.085242000
1	-0.315554000	1.776565000	2.535385000
1	-0.995847000	-0.449404000	2.221303000

α -[LFe(CO)(NMe₃)₂]:

26	0.000000000	0.000000000	0.000000000
8	3.312509000	0.000000000	0.000000000
8	1.317948000	2.577382000	0.000000000
14	2.402382000	-1.282609000	-2.641194000
14	2.338308000	-0.503415000	2.909921000
6	2.227043000	-0.620924000	0.077846000
6	1.445763000	-0.875828000	1.305163000
6	0.475335000	-1.874959000	0.957048000
6	-0.196004000	-2.829267000	1.908261000
1	0.573401000	-3.193023000	2.595954000
1	-0.930000000	-2.333497000	2.547650000
6	-0.833617000	-4.027161000	1.189622000
1	-0.060060000	-4.777195000	0.991550000
1	-1.572152000	-4.496666000	1.844390000
6	-1.463735000	-3.630262000	-0.143775000
1	-2.224071000	-2.859739000	0.020358000
1	-1.968317000	-4.488501000	-0.594931000
6	-0.392754000	-3.100824000	-1.098481000
1	0.274685000	-3.926274000	-1.380524000
1	-0.854216000	-2.764411000	-2.029050000
6	0.430389000	-2.023480000	-0.450856000
6	1.435718000	-1.162346000	-1.040122000
6	3.006317000	0.407479000	-3.212165000
1	3.788680000	0.291669000	-3.969767000
1	3.420993000	0.944823000	-2.357110000
1	2.212871000	1.018267000	-3.651363000
6	1.568068000	-2.137699000	-4.105398000
1	2.356536000	-2.388056000	-4.824074000
1	0.840428000	-1.514104000	-4.627794000
1	1.075553000	-3.071845000	-3.820876000
6	3.897406000	-2.356539000	-2.233534000
1	4.601661000	-2.383291000	-3.071540000
1	3.584603000	-3.385215000	-2.025703000
1	4.414379000	-1.967295000	-1.353589000
6	1.444731000	-0.967668000	4.509881000
1	2.203161000	-1.069631000	5.294071000

1	0.912332000	-1.919826000	4.445598000
1	0.736844000	-0.204697000	4.841363000
6	2.820256000	1.312451000	3.001731000
1	3.516207000	1.483241000	3.829963000
1	1.956273000	1.964117000	3.154748000
1	3.304563000	1.602178000	2.067336000
6	3.903887000	-1.551757000	2.856860000
1	4.539633000	-1.354106000	3.726210000
1	4.467545000	-1.328464000	1.948407000
1	3.658670000	-2.619008000	2.853225000
6	0.723228000	1.575741000	-0.008915000
7	-1.564513000	0.538340000	1.458998000
6	-2.153356000	1.883070000	1.253468000
1	-2.812874000	1.881674000	0.391350000
1	-2.747553000	2.158410000	2.132769000
1	-1.360434000	2.614983000	1.114517000
6	-2.701395000	-0.398397000	1.641087000
1	-2.327817000	-1.396479000	1.838877000
1	-3.312757000	-0.070978000	2.490183000
1	-3.323177000	-0.421448000	0.753850000
6	-0.877654000	0.610331000	2.766517000
1	-0.040809000	1.299790000	2.696992000
1	-1.579322000	0.959459000	3.534599000
1	-0.516362000	-0.374394000	3.035674000
7	-1.270918000	0.433661000	-1.733005000
6	-2.636525000	-0.136801000	-1.679944000
1	-3.231540000	0.391458000	-0.941942000
1	-3.125778000	-0.024097000	-2.654492000
1	-2.582343000	-1.193037000	-1.424423000
6	-1.395878000	1.888653000	-2.003030000
1	-0.404550000	2.304710000	-2.167190000
1	-2.000042000	2.039025000	-2.905509000
1	-1.870417000	2.401213000	-1.175180000
6	-0.647159000	-0.108565000	-2.956107000
1	-0.560417000	-1.184556000	-2.883850000
1	-1.266053000	0.145257000	-3.825645000
1	0.335931000	0.333945000	-3.074444000

β -[LFe(CO)(NMe₃)₂]:

26	0.000000000	0.000000000	0.000000000
8	3.359471000	0.000000000	0.000000000
8	-1.946360000	2.133331000	0.000000000
14	2.462464000	-2.873125000	0.858427000
14	2.084053000	2.845055000	1.275397000
6	2.268061000	-0.048307000	0.630974000
6	1.462412000	1.089884000	1.094668000
6	0.432519000	0.533852000	1.943632000
6	-0.407847000	1.246403000	2.973920000
1	0.044652000	2.207355000	3.221391000
1	-1.410130000	1.464685000	2.595851000
6	-0.528747000	0.375251000	4.226267000
1	0.459272000	0.253259000	4.684949000

