Supporting Information for:

Three-Coordinate Terminal Imidoiron(III) Complexes: Structure, Spectroscopy, and Mechanism of Formation

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Full Citation for Reference 66

Gaussian 03, Revision D.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

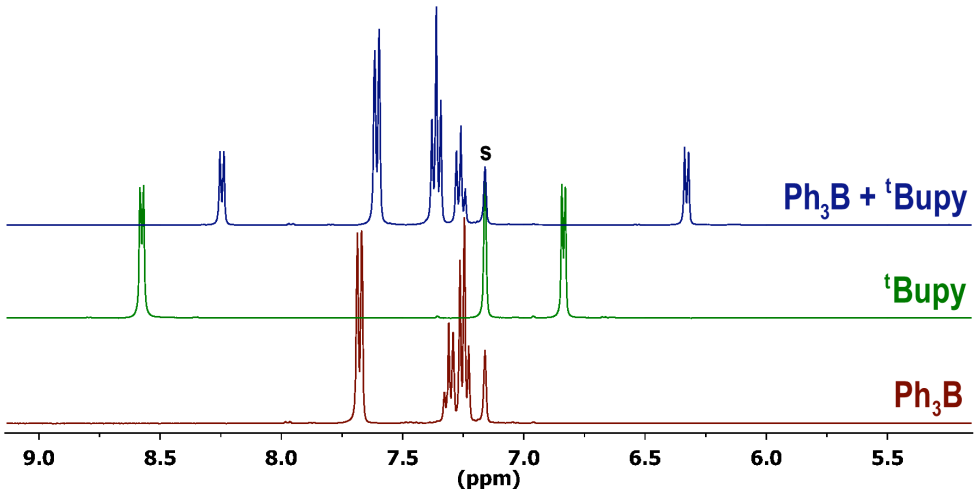


Figure S-1. ^{1}H NMR spectra of Ph_3B, ^{t}Bupy, and a 1:1 mixture of Ph_3B:^{t}Bupy in C_6D_6. The residual C_6D_5H peak is marked with "**s**". An additional peak for ^{t}Bu-*H* is present at δ 1.002 (^{t}Bupy) and δ 0.745 (BPh_3:^{t}Bupy) ppm, respectively.

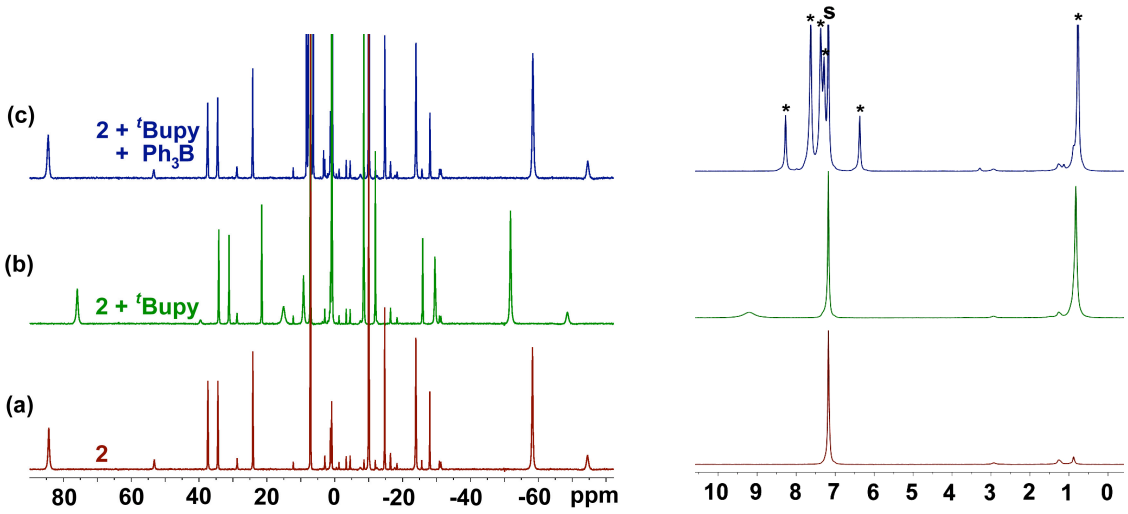


Figure S-2. ^{1}H NMR spectra of (a) compound **2**; (b) compound **2** with added ^{t}Bupy; and (c) upon addition of BPh_3 to the mixture in (b). Right: inset of the 0 – 10 ppm region. Peaks marked with asterisks match the compound "Ph_3B:^{t}Bupy" in the spectrum shown in Figure S-1.

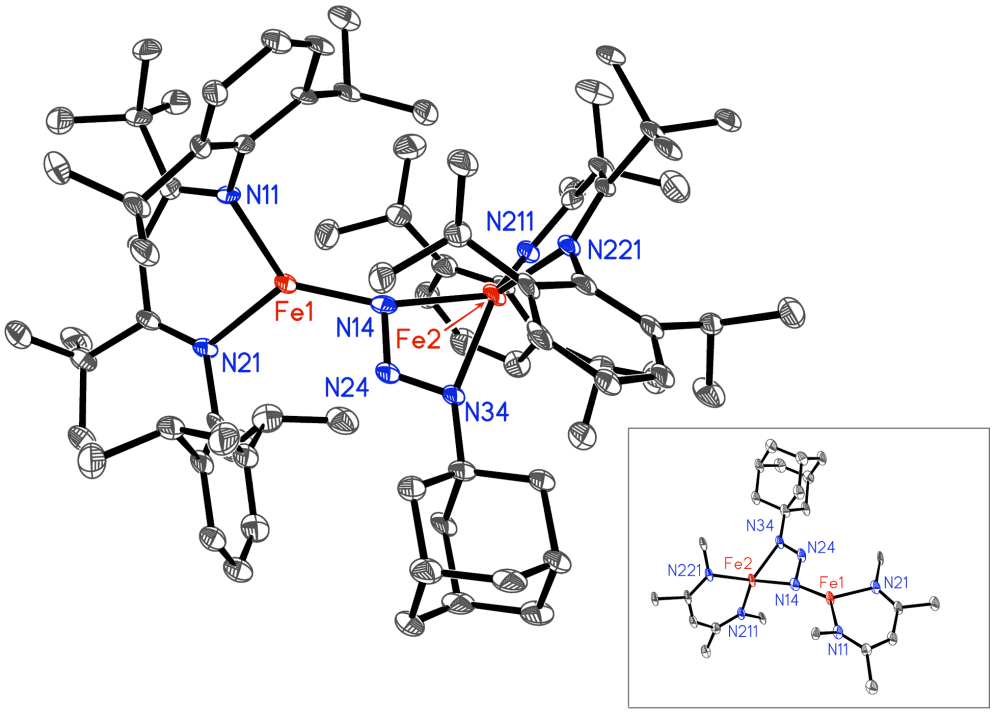


Figure S-3. Thermal ellipsoid plot of $L^{tBu}Fe(\mu\text{-}N_3Ad)FeL^{tBu}$ at 50% probability. Hydrogens and co-crystallized pentane molecules are removed for clarity. *Inset*: Alternate view with the 2,6-diisopropylphenyl and *tert*-butyl groups removed for clarity.