1	-1.172648000	0.867552000	4.960435000
6	-1.099016000	-0.993313000	3.859889000
1	-2.089764000	-0.847085000	3.415715000
1	-1.243133000	-1.601966000	4.756295000
6	-0.182826000	-1.755714000	2.892202000
1	0.641236000	-2.188910000	3.472582000
1	-0.714679000	-2.610282000	2.466991000
6	0.468301000	-0.880200000	1.852806000
6	1.510780000	-1.263797000	0.930147000
6	3.219653000	-3.229183000	-0.826284000
1	3.855105000	-4.119094000	-0.758624000
1	3.832463000	-2.389870000	-1.160064000
1	2.456498000	-3.424299000	-1.584607000
6	1.520700000	-4.433587000	1.346789000
1	2.265300000	-5.226698000	1.481375000
1	0.825393000	-4.773208000	0.576143000
1	0.970871000	-4.335942000	2.285721000
6	3.848738000	-2.665958000	2.121668000
1	4.532657000	-3.520808000	2.116739000
1	3.434323000	-2.569854000	3.130651000
1	4.418722000	-1.759272000	1.903052000
6	0.713403000	4.123523000	1.099725000
1	1.112862000	5.119012000	1.322092000
1	-0.125543000	3.938751000	1.774306000
1	0.318179000	4.139836000	0.080116000
6	3.480588000	3.325386000	0.106786000
1	3.991281000	4.201195000	0.521654000
1	3.129480000	3.588616000	-0.893265000
1	4.202586000	2.511592000	0.012589000
6	2.821359000	2.948229000	3.012648000
1	3.181184000	3.960160000	3.225563000
1	3.672576000	2.264252000	3.092491000
1	2.104240000	2.673312000	3.790237000
6	-1.178986000	1.256341000	-0.041498000
7	0.677236000	0.423708000	-2.019371000
6	-0.333414000	0.829143000	-3.028793000
1	-0.976019000	1.603971000	-2.613825000
1	0.183932000	1.228865000	-3.908125000
1	-0.931888000	-0.013789000	-3.345091000
6	1.602522000	1.580437000	-1.941094000
1	2.434517000	1.337417000	-1.289013000
1	1.980113000	1.808092000	-2.946905000
1	1.052177000	2.440775000	-1.564889000
6	1.441256000	-0.724464000	-2.551821000
1	0.783497000	-1.586595000	-2.648893000
1	1.856607000	-0.480434000	-3.538694000
1	2.248883000	-0.946292000	-1.859423000
7	-1.453207000	-1.500407000	-0.504331000
6	-2.127775000	-1.421462000	-1.818771000
1	-1.425575000	-1.678167000	-2.607109000
1	-2.948975000	-2.146784000	-1.844494000
1	-2.528694000	-0.422585000	-1.973392000

6	-0.876151000	-2.858959000	-0.424124000
1	-0.528303000	-3.040676000	0.584335000
1	-1.635290000	-3.605492000	-0.687858000
1	-0.037092000	-2.937062000	-1.111877000
6	-2.541747000	-1.403928000	0.500404000
1	-3.067532000	-0.460290000	0.370237000
1	-3.248006000	-2.231195000	0.359241000
1	-2.124253000	-1.445829000	1.497800000

γ -[LFe(CO)(NMe₃)₂]:

26	0.000000000	0.000000000	0.000000000
8	3.498668000	0.000000000	0.000000000
8	-1.484264000	2.474924000	0.000000000
14	2.241660000	2.761889000	-1.057978000
14	2.392277000	-2.975695000	-0.540239000
6	2.373528000	-0.081601000	-0.541094000
6	1.577969000	-1.309821000	-0.764808000
6	0.627469000	-0.962819000	-1.787147000
6	0.050378000	-1.885112000	-2.832613000
1	0.693975000	-2.763385000	-2.915635000
1	-0.941625000	-2.271284000	-2.588355000
6	-0.017036000	-1.156867000	-4.180121000
1	1.001973000	-0.951058000	-4.526826000
1	-0.490640000	-1.804351000	-4.923057000
6	-0.785456000	0.157871000	-4.054220000
1	-1.805211000	-0.051863000	-3.719109000
1	-0.874595000	0.636150000	-5.033136000
6	-0.092087000	1.133603000	-3.089609000
1	0.698144000	1.656797000	-3.641036000
1	-0.793266000	1.904700000	-2.761669000
6	0.572666000	0.447459000	-1.926138000
6	1.551032000	1.029669000	-1.018322000
6	2.859207000	3.345022000	0.620698000
1	3.347796000	4.319456000	0.512426000
1	3.581868000	2.644240000	1.044026000
1	2.034610000	3.466319000	1.329551000
6	1.017129000	4.064419000	-1.647969000
1	1.518123000	5.038992000	-1.626608000
1	0.142565000	4.123201000	-0.996966000
1	0.668772000	3.889848000	-2.668451000
6	3.692641000	2.723530000	-2.260857000
1	4.202085000	3.690793000	-2.319322000
1	3.348488000	2.459622000	-3.266318000
1	4.415470000	1.966837000	-1.943541000
6	1.223366000	-4.453158000	-0.512132000
1	1.832658000	-5.364098000	-0.511267000
1	0.559124000	-4.502640000	-1.378242000
1	0.607211000	-4.468612000	0.390346000
6	3.426322000	-3.067466000	1.027878000
1	4.033376000	-3.979146000	1.008912000
1	2.815891000	-3.099024000	1.933918000
1	4.089188000	-2.202984000	1.091357000

6	3.554307000	-3.167183000	-2.014911000
1	4.101987000	-4.114495000	-1.980415000
1	4.281359000	-2.349475000	-2.017086000
1	3.005896000	-3.125548000	-2.960787000
6	-0.912922000	1.458068000	0.048856000
7	-1.853104000	-1.141027000	0.150422000
6	-2.758480000	-0.841327000	1.285608000
1	-2.949820000	0.229537000	1.325520000
1	-3.709174000	-1.366476000	1.137430000
1	-2.332007000	-1.175996000	2.225462000
6	-2.646357000	-0.775075000	-1.049812000
1	-2.062557000	-0.933430000	-1.944563000
1	-3.555244000	-1.387956000	-1.090084000
1	-2.925611000	0.274734000	-0.989220000
6	-1.637865000	-2.603828000	0.130834000
1	-1.155299000	-2.912287000	1.053569000
1	-2.597577000	-3.126591000	0.035901000
1	-0.999464000	-2.865846000	-0.704276000
7	0.461299000	-0.088808000	2.107467000
6	-0.371737000	0.845286000	2.904332000
1	-1.426468000	0.635017000	2.768335000
1	-0.119080000	0.748289000	3.967223000
1	-0.163017000	1.863367000	2.580347000
6	0.334708000	-1.447132000	2.683494000
1	0.883767000	-2.145536000	2.057994000
1	0.749276000	-1.459962000	3.698924000
1	-0.704504000	-1.751899000	2.738835000
6	1.862725000	0.314291000	2.361498000
1	2.043442000	1.288054000	1.919260000
1	2.033449000	0.355896000	3.444975000
1	2.539766000	-0.402390000	1.911309000

α -[LFe(CO)(NMe₃):

26	0.000000000	0.000000000	0.000000000
8	3.233148000	0.000000000	0.000000000
8	-1.990204000	2.104434000	0.000000000
14	2.295741000	-2.943546000	0.696855000
14	1.898881000	2.790203000	0.841349000
6	2.168187000	-0.084660000	0.659872000
6	1.365583000	1.033129000	1.176438000
6	0.302586000	0.459919000	1.960069000
6	-0.603975000	1.142834000	2.951045000
1	0.017831000	1.758096000	3.607591000
1	-1.288532000	1.831425000	2.452248000
6	-1.395833000	0.129180000	3.789682000
1	-0.753767000	-0.262914000	4.586875000
1	-2.232826000	0.637402000	4.274775000
6	-1.889100000	-1.048776000	2.947663000
1	-2.472323000	-0.679175000	2.097192000
1	-2.542612000	-1.693837000	3.540377000
6	-0.695610000	-1.856822000	2.434303000
1	-0.208123000	-2.353113000	3.283709000

1	-1.017033000	-2.649553000	1.755319000
6	0.297859000	-0.960451000	1.761295000
6	1.396952000	-1.315171000	0.910631000
6	2.875581000	-3.207647000	-1.074553000
1	3.619304000	-4.010955000	-1.099252000
1	3.346373000	-2.293451000	-1.444341000
1	2.073078000	-3.488160000	-1.761615000
6	1.319492000	-4.448074000	1.268446000
1	1.943621000	-5.334722000	1.111016000
1	0.382535000	-4.604959000	0.729656000
1	1.091575000	-4.388618000	2.336103000
6	3.825065000	-2.837457000	1.790923000
1	4.454972000	-3.723326000	1.659504000
1	3.551785000	-2.771996000	2.848532000
1	4.412938000	-1.953477000	1.531216000
6	0.716223000	4.057139000	1.567434000
1	1.067779000	5.062968000	1.313971000
1	0.661745000	3.986645000	2.657070000
1	-0.293875000	3.943565000	1.166382000
6	2.008861000	3.037914000	-1.020659000
1	2.484998000	3.992743000	-1.266829000
1	1.017546000	3.022049000	-1.483079000
1	2.603841000	2.231990000	-1.459063000
6	3.611538000	3.015570000	1.583690000
1	4.034849000	3.993869000	1.334172000
1	4.274036000	2.240504000	1.188995000
1	3.589572000	2.919032000	2.673812000
6	-1.207995000	1.245418000	-0.060048000
7	-0.861565000	-1.198112000	-1.345488000
6	-0.819570000	-2.662048000	-1.201265000
1	-1.618498000	-2.965463000	-0.526889000
1	-0.961111000	-3.145861000	-2.172302000
1	0.137202000	-2.949454000	-0.782733000
6	-2.166591000	-0.810914000	-1.928232000
1	-2.162723000	0.250501000	-2.162852000
1	-2.347096000	-1.384059000	-2.842788000
1	-2.949571000	-1.024215000	-1.202604000
6	0.271952000	-0.649149000	-2.106183000
1	1.076980000	-1.368531000	-2.208573000
1	-0.031454000	-0.252819000	-3.074861000
1	0.700729000	0.283547000	-1.581500000