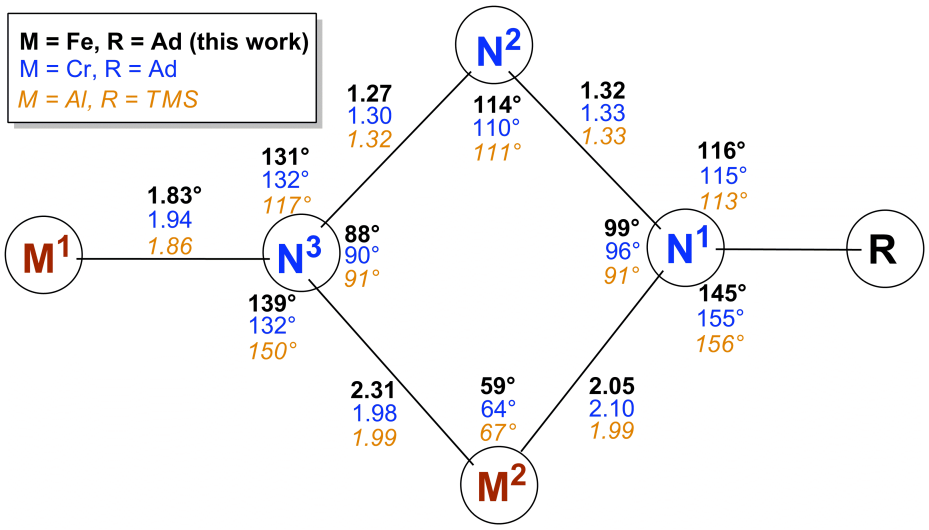


Figure S-4. Comparison of core bond metrics in the DFT model of $\{L^{Me}Fe\}_2(\mu\text{-}N_3Ad)$ to two crystallographically characterized literature complexes (Cr: Ni, C.; Ellis, B. D.; Long, G. J.; Power, P. P. *Chem. Commun.* **2009**, 2332-2334; Al: Uhl, W.; Gerding, R.; Pohl, S.; Saak, W. *Chem. Ber.* **1995**, *128*, 81-85).

Table S-1. Crystal data for **2**, **3**, and $L^{tBu}Fe(\mu\text{-}N_3Ad)FeL^{tBu}$.

	$L^{Me}Fe{=}NAd$ (**2**)	$L^{Me}FeNHAd$ (**3**)	$L^{tBu}Fe(\mu\text{-}N_3Ad)FeL^{tBu} \cdot 2C_5H_{12}$
Empirical formula	$C_{39}\ H_{56}\ Fe\ N_3$	$C_{39}\ H_{57}\ Fe\ N_3$	$C_{90}\ H_{145}\ Fe_2\ N_7$
Formula weight	622.72	623.73	1436.83
Data collection temperature (°C)	–100	–80	–100
Color, habit	Dark yellow, plate	Yellow, plate	Dark orange, rod
crystal size (mm^3)	0.24 × 0.16 × 0.04	0.47 × 0.42 × 0.10	0.28 × 0.12 × 0.08
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	$P2_1/c$	$P\bar{1}$
a (Å)	11.134(3)	10.9816(7)	13.282(3)
b (Å)	12.925(4)	13.1386(8)	15.629(3)
c (Å)	25.274(8)	25.7345(15)	21.057(4)
α (º)	90	90	94.791(4)
β (º)	93.059(6)	95.0910(10)	102.722(4)
γ (º)	90	90	93.567(4)
V ($Å^3$)	3631.8(19)	3698.4(4)	4234.4(15)
Z	4	4	2
θ range for data collection (º)	1.77 to 33.14	1.74 to 28.30	1.57 to 25.03
ρ (calcd) (g/cm^3)	1.139	1.120	1.127
μ (mm^{-1})	0.444	0.436	0.389
R(int)	0.0887	0.0411	0.1404
$R1$ (F^2, $I > 2\sigma(I)$)	0.0519	0.0551	0.0898
$wR2$ (F^2, all data)	0.1297	0.1436	0.2449
GOF	1.014	1.044	1.027
largest residual density ($e \cdot Å^{-3}$)	0.529 and –0.325	0.628 and –0.531	1.311 and –1.153