α' -[LFe(CO)(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.291002000	0.000000000	0.000000000
8	1.239918000	2.625081000	0.000000000
14	1.946043000	-0.722625000	-2.856627000
14	1.785456000	-0.419913000	2.993521000
6	2.203104000	-0.609270000	0.045940000
6	1.381404000	-0.916206000	1.240630000
6	0.394498000	-1.875140000	0.818393000
6	-0.460974000	-2.772702000	1.673908000

1	0.049057000	-2.970888000	2.619376000
1	-1.411692000	-2.293517000	1.931019000
6	-0.737012000	-4.085415000	0.934080000
1	0.200698000	-4.642807000	0.829040000
1	-1.419870000	-4.704775000	1.521121000
6	-1.325586000	-3.811707000	-0.449067000
1	-2.257989000	-3.250913000	-0.320057000
1	-1.593550000	-4.748101000	-0.944709000
6	-0.348362000	-3.034469000	-1.340855000
1	0.407033000	-3.731805000	-1.724871000
1	-0.857509000	-2.637837000	-2.220242000
6	0.395714000	-1.964101000	-0.594651000
6	1.379341000	-1.045548000	-1.110898000
6	2.313138000	1.105249000	-3.082227000
1	2.796755000	1.285474000	-4.047794000
1	2.970737000	1.463839000	-2.287535000
1	1.391789000	1.693365000	-3.049777000
6	0.664247000	-1.210820000	-4.143829000
1	1.045851000	-0.949087000	-5.136814000
1	-0.275946000	-0.670638000	-4.003461000
1	0.446895000	-2.281457000	-4.142041000
6	3.515045000	-1.721863000	-3.150964000
1	3.938681000	-1.513721000	-4.138871000
1	3.315653000	-2.796255000	-3.088198000
1	4.264712000	-1.470424000	-2.395647000
6	0.205239000	-0.136483000	3.979588000
1	0.453221000	0.184611000	4.996785000
1	-0.410481000	-1.036420000	4.052828000
1	-0.400482000	0.651691000	3.522532000
6	2.785392000	1.166446000	3.004722000
1	3.113123000	1.408925000	4.020792000
1	2.185767000	2.000698000	2.630952000
1	3.660694000	1.069630000	2.359860000
6	2.777156000	-1.813152000	3.784622000
1	3.057293000	-1.576354000	4.816009000
1	3.694978000	-1.997816000	3.217490000
1	2.202259000	-2.744283000	3.797191000
6	0.683009000	1.605961000	-0.012976000
7	-1.748433000	0.421670000	-0.883057000
6	-1.912828000	1.761971000	-1.489149000
1	-1.382763000	1.779735000	-2.439960000
1	-2.974571000	1.967556000	-1.658154000
1	-1.495178000	2.515135000	-0.826884000
6	-2.503979000	-0.558684000	-1.684269000
1	-2.468061000	-1.528402000	-1.200846000
1	-3.545441000	-0.238515000	-1.782502000
1	-2.054352000	-0.623016000	-2.672722000
6	-2.090821000	0.382077000	0.539919000
1	-2.589033000	1.288918000	0.880050000
1	-2.672705000	-0.499237000	0.794739000
1	-1.141546000	0.370546000	1.213586000

β -[LFe(CO)(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.289588000	0.000000000	0.000000000
8	-2.041481000	2.058081000	0.000000000
14	1.931888000	2.783635000	-0.919629000
14	2.047902000	-3.063262000	-0.572278000
6	2.205933000	-0.102069000	-0.625831000
6	1.415440000	-1.321005000	-0.842176000
6	0.340825000	-0.975875000	-1.749095000
6	-0.580895000	-1.904975000	-2.498766000
1	-0.009698000	-2.767128000	-2.853940000
1	-1.352520000	-2.302417000	-1.833201000
6	-1.232258000	-1.197659000	-3.692351000
1	-0.492959000	-1.094373000	-4.495213000
1	-2.045178000	-1.815381000	-4.082488000
6	-1.740203000	0.193266000	-3.313838000
1	-2.430350000	0.112583000	-2.466613000
1	-2.295050000	0.637229000	-4.144248000
6	-0.571258000	1.104348000	-2.933809000
1	0.016762000	1.334333000	-3.831684000
1	-0.933103000	2.058328000	-2.549191000
6	0.342098000	0.431515000	-1.952246000
6	1.387598000	1.013082000	-1.139378000
6	2.093968000	3.144886000	0.916075000
1	2.574322000	4.112531000	1.091668000
1	2.689962000	2.368712000	1.401631000
1	1.108708000	3.166082000	1.389637000
6	0.717782000	4.017756000	-1.654677000
1	1.074579000	5.030493000	-1.436981000
1	-0.278717000	3.917503000	-1.216409000
1	0.626956000	3.920811000	-2.739411000
6	3.609977000	2.996067000	-1.744477000
1	4.003798000	4.003969000	-1.578076000
1	3.550235000	2.829139000	-2.824277000
1	4.317161000	2.274882000	-1.326469000
6	0.658656000	-4.325628000	-0.412901000
1	1.094359000	-5.283399000	-0.108156000
1	0.124354000	-4.484780000	-1.351849000
1	-0.077313000	-4.044776000	0.345181000
6	3.142665000	-3.259147000	0.942815000
1	3.671664000	-4.215284000	0.867087000
1	2.564588000	-3.279298000	1.870535000
1	3.880177000	-2.457032000	1.011556000
6	3.069970000	-3.461309000	-2.104240000
1	3.435939000	-4.492737000	-2.087776000
1	3.935673000	-2.794525000	-2.164644000
1	2.478741000	-3.322636000	-3.014366000
6	-1.244411000	1.211532000	0.009704000
7	0.265181000	-0.139952000	1.982505000
6	-0.569066000	-1.299297000	1.666604000
1	-0.007188000	-2.225579000	1.714177000
1	-1.465796000	-1.349604000	2.283248000

1	-1.030511000	-1.234793000	0.595142000
6	1.590605000	-0.482261000	2.528675000
1	2.137073000	0.444215000	2.689149000
1	1.479226000	-1.010208000	3.481025000
1	2.137222000	-1.082341000	1.811117000
6	-0.407734000	0.808744000	2.894905000
1	-1.417117000	1.008501000	2.543789000
1	-0.448827000	0.383353000	3.902663000
1	0.160477000	1.735952000	2.914783000

β' -[LFe(CO)(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.282361000	0.000000000	0.000000000
8	-2.106284000	1.991048000	0.000000000
14	1.921914000	2.816877000	-0.798583000
14	2.050975000	-3.037299000	-0.711441000
6	2.199731000	-0.076300000	-0.631062000
6	1.409289000	-1.286898000	-0.897241000
6	0.333813000	-0.906188000	-1.787865000
6	-0.591218000	-1.805025000	-2.569504000
1	-0.021691000	-2.653111000	-2.959435000
1	-1.360973000	-2.227598000	-1.917407000
6	-1.245506000	-1.051483000	-3.732882000
1	-0.508149000	-0.918064000	-4.533015000
1	-2.060011000	-1.653011000	-4.144426000
6	-1.751328000	0.323971000	-3.299067000
1	-2.437980000	0.210805000	-2.452840000
1	-2.309546000	0.799742000	-4.109326000
6	-0.580882000	1.219517000	-2.887541000
1	0.004676000	1.485086000	-3.777110000
1	-0.941974000	2.157116000	-2.464066000
6	0.334481000	0.507879000	-1.935672000
6	1.382886000	1.057457000	-1.103445000
6	2.097067000	3.086285000	1.051495000
1	2.576843000	4.045042000	1.271679000
1	2.697509000	2.287409000	1.492823000
1	1.115182000	3.081852000	1.532510000
6	0.699616000	4.082259000	-1.462844000
1	1.054039000	5.084305000	-1.197368000
1	-0.293864000	3.956348000	-1.024084000
1	0.601996000	4.038608000	-2.550472000
6	3.594511000	3.076527000	-1.621918000
1	3.996316000	4.068236000	-1.389985000
1	3.525928000	2.984848000	-2.710167000
1	4.300393000	2.324676000	-1.259208000
6	0.669801000	-4.310948000	-0.575799000
1	1.113763000	-5.282732000	-0.334113000
1	0.107978000	-4.421141000	-1.505774000
1	-0.044086000	-4.070966000	0.216654000
6	3.188813000	-3.292106000	0.762615000
1	3.740844000	-4.226773000	0.616271000
1	2.636912000	-3.383240000	1.701975000

1	3.905770000	-2.474401000	0.859291000
6	3.038381000	-3.366396000	-2.282315000
1	3.412534000	-4.394616000	-2.312747000
1	3.897439000	-2.690604000	-2.337203000
1	2.425594000	-3.198810000	-3.173010000
6	-1.252145000	1.203960000	0.052889000
7	0.255470000	-0.240895000	1.971894000
6	-0.607973000	-1.362250000	1.600798000
1	-0.077849000	-2.307833000	1.626029000
1	-1.517536000	-1.403338000	2.198744000
1	-1.047055000	-1.248195000	0.524104000
6	1.572598000	-0.642077000	2.497097000
1	2.149218000	0.260965000	2.683995000
1	1.451048000	-1.198599000	3.431788000
1	2.095015000	-1.233835000	1.755476000
6	-0.392342000	0.679940000	2.929754000
1	-1.397293000	0.919787000	2.590754000
1	-0.441417000	0.209702000	3.917021000
1	0.197876000	1.591461000	2.990239000