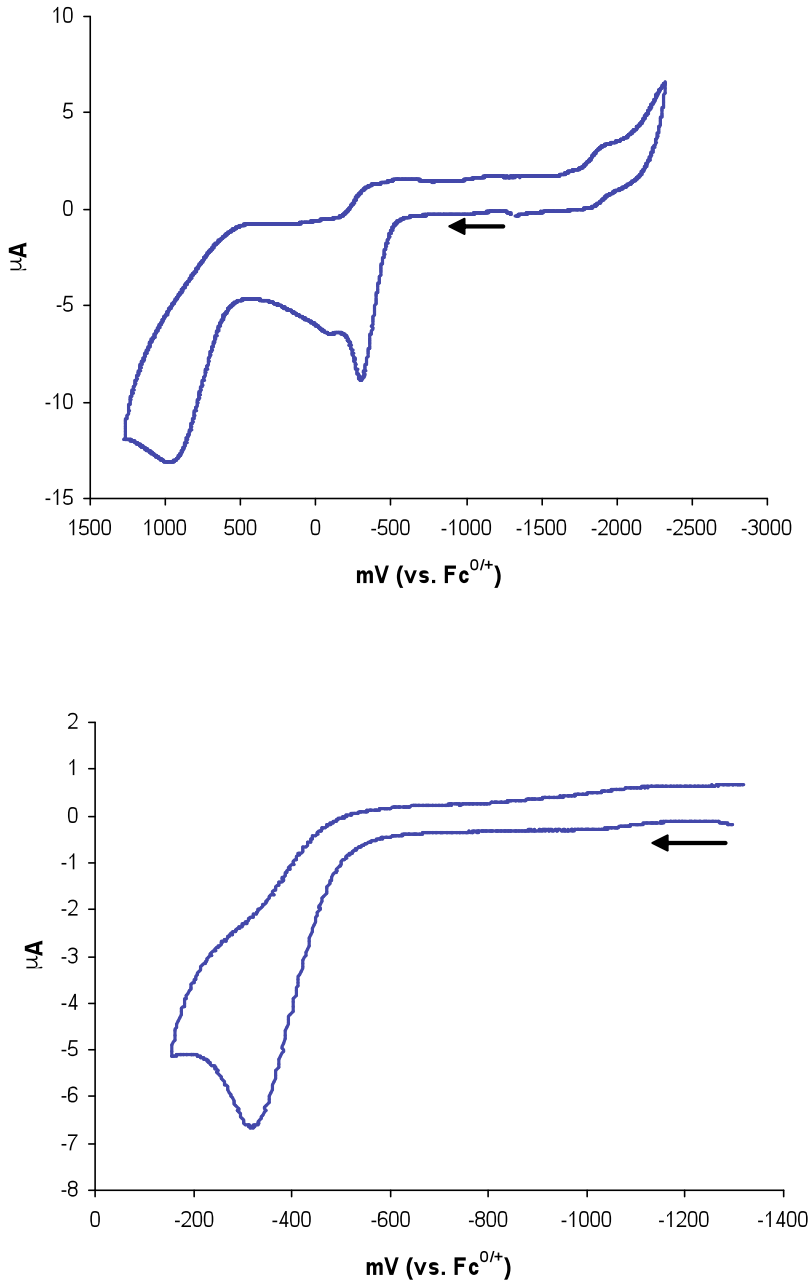


Figure S-5. Cyclic voltammograms of **2** in Et_2O (2 mM), with 0.1 M [$^nBu_4N$][BAr^F] supporting electrolyte. CV measurements were obtained using a Cypress Systems 3100 potentiostat. The working electrode was glassy carbon with a 1 mm diameter working area, and Ag wires were used as auxiliary and reference electrodes. All measurements were referenced with a ferrocene standard, and reported relative to the $Cp_2Fe^{+/0}$ couple.

Table S-2. Calculated Lowest Energy Linkage Isomers of L'Fe(N_3Me) (L' = $N_2C_3H_5$)[a]

Isomer	Multiplicity	ΔG_{rel} [b]
κN^1	6	0.00
κN^1	4	+1.58
κN^3	6	+11.47
κN^3	4	+0.08
η^2	4	+1.44

[a] Calculated at B3LYP/6-311+G(d) level
[b] Relative to the lowest energy linkage isomer (1 atm, 298.15 K)

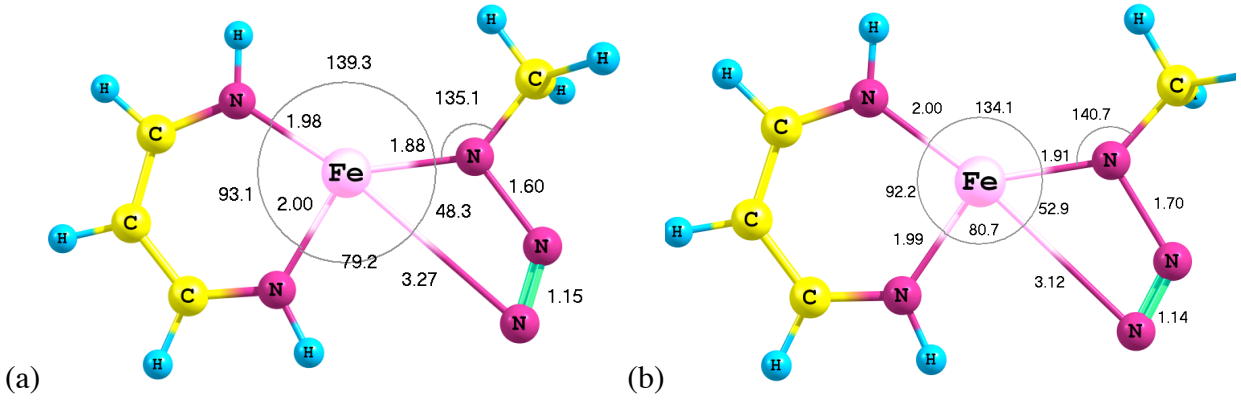
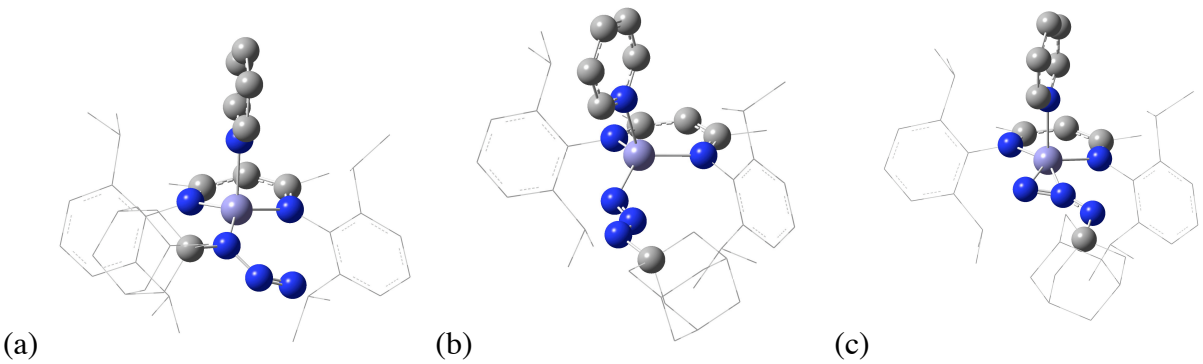


Figure S-6. Calculated B3LYP/6-311+G(d) transition states for N_2 elimination from (a) ^{4}L'Fe(N_3Me-κN^1), and (b) ^{6}L'Fe(N_3Me-κN^1), and their corresponding bond lengths (Å) and angles (°).

Table S-3. Calculated Lowest Energy Linkage Isomers of $L^{Me}Fe(N_3Ad)(py)$[a]

Isomer	Multiplicity	ΔG_{rel} [b]
κN^1	4	+8.5
κN^1	6	+7.4
κN^3	4	+0.0
κN^3	6	+6.9
η^2	4	+2.3
η^2	6	[c]

[a] Calculated at the B3LYP/6-311+G(d):UFF level of theory
[b] Relative to the lowest energy linkage isomer in kcal/mol (1 atm, 298.15 K)
[c] This complex is not stable at this level of theory, and converts upon QM/MM geometry optimization to the sextet κN^3 isomer.



(a) (b) (c)

Figure S-7. QM/MM optimized geometries of three low energy linkage isomers of $L^{Me}Fe(N_3Ad)(py)$: (a) sextet κN^1, (b) quartet κN^3, and (c) quartet η^2. QM atoms are shown as spheres, and MM atoms are shown in wireframe. Hydrogens omitted from figure for clarity.