γ -[LFe(CO)(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.252792000	0.000000000	0.000000000
8	1.258301000	2.613855000	0.000000000
14	1.950888000	-0.457494000	-2.946048000
14	2.039979000	-0.775366000	2.835038000
6	2.170777000	-0.620499000	-0.041496000
6	1.345610000	-1.060494000	1.118237000
6	0.358664000	-1.975719000	0.595446000
6	-0.420778000	-3.042463000	1.318943000
1	0.206997000	-3.458519000	2.110478000
1	-1.309369000	-2.646164000	1.820388000
6	-0.838075000	-4.153323000	0.347116000
1	0.051420000	-4.719337000	0.048409000
1	-1.510969000	-4.849538000	0.853943000
6	-1.507650000	-3.579943000	-0.901774000
1	-2.392883000	-3.010470000	-0.608137000
1	-1.861179000	-4.387119000	-1.548004000
6	-0.543724000	-2.688156000	-1.696261000
1	0.091833000	-3.316872000	-2.331491000
1	-1.098206000	-2.039763000	-2.381577000
6	0.365721000	-1.879726000	-0.817614000
6	1.361480000	-0.932147000	-1.240112000
6	2.366864000	1.372140000	-3.019696000
1	2.874371000	1.607775000	-3.960911000
1	3.018346000	1.654756000	-2.190303000
1	1.460374000	1.981052000	-2.962068000
6	0.662348000	-0.802519000	-4.272038000
1	1.032908000	-0.428503000	-5.232667000
1	-0.280818000	-0.290150000	-4.059364000
1	0.451635000	-1.868345000	-4.387539000
6	3.497891000	-1.465012000	-3.312513000

1	3.933003000	-1.188100000	-4.278245000
1	3.272669000	-2.535851000	-3.336847000
1	4.249550000	-1.293808000	-2.536704000
6	0.977581000	-1.425094000	4.245923000
1	1.555896000	-1.329872000	5.171548000
1	0.715971000	-2.479508000	4.127309000
1	0.054369000	-0.858704000	4.379333000
6	2.322328000	1.064772000	3.087422000
1	2.870446000	1.254447000	4.015971000
1	1.375768000	1.609706000	3.137467000
1	2.898670000	1.466270000	2.251168000
6	3.686232000	-1.687483000	2.887940000
1	4.186202000	-1.547587000	3.851533000
1	4.340086000	-1.314279000	2.096087000
1	3.542223000	-2.761555000	2.732480000
6	0.679929000	1.607013000	-0.015127000
7	-1.733689000	0.438363000	1.015526000
6	-2.128945000	1.853249000	0.795539000
1	-2.159854000	2.062022000	-0.273474000
1	-3.119105000	2.032674000	1.228694000
1	-1.400923000	2.505701000	1.272480000
6	-2.783717000	-0.421781000	0.418208000
1	-2.597764000	-1.455828000	0.690363000
1	-3.772097000	-0.124273000	0.784300000
1	-2.768959000	-0.316228000	-0.668721000
6	-1.674254000	0.202941000	2.471010000
1	-0.902465000	0.839825000	2.897972000
1	-2.640226000	0.442196000	2.930529000
1	-1.432932000	-0.838631000	2.659432000

γ' -[LFe(CO)(NMe₃)]:

26	0.000000000	0.000000000	0.000000000
8	3.200606000	0.000000000	0.000000000
8	-1.776030000	2.286676000	0.000000000
14	1.972649000	2.710721000	-1.199868000
14	2.267866000	-2.979542000	-0.456519000
6	2.143081000	-0.126340000	-0.668892000
6	1.376116000	-1.375812000	-0.852822000
6	0.273252000	-1.073336000	-1.718931000
6	-0.705379000	-2.022067000	-2.357228000
1	-0.162317000	-2.886580000	-2.746510000
1	-1.395680000	-2.411122000	-1.603951000
6	-1.497686000	-1.354261000	-3.489013000
1	-0.868924000	-1.299356000	-4.385019000
1	-2.360195000	-1.975888000	-3.741834000
6	-1.939015000	0.063070000	-3.122234000
1	-2.526713000	0.041261000	-2.197557000
1	-2.578576000	0.476885000	-3.905830000
6	-0.718578000	0.964302000	-2.923464000
1	-0.213317000	1.108064000	-3.887160000
1	-1.016592000	1.954896000	-2.578743000
6	0.259916000	0.335588000	-1.976529000

6	1.352874000	0.952999000	-1.268212000
6	2.174582000	3.229351000	0.594391000
1	2.673405000	4.200866000	0.671220000
1	2.774653000	2.487327000	1.127543000
1	1.203941000	3.304546000	1.093445000
6	0.841912000	3.941560000	-2.062545000
1	1.289322000	4.938250000	-1.978418000
1	-0.152179000	3.983795000	-1.610522000
1	0.727389000	3.717167000	-3.126478000
6	3.651074000	2.770125000	-2.052606000
1	4.114689000	3.755096000	-1.936617000
1	3.559222000	2.566687000	-3.124298000
1	4.317262000	2.020773000	-1.616807000
6	1.341683000	-4.521212000	-1.013009000
1	1.921060000	-5.399447000	-0.708110000
1	1.242131000	-4.553446000	-2.101409000
1	0.343058000	-4.615959000	-0.580392000
6	2.686187000	-3.133633000	1.373194000
1	3.443987000	-3.912613000	1.507134000
1	1.832679000	-3.403427000	2.000417000
1	3.100997000	-2.189949000	1.736199000
6	3.896265000	-2.910318000	-1.396926000
1	4.510816000	-3.787250000	-1.169403000
1	4.446106000	-2.012139000	-1.106844000
1	3.733300000	-2.877272000	-2.478633000
6	-1.089360000	1.349953000	0.056363000
7	-0.988936000	-1.132024000	1.314056000
6	0.107228000	-0.596164000	2.136016000
1	0.682982000	0.239248000	1.583050000
1	-0.254798000	-0.088266000	3.028320000
1	0.836019000	-1.359664000	2.385227000
6	-2.325132000	-0.694544000	1.777450000
1	-3.047966000	-0.895718000	0.988612000
1	-2.603470000	-1.244718000	2.681516000
1	-2.309194000	0.370174000	1.994174000
6	-0.982072000	-2.601648000	1.219028000
1	-0.014080000	-2.932791000	0.863117000
1	-1.191109000	-3.045187000	2.196907000
1	-1.753142000	-2.908291000	0.514519000

α -[LFe(CO)]:

Fe	0.34089719445368	3.57746731322543	-0.30443514414796
O	0.25118064383023	6.93021348219153	-0.16290256853028
Si	-2.68058425060214	5.47279486582809	-0.09495239195135
Si	3.02383038383523	5.66720523139074	-1.33989708783800
C	0.14679395582785	5.87076551306801	-0.78890210909624
C	1.24442758136113	5.07567089975294	-1.42553420362907
C	0.59767583959834	4.12799428239049	-2.30086713669313
C	1.23476900785542	3.24194280147383	-3.33293373703442
H	1.89273860474572	3.84500090386510	-3.96406347651225
H	1.88123708549329	2.50365097526047	-2.84164372190595
C	0.18169396333784	2.52850102539850	-4.18606576296259

H	-0.24994575707340	3.24056953494741	-4.89821195681057
H	0.66024057211883	1.73813660358486	-4.76900483158951
C	-0.93762914234695	1.95793910525037	-3.31658273145512
H	-0.50432941779728	1.29209198342690	-2.55982593630504
H	-1.62396160936545	1.35608731611177	-3.91685721572428
C	-1.71437359448917	3.08077260917896	-2.62113453181856
H	-2.33664178284998	3.61198291633034	-3.35246128199573
H	-2.39847615496748	2.66901609841861	-1.87628233354773
C	-0.78237564075004	4.06745336956599	-1.98062837811788
C	-1.06089673704117	4.99189949725357	-0.90715656106641
C	-2.37943776639817	5.82550152646737	1.72231560168541
H	-3.27149233128966	6.27125585934190	2.17410231458099
H	-1.54203224492792	6.51397017768868	1.85353031204494
H	-2.15110881979254	4.90383164354323	2.26457318060163
C	-3.97102279481086	4.11352493943423	-0.22285260162847
H	-4.85468067881499	4.40901423620373	0.35284355535247
H	-3.60329435359329	3.17150007809832	0.19481772957006
H	-4.28987462601223	3.93038616382882	-1.25171473815704
C	-3.29750104840665	7.02750682966476	-0.95436310154042
H	-4.22327801299287	7.38574365680537	-0.49289621568748
H	-3.49620953207598	6.84344693157537	-2.01436504533143
H	-2.54875676937101	7.82088658870779	-0.88008406375948
C	4.20367742520049	4.49924735085200	-2.21598330243471
H	5.23071455278548	4.83689844880486	-2.04173027045851
H	4.03926020719220	4.47865412299109	-3.29605559332048
H	4.11812478307435	3.47740402912965	-1.83595594414580
C	3.52761260756739	5.81344374914711	0.46211987855047
H	4.49109295252959	6.32489874242791	0.55414978181071
H	3.62167720641363	4.82725471337516	0.92456518740690
H	2.78098788402224	6.38167433177811	1.02179674304974
C	3.07671003160304	7.36035256024111	-2.15239111123423
H	4.08706076235253	7.77997077523322	-2.12192231208704
H	2.40389020217230	8.04416485606070	-1.62812176453587
H	2.75859348808409	7.30854434874119	-3.19820368261677
C	0.68354067974468	4.00120534507011	1.36324537814886
O	0.88552445056966	4.41444966687431	2.42701818286764

β -[LFe(CO)]:

Fe	0.33035962270926	3.78958481351742	-0.31166908677456
O	0.25416104556605	6.79227404233496	-0.09580223110522
O	2.59381981808201	1.96364684533197	-0.16801484864333
Si	-2.68558404042501	5.52313819981241	-0.19373053632705
Si	2.98631809263491	5.71974479706846	-1.43622197282815
C	0.11933641199031	5.83425820159458	-0.89456133720265
C	1.21591667877200	5.10925589068825	-1.56738760639332
C	0.61341093003491	4.02674559179170	-2.30155102625576
C	1.25328191134840	3.10850401863372	-3.30523536424727
H	1.82335362648825	3.71794410987639	-4.01159242395906
H	1.97723803284726	2.45219606947941	-2.81626833858836
C	0.21113404585223	2.27284227512563	-4.05822385953797
H	-0.26377184678986	2.89347019620817	-4.82628650607819
H	0.71204371974561	1.45017339331948	-4.57377769113896