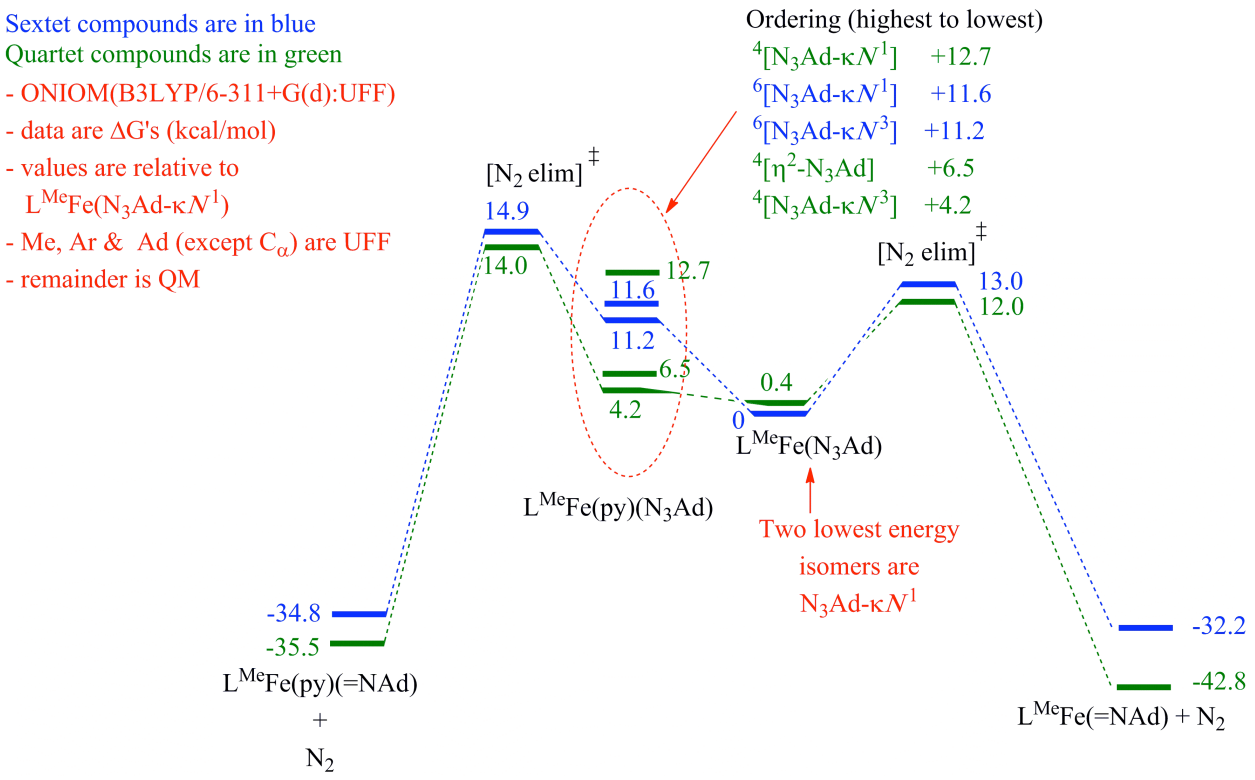


Figure S-8. Potential energy surface showing the relative energies of intermediates and transition states for N_2 loss. The energies (ΔG, kcal/mol) are given relative to $^6L^{Me}Fe(N_3Ad\text{-}\kappa N^1)$. Species with sextet spin states are blue and species with quartet spin states are green.

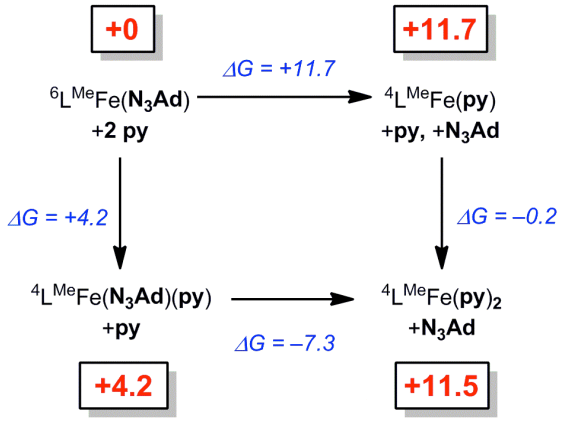


Figure S-9. Calculated thermodynamic cycle for pyridine coordination/exchange from $L^{Me}Fe(N_3Ad)$. The energies (ΔG, kcal/mol) are given relative to $^6L^{Me}Fe(N_3Ad\text{-}\kappa N^1)$.

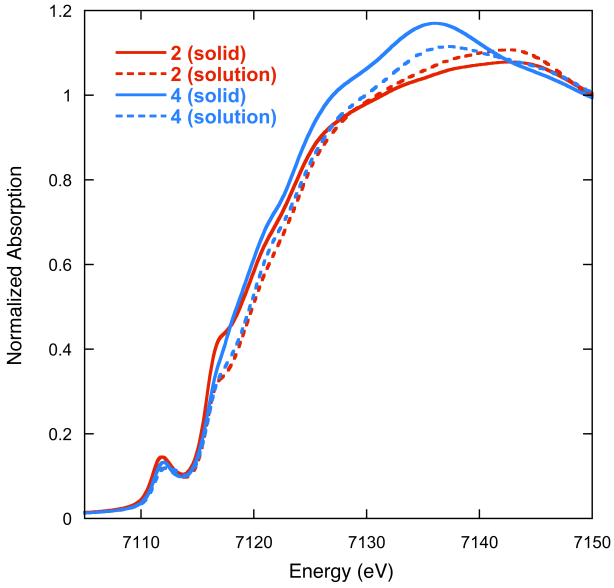


Figure S-10. Comparison of the normalized Fe K-edge XAS data for **2** (red) and **4** (blue) as solids and in solution.

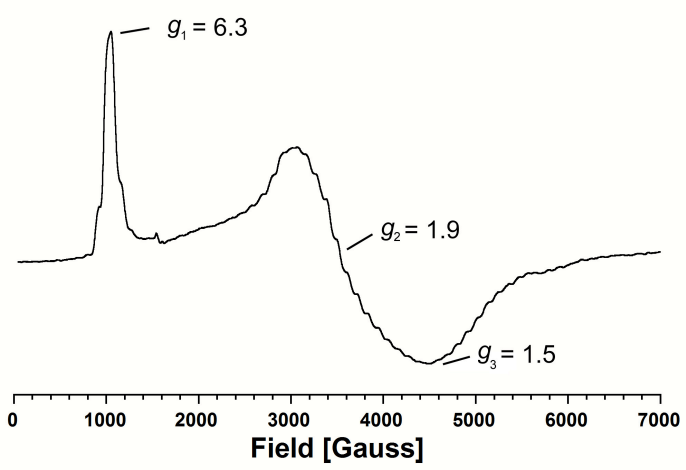


Figure S-11. X-band EPR spectrum of a 9.8 mM sample of **2** in THF. Parameters: T = 7 K; ν = 9.4110 GHz; time constant = 100 ms; modulation = 15 G; power = 167 μW.

Table S-4. Compounds used in the Fe–$N_{diketiminate}$ bond length analysis from the CSD v. 5.31 (Feb 2010 update). Only neutral molecules with η^1-coordinated ligands and unambiguous oxidation states are considered in the survey.