C	-0.87161252349881	1.74653780841330	-3.11713509066512
H	-0.40911868819013	1.18020827229047	-2.30115616279328
H	-1.54211725521664	1.06552336117629	-3.64645942942089
C	-1.68282354568184	2.90928072640584	-2.53840962182018
H	-2.29706508747464	3.35642408927803	-3.33053010512423
H	-2.37473678425140	2.55851220220638	-1.77046023109195
C	-0.78640657300609	3.97491394286361	-1.98637215800380
C	-1.10460046950556	5.02971894239794	-1.07423091828273
C	-2.36820294004245	5.47930678255375	1.65829892870689
H	-3.24164453466471	5.84265906740101	2.20920985869804
H	-1.51426579990229	6.11166202344721	1.91314182071656
H	-2.15697667748323	4.46171745609402	2.00373692897216
C	-4.10278327824644	4.36366564951922	-0.60229587993975
H	-5.00954443113352	4.72948685394475	-0.10861333492449
H	-3.91615201156228	3.34861671515679	-0.24125443796625
H	-4.30269664280318	4.31573528509042	-1.67589349715158
C	-3.12758772345136	7.27316671997609	-0.71571656884550
H	-4.01826651162356	7.61774544732486	-0.18077634225624
H	-3.33327468658478	7.33172716563046	-1.78871978509088
H	-2.30391797010239	7.95362582273028	-0.48633160670924
C	4.16897818932748	4.65870594405755	-2.43496313196684
H	5.18782693321892	5.03365912588603	-2.29197868632788
H	3.94792892942939	4.69239015204218	-3.50473835302547
H	4.14977346931484	3.61422262562858	-2.11294399325771
C	3.50813679371702	5.71604297705189	0.36793389496650
H	4.45931776902151	6.24356833955830	0.49344653330359
H	3.63417729212058	4.69975530024821	0.75039535247853
H	2.75214013815821	6.21947652626905	0.97549719336778
C	2.99880037778009	7.48504925664894	-2.07634263514095
H	3.99712079645541	7.92505944950228	-1.99008007526046
H	2.30309035086160	8.09207401556860	-1.49121252748258
H	2.69176885501513	7.53303324418128	-3.12559760189129
C	1.68040507814879	2.67482729167379	-0.14552953169093

γ -[LFe(CO)]:

26	0.000000000	0.000000000	0.000000000
8	3.075553000	0.000000000	0.000000000
8	-1.951799000	2.157827000	0.000000000
14	1.807954000	2.604096000	-1.390575000
14	1.823829000	-2.953108000	0.285288000
6	2.048053000	-0.211666000	-0.683909000
6	1.257029000	-1.459101000	-0.703854000
6	0.152602000	-1.243952000	-1.585294000
6	-0.902608000	-2.225465000	-2.009244000
1	-0.426951000	-3.176070000	-2.262123000
1	-1.567269000	-2.432801000	-1.162189000
6	-1.719333000	-1.702710000	-3.195030000
1	-1.119667000	-1.782151000	-4.108607000
1	-2.601257000	-2.332968000	-3.331689000
6	-2.124264000	-0.241864000	-2.996346000
1	-2.680783000	-0.140273000	-2.057594000
1	-2.785079000	0.084530000	-3.802746000

6	-0.887327000	0.659596000	-2.954513000
1	-0.425626000	0.689292000	-3.949777000
1	-1.159692000	1.686023000	-2.707873000
6	0.134064000	0.131983000	-1.995444000
6	1.242263000	0.815885000	-1.373932000
6	2.014164000	3.199153000	0.378991000
1	2.440277000	4.207538000	0.394443000
1	2.682280000	2.531287000	0.927657000
1	1.055448000	3.228090000	0.904618000
6	0.590898000	3.726295000	-2.277809000
1	0.982047000	4.749145000	-2.263572000
1	-0.387524000	3.740603000	-1.790658000
1	0.449200000	3.438020000	-3.322507000
6	3.469243000	2.673409000	-2.265524000
1	3.856626000	3.696990000	-2.277507000
1	3.392220000	2.330266000	-3.301601000
1	4.192404000	2.038335000	-1.747395000
6	0.621955000	-4.389644000	0.164438000
1	0.971187000	-5.195432000	0.818653000
1	0.555419000	-4.790436000	-0.850147000
1	-0.383494000	-4.107995000	0.488691000
6	1.972119000	-2.418596000	2.080585000
1	2.422261000	-3.207348000	2.691642000
1	0.990611000	-2.187462000	2.507957000
1	2.597361000	-1.525446000	2.152732000
6	3.500851000	-3.465534000	-0.383278000
1	3.907973000	-4.309106000	0.182663000
1	4.203334000	-2.631054000	-0.312521000
1	3.429604000	-3.762277000	-1.434194000
6	-1.173199000	1.304591000	0.084104000