Compound	*Fe Ox. State*	*Coordination Number*	*CSD Refcode*	*Fe–N_{avg} (Å)*
$L^{Me,iPr2}Fe(PPh_3)$	1	3	PECMOA	1.956
$L^{tBu,iPr2}Fe(\mu\text{-}Cl)K(18\text{-}c\text{-}6)$	1	3	PECNOB	1.934
$L^{tBu,iPr2}Fe(CO)_2$	1	4	WOBGUQ	1.967
$L^{Me,iPr2}Fe(CN^tBu)_2$	1	4	AFUDOV	1.9695
$L^{Me,iPr2}Fe(CO)_3$	1	5	PECMUG	1.983
$L^{tBu,iPr2}Fe(CO)_3$	1	5	PECNAN	1.9655
$L^{tBu,iPr2}Fe(CN^tBu)_3$	1	5	COWFUQ	2.039
$L^{tBu,iPr2}Fe$(3-hexenyl)	2	3	AQUGAU	1.989
$L^{tBu,iPr2}Fe(N(Ph)NHPh)$	2	3	AQUGIC	1.99
$L^{tBu,iPr2}Fe(NHPh)$	2	3	AQUGOI	1.972
$L^{Me,iPr2}Fe(NCMe)(\mu\text{-}S)FeL^{Me,iPr2}$	2	3	BEQJOX	1.997
$L^{tBu,iPr2}Fe(^iBu)$	2	3	BIJHUY	1.9895
$L^{Me,iPr2}Fe(Me)$	2	3	BIJJAG	1.9725
$L^{Me,iPr2}Fe(CH_2CH_2CF_3)$	2	3	BIJJEK	1.974
$L^{Me,iPr2}Fe(CH_2CH_2CF_3)$	2	3	BIJJEK	1.9735
$L^{Me,iPr2}Fe(CH(Me)Ph)$	2	3	BIJJIO	1.988
$L^{Me,iPr2}Fe(OCHPh_2)$	2	3	BIJJOU	1.9655
$L^{Me,iPr2}Fe(N(Me)CH_2Ph)$	2	3	BIJJUA	1.973
$L^{Me,iPr2}Fe(Cy)$	2	3	BIJKEL	1.985
$L^{Me,iPr2}Fe(NHdipp)$	2	3	DABQUT	1.996
$L^{Me,iPr2}Fe(OtBu)$	2	3	DABREE	1.9755
$L^{tBu,iPr2}Fe(CCPh)$	2	3	DABRUU	1.970
$L^{tBu,iPr2}Fe(CCPh)$	2	3	DABRUU	1.966
$L^{tBu,iPr2}Fe(NHdipp)$	2	3	DABSAB	1.9955
$L^{tBu,iPr2}Fe(NHtBu)$	2	3	DABSEF	1.984
$L^{tBu,iPr2}Fe(NHtol)$	2	3	DABSIJ	1.972
$L^{tBu,iPr2}Fe(NHxyl)$	2	3	DABSOP	1.997
$L^{tBu,iPr2}Fe(CH_2Ph)$	2	3	HUJDEV	1.995
$L^{tBu,iPr2}Fe(^iPr)$	2	3	HUJDIZ	1.9945
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}O)$	2	3	MARBEN	1.9855
$L^{Me,iPr2}Fe(CH_2SiMe_3)$	2	3	MEGHOW	1.992
$L^{Me,iPr2}Fe(N(SiMe_3)_2)$	2	3	MONYIX	2.007
$L^{Me,C6F5}Fe(N(SiMe_3)_2)$	2	3	MONYOD	2.0005
$L^{Me,C6F5}Fe(N(SiMe_3)_2)$	2	3	MONYOD	2.0075
$L^{Me,Me3}Fe(N(SiMe_3)_2)$	2	3	MONYUJ	1.997
$L^{Me,Me2}Fe(N(SiMe_3)_2)$	2	3	MONZAQ	1.9945
$L^{Me,Me2}Fe(N(SiMe_3)_2)$	2	3	MONZAQ	1.994
$L^{tBu,iPr2}Fe(OtBu)$	2	3	MUNDII	1.979
$L^{tBu,iPr2}Fe(F)$	2	3	NASJAT	1.961
$L^{tBu,iPr2}Fe(SSiMe_3)$	2	3	NASJIB	1.9725
$L^{tBu,iPr2}Fe(SSiMe_3)$	2	3	NASJIB	1.9715
$L^{tBu,iPr2}Fe(CCSiMe_3)$	2	3	NASJOH	1.9585
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}(OC(Me)(Ph))_2)$	2	3	PECNER	1.976
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}(OC(Me)(Ph))_2)$	2	3	PECNER	1.9845
$L^{tBu,iPr2}Fe(Cl)(NCMe)$	2	3	REWZUO	1.948

$L^{Me,iPr2}Fe(CH_2Ph)$	2	3	UGEMIC	1.982
$L^{Me,iPr2}Fe(CH_2Ph)$	2	3	UGEMIC	1.9785
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}CO_3)$	2	3	WIYFEQ	1.966
$L^{tBu,iPr2}Fe(^tBu)$	2	3	WUFSIZ	2.0155
$L^{Me,iPr2}Fe(^iBu)$	2	3	WUFSOF	1.983
$L^{Me,iPr2}Fe(Et)$	2	3	WUFSUL	1.9845
$L^{tBu,iPr2}Fe(Me)$	2	3	XOXHUN	1.973
$L^{tBu,iPr2}Fe(NCH^tBu)$	2	3	AFUFEN	1.9715
$L^{tBu,iPr2}Fe(NCH^tBu)$	2	3	AFUFEN	1.9695
$L^{Me,iPr2}Fe(C(Ph)CHPh)$	2	3	AFUFIR	1.9785
$L^{Me,iPr2}Fe(Ph)$	2	3	COGQIZ	1.972
$[^{LtBu,iPr3}Fe]_2(\mu\text{-}CO_3)$	2	3	BOTNOO	1.9625
$[^{LtBu,iPr2}Fe(H)]_2$	2	4	AQUFUN	2.0055
$L^{tBu,iPr2}Fe(H)(^tBupy)$	2	4	AQUGEY	2.0265
$L^{Me,iPr2}Fe(NCMe)(\mu\text{-}S)FeL^{Me,iPr2}$	2	4	BEQJOX	2.0345
$[L^{Me,iPr2}Fe(NH_2NHMe)]_2(\mu\text{-}S)$	2	4	BEQJUD	2.0245
$[L^{Me,iPr2}Fe(NH_2NHMe)]_2(\mu\text{-}S)$	2	4	BEQJUD	2.0315
$[L^{Me,iPr2}Fe(NH_2NMe_2)]_2(\mu\text{-}S)$	2	4	BEQKAK	2.014
$[L^{Me,iPr2}Fe(NH_2NMe_2)]_2(\mu\text{-}S)$	2	4	BEQKAK	2.0295
$[L^{Me,iPr2}Fe(NH_3)]_2(m\text{-}S)$	2	4	BEQKEO	2.031
$[L^{Me,iPr2}Fe(CH_2CN)]_2$	2	4	BIJKAH	1.9985
$[L^{Me,iPr2}Fe(Cl)]_2$	2	4	DABPIG	2.004
$L^{Me,iPr2}Fe(NHdipp)(thf)$	2	4	DABPUS	2.0285
$L^{Me,iPr2}Fe(NHxyl)(thf)$	2	4	DABQAZ	2.030
$L^{Me,iPr2}Fe(\mu\text{-}Cl)(\mu\text{-}thf)Li(OEt_2)$	2	4	DABQIH	2.0295
$L^{Me,iPr2}Fe(NHdipp)(NH_2dipp)$	2	4	DABQUT	2.038
$L^{Me,iPr2}Fe(\mu\text{-}Cl)(\mu\text{-}NHtol)Li(OEt_2)_2$	2	4	DABRAA	2.018
$L^{tBu,iPr2}Fe(NHdipp)(NCMe)$	2	4	DABRII	2.016
$L^{tBu,iPr2}Fe(NHdipp)(^tBupy)$	2	4	DABROO	2.0385
$L^{Me,iPr2}Fe(^iBu)(NCMe)$	2	4	JEWTEL	2.0245
$L^{Me,iPr2}Fe(CH_2tBu)(NCMe)$	2	4	JEWTIP	2.028
$L^{Me,iPr2}Fe(Cl)(tBupy)$	2	4	JEWTOV	2.0055
$L^{Me,iPr2}Fe(Cl)(tBupy)$	2	4	JEWTOV	2.0045
$L^{tBu,iPr2}Fe(Cl)(NCMe)$	2	4	JEWTUB	1.9985
$L^{tBu,iPr2}Fe(Cl)(NCMe)$	2	4	JEWTUB	2.001
$L^{Me,iPr2}Fe(\mu\text{-}Me_2pz)(\mu\text{-}Cl)Li(thf)_2$	2	4	LECPAL	2.011
$[L^{tBu,iPr3}Fe(H)]_2$	2	4	LIHTEC	1.983
$[L^{tBu,iPr3}Fe(H)]_2$	2	4	LIHTEC	2.0265
$L^{Me,iPr2}Fe(CH_2Ph)(py)$	2	4	MEGHUC	2.032
$(L^{Me,C6F5})_2Fe$	2	4	MONZIY	2.0255
$(L^{Me,C6F5})_2Fe$	2	4	MONZIY	2.0075
$[L^{Me,iPr2}Fe(F)]_2$	2	4	NASHUL	2.012
$L^{tBu,iPr2}Fe(F)(^tBupy)$	2	4	NASJEX	2.011
$L^{Me,iPr2}Fe(F)(^tBupy)$	2	4	NASJUN	2.0105
$L^{Me,iPr2}Fe(F)(CF_3py)$	2	4	NASKAU	2.011
$L^{tBu,iPr2}Fe(F)(NCMe)$	2	4	NASKEY	2.012
$L^{tBu,iPr2}Fe(FBF_3)(OEt_2)$	2	4	NASKIC	1.992
$[L^{Me,iPr2}Fe(H)]_2$	2	4	NASKOI	1.9735
$[L^{Me,iPr2}Fe(H)]_2$	2	4	NASKOI	1.9825
$L^{Me,iPr2}Fe(\mu\text{-}Cl)_2Li(thf)_2$	2	4	REWPOY	2.001
$L^{Me,iPr2}Fe(\mu\text{-}Cl)_2Li(thf)_2$	2	4	REWPOY	1.9995
$L^{Me,iPr2}Fe(\mu\text{-}Cl)_2Li(thf)_2$	2	4	REWPOY	2.0065
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$L^{Me,iPr2}Fe(\mu\text{-}Cl)_2Li(OEt_2)_2$	2	4	REWSOB	2.006
$[L^{Me,iPr2}Fe(Cl)]_2(\mu\text{-}MgCl_2(thf)_4)$	2	4	REWZOI	2.0125

$[L^{tBu,iPr2}Fe]_2(\mu\text{-}CO_3)$	2	4	WIYFEQ	1.989
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}CO_3)$	2	4	WIYFEQ	1.9885
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}CO_3)$	2	4	WIYFEQ	2.0005
$L^{Me,iPr2}Fe(NHAd)(tBupy)$	2	4	XEPHEG	2.0285
$[L^{tBu,iPr2}Fe(N_3)]_2$	2	4	AFUDIP	1.9885
$[L^{Me,iPr2}Fe(NCHMe)]_2$	2	4	AFUDUB	2.050
$[L^{Me,iPr2}Fe]_2(\mu\text{-}NCH^tBu)(m\text{-}H)$	2	4	AFUFAJ	2.0335
$[L^{Me,iPr2}Fe]_2(\mu\text{-}NCH^tBu)(m\text{-}H)$	2	4	AFUFAJ	2.037
$[L^{Me,iPr2}Fe]_2(\mu\text{-}NCH^tBu)(m\text{-}H)$	2	4	AFUFAJ	2.035
$[L^{Me,iPr2}Fe]_2(\mu\text{-}NCH^tBu)(m\text{-}H)$	2	4	AFUFAJ	2.0405
$[L^{Me,iPr2}Fe(HCO_2)]_2$	2	4	AFUGAK	1.975
$[L^{tBu,iPr2}Fe(HCO_2)]_2$	2	4	AFUGEO	2.006
$L^{tBu,iPr2}Fe(\kappa^2\text{-}^iPrNCHN^iPr)$	2	4	AFUGIS	2.0285
$[L^{Me,iPr2}Fe(OH)]_2$	2	4	AFUGOY	2.0395
$[L^{tBu,iPr2}Fe]_2(\mu\text{-}N_6Ad_2)$	2	4	IFECUS	2.0305
$[L^{Me,iPr2}Fe]_2(\mu\text{-}N_6Ad_2)$	2	4	IFEDAZ	2.0185
$[L^{tBu,iPr3}Fe]_2(\mu\text{-}CO_3)$	2	4	BOTNOO	1.9755
$L^{tBu,iPr2}Fe(OtBu)(OTf)$	3	4	DABPEC	1.966
$L^{tBu,iPr2}Fe(OtBu)(OTf)$	3	4	DABPEC	1.973
$L^{tBu,iPr2}Fe(NHdipp)(OTf)$	3	4	DABPOM	1.971
$L^{Me,iPr2}Fe(OtBu)(Cl)$	3	4	DABQED	1.977
$L^{Me,iPr2}Fe(OtBu)(OTf)$	3	4	DABQON	1.9645
$[L^{Me,iPr2}Fe(PPh)]_2$	3	4	MECCIH	2.013
$L^{Me,iPr2}Fe(Cl)_2$	3	4	MONZUK	1.9645

Table S-5. Average Fe–$N_{diketiminate}$ bond lengths (Å) from the CSD v. 5.31 (Feb 2010 update) organized by iron oxidation state and coordination number.

3-coordinate					
Fe(I)	1.945	±	0.013	*N* =	2
Fe(II)	1.982	±	0.017	*N* =	50
4-coordinate					
Fe(I)	1.968	±	0.001	*N* =	2
Fe(II)	2.014	±	0.020	*N* =	61
Fe(III)	1.976	±	0.021	*N* =	7
5-coordinate					
Fe(I)	1.996	±	0.038	*N* =	3
Fe(II)	1.987	±	0.005	*N* =	1

Table S-6. Imido complexes of Fe, Co, and Ni used in the bond metric analysis from the CSD.

CSD Refcode	*metal*	*coordination number*	*Geometry*	*M=N–C angle (°)*	*M=N bond length (Å)*
PEKWUY	Fe	4	square planar	159.00	1.716
PEKXAF	Fe	4	square planar	165.68	1.705
MOBNUN	Fe	4	tetrahedral	176.83	1.618
MOBNEX	Fe	4	tetrahedral	177.01	1.625
SESQEM	Fe	4	tetrahedral	178.64	1.635
CEKBOK	Fe	4	tetrahedral	173.72	1.609
CEKBUQ	Fe	4	tetrahedral	176.26	1.634
CEKBEA	Fe	4	tetrahedral	173.01	1.630
CEKBIE	Fe	4	tetrahedral	172.27	1.650
OLAXOO	Fe	4	tetrahedral	175.97	1.638
SEYGUZ	Fe	4	tetrahedral	176.31	1.622
DEQKEQ	Fe	4	tetrahedral	179.17	1.635
FIMPOH	Fe	4	tetrahedral	176.33	1.641
OJAPEU	Fe	4	tetrahedral	168.63	1.660
FIMPIB	Fe	4	tetrahedral	178.57	1.651
FEMPOD	Co	4	tetrahedral	168.65	1.675
WEZFIR	Co	4	tetrahedral	179.69	1.659
LUFQAE	Co	4	tetrahedral	169.49	1.658
NALROI	Co	4	tetrahedral	176.68	1.633
OLAXUU	Co	4	tetrahedral	173.15	1.667
YALHOJ	Co	4	tetrahedral	178.34	1.655
REVKOT	Co	4	tetrahedral	179.36	1.660
QOXBUB	Fe	4	tetrahedral	177.74	1.653
XOMYAA	Fe	3	trigonal	156.60	1.642
XOMYAA	Fe	3	trigonal	160.70	1.619
compound **2** (this work)	Fe	3	trigonal	170.40	1.670
ABATUT	Co	3	trigonal	161.55	1.624
[a]	Co	3	trigonal	172.10	1.621
JATZEK	Ni	3	trigonal	164.49	1.662
MIQBIX	Ni	3	trigonal	162.79	1.702
SOQJAE	Ni	3	trigonal	163.00	1.673
SOQHOQ	Ni	3	trigonal	180.00	1.703

[a] This structure is from: Jones, C.; Schulten, C.; Rose, R. P.; Stasch, A.; Aldridge, S.; Woodul, W. D.; Murray, K. S.; Moubaraki, B.; Brynda, M.; La Macchia, G.; Gagliardi, L. *Angew. Chem. Int. Ed.* **2009**, *48*, 7406 - 7410.

Table S-7. ONIOM(B3LYP/6-311+G(d):UFF) Optimized Free Energies (a.u.) for Stationary Points[a]

Compound	*Multiplicity*	*Stoichiometry*	*G*	*Comment*
Py	0	C_5H_5N	-248.28122	Pyridine
AdN_3	0	$C_{10}H_{15}N_3$	-203.88027	1-Adamantyl Azide
N_2	0	N_2	-109.57256	Dinitrogen
$L^{Me}Fe(py)(N_3Ad-\kappa N^1)$	4	$C_{44}H_{61}FeN_6$	-1942.07341	N_3Ad coordinated through internal N
$L^{Me}Fe(py)(N_3Ad-\kappa N^1)$	6	$C_{44}H_{61}FeN_6$	-1942.07513	N_3Ad coordinated through internal N
$L^{Me}Fe(py)(N_3Ad-\kappa N^3)$	4	$C_{44}H_{61}FeN_6$	-1942.08689	N_3Ad coordinated through terminal N
$L^{Me}Fe(py)(N_3Ad-\kappa N^3)$	6	$C_{44}H_{61}FeN_6$	-1942.07585	N_3Ad coordinated through terminal N
$L^{Me}Fe(py)(\eta^2-N_3Ad)$	4	$C_{44}H_{61}FeN_6$	-1942.08329	η^2-N_3Ad
$L^{Me}Fe(py)(\eta^2-N_3Ad)$	6	$C_{44}H_{61}FeN_6$	*n/a*	η^2-N_3Ad; reverts to sextet ($N_3Ad-\kappa N^3$)
$L^{Me}Fe(N_3Ad-\kappa N^1)$	4	$C_{39}H_{56}FeN_5$	-1693.81174	N_3Ad coordinated through internal N
$L^{Me}Fe(N_3Ad-\kappa N^1)$	6	$C_{39}H_{56}FeN_5$	-1693.81243	N_3Ad coordinated through internal N
$L^{Me}Fe(N_3Ad-\kappa N^3)$	4	$C_{39}H_{56}FeN_5$	-1693.80451	N_3Ad coordinated through terminal N
$L^{Me}Fe(N_3Ad-\kappa N^3)$	6	$C_{39}H_{56}FeN_5$	-1693.78608	N_3Ad coordinated through terminal N
$L^{Me}Fe(\eta^2-N_3Ad)$	4	$C_{39}H_{56}FeN_5$	-1693.80107	η^2-N_3Ad
$L^{Me}Fe(\eta^2-N_3Ad)$	6	$C_{39}H_{56}FeN_5$	*n/a*	η^2-N_3Ad; reverts to sextet ($N_3Ad-\kappa N^3$)
$L^{Me}Fe(N_3Ad-\kappa N^1N^3)$	4	$C_{39}H_{56}FeN_5$	-1693.76057	triazametallocyclobutene core
$L^{Me}Fe(N_3Ad-\kappa N^1N^3)$	6	$C_{39}H_{56}FeN_5$	-1693.74429	triazametallocyclobutene core
$L^{Me}Fe(py)$	4	$C_{34}H_{46}FeN_3$	-1738.19466	Pyridine Complex
$L^{Me}Fe(py)$	6	$C_{34}H_{46}FeN_3$	-1738.14685	Pyridine Complex
$L^{Me}Fe(py)_2$	4	$C_{39}H_{51}FeN_4$	-1986.47628	Bis(pyridine) Complex
$L^{Me}Fe(py)_2$	6	$C_{39}H_{51}FeN_4$	-1986.45761	Bis(pyridine) Complex
$L^{Me}Fe(NAd)$	4	$C_{39}H_{56}FeN_3$	-1584.30802	Imide
$L^{Me}Fe(NAd)$	6	$C_{39}H_{56}FeN_3$	-1584.29124	Imide
$L^{Me}Fe(py)(NAd)$	4	$C_{44}H_{61}FeN_4$	-1832.57769	Imide/Pyridine Adduct
$L^{Me}Fe(py)(NAd)$	6	$C_{44}H_{61}FeN_4$	-1832.57655	Imide/Pyridine Adduct
$L^{Me}Fe(N_3Ad)$ - N_2 TS	4	$C_{39}H_{56}FeN_5$	-1693.79334	TS for N_2 Elimination
$L^{Me}Fe(N_3Ad)$ - N_2 TS	6	$C_{39}H_{56}FeN_5$	-1693.79168	TS for N_2 Elimination
$L^{Me}Fe(py)(N_3Ad)$ - N_2 TS	4	$C_{44}H_{61}FeN_6$	-1942.07134	TS for N_2 Elimination
$L^{Me}Fe(py)(N_3Ad)$ - N_2 TS	6	$C_{44}H_{61}FeN_6$	-1942.06997	TS for N_2 Elimination
$L^{Me}FeNNFeL^{Me}$	7	$C_{58}H_{82}Fe_2N_6$	-3089.41461	Diiron Dinitrogen Complex
$L^{Me}Fe$	4	$C_{29}H_{41}FeN_2$	-1489.87940	Fe-β-Diketiminate Fragment
$L^{Me}Fe(N_3Ad)FeL^{Me}$	7	$C_{68}H_{97}Fe_2N_7$	-3183.74110	$L^{Me}Fe(\mu-N_3Ad)FeL^{Me}$
$L^{Me}Fe(N_2)(N_3Ad)FeL^{Me}$	7	$C_{68}H_{97}Fe_2N_9$	-3293.28138	$L^{Me}Fe(\mu-N_2)(\mu-N_3Ad)FeL^{Me}$
$L^{Me}Fe(AdNNNNNNAd)FeL^{Me}$	7	$C_{78}H_{112}Fe_2N_{10}$	-3387.62685	$L^{Me}Fe(\mu-AdNNNNNNAd)FeL^{Me}$

[a] Ad = 1-adamantyl; L^{Me} = 2,4-bis(2,6-diisopropylphenylimido)pentyl anion; py = pyridine;
n/a = not available (geometry not stable at the level of theory utilized; see comment)

Table S-8. ONIOM(B3LYP/6-311+G(d):UFF) Optimized Cartesian Coordinates (Å) for Stationary Points

Py (Pyridine, C_5H_5N)

C	0.000000	-1.141419	-0.709904
C	0.000000	-1.196822	0.683008
C	0.000000	0.000000	1.394554
C	0.000000	1.196822	0.683008
C	0.000000	1.141419	-0.709904
H	0.000000	-2.056251	-1.297529
H	0.000000	-2.154730	1.192007
H	0.000000	0.000000	2.479920
H	0.000000	2.154730	1.192007
H	0.000000	2.056251	-1.297529
N	0.000000	0.000000	-1.405553

AdN_3 (1-Adamantyl Azide, $C_{10}H_{15}N_3$)

N	-0.495411	-0.689858	-1.023386
N	-1.442510	-1.231032	-1.341788
N	-2.370934	-1.927005	-1.737939
C	-3.766129	-1.457031	-1.563131
C	-4.003434	-0.129430	-2.312450
C	-4.685819	-2.535247	-2.153103
C	-4.106171	-1.268762	-0.070071
H	-3.754113	-0.248014	-3.390304
H	-3.339868	0.666155	-1.907045
C	-5.478697	0.306236	-2.162504
H	-4.522110	-3.505976	-1.633787
H	-4.449033	-2.695583	-3.228755
C	-6.166197	-2.114195	-2.006994
H	-3.444703	-0.496759	0.381706
H	-3.931679	-2.217081	0.485119
C	-5.581710	-0.836170	0.085938
H	-5.640919	1.264161	-2.702757
C	-6.396749	-0.783958	-2.756812
C	-5.808105	0.495056	-0.664857
H	-6.821904	-2.902035	-2.437328
C	-6.499642	-1.925018	-0.511018
H	-5.818061	-0.700320	1.163663
H	-6.179303	-0.915319	-3.839647
H	-7.461628	-0.475642	-2.667152
H	-5.162811	1.290402	-0.231187
H	-6.864074	0.823564	-0.546326
H	-7.565844	-1.631380	-0.392470
H	-6.356799	-2.883716	0.034477

AdN_3^- (1-Adamantyl Azide anion, $C_{10}H_{15}N_3^-$)

N	-0.269037	-1.085337	-1.213637

N	-1.472988	-1.042670	-1.247424
N	-2.365805	-1.903143	-1.724886
C	-3.751077	-1.433774	-1.550234
C	-4.016868	-0.100483	-2.302941
C	-4.668072	-2.521639	-2.144725
C	-4.120342	-1.242865	-0.052860
H	-3.760078	-0.213717	-3.379513
H	-3.371731	0.708763	-1.895404
C	-5.499387	0.310450	-2.161349
H	-4.498386	-3.490922	-1.624561
H	-4.425062	-2.681342	-3.219116
C	-6.153498	-2.117982	-2.008092
H	-3.477651	-0.460195	0.407079
H	-3.938794	-2.186959	0.507046
C	-5.602782	-0.831032	0.086927
H	-5.673542	1.265515	-2.703032
C	-6.396468	-0.792821	-2.761220
C	-5.840840	0.495807	-0.666655
H	-6.796476	-2.914364	-2.441996
C	-6.499747	-1.933072	-0.515375
H	-5.851299	-0.696907	1.162171
H	-6.168932	-0.922339	-3.842220
H	-7.466272	-0.499462	-2.680212
H	-5.209361	1.300155	-0.229235
H	-6.901855	0.810467	-0.555693
H	-7.570920	-1.654817	-0.404623
H	-6.347089	-2.889275	0.031872

N_2 (N_2)

N	0.000000	0.000000	0.547768
N	0.000000	0.000000	-0.547768

$L^{Me}Fe(py)(N_3Ad\text{-}\kappa N^1)$ ($C_{44}H_{61}FeN_6$)

N	2.405993	0.308417	0.416228
N	-0.165667	1.693550	1.017128
C	2.823322	1.122575	1.393403
C	0.665313	2.447995	1.736465
C	1.988227	2.053601	2.045780
H	2.485349	2.672525	2.790691
N	-0.561543	-1.102297	-1.305574
N	0.227192	-1.424276	-2.402433
N	1.390861	-1.279403	-2.544051
C	-1.983773	-1.474079	-1.566789
C	-2.801644	-1.208949	-0.293577
C	-2.588130	-0.627497	-2.711310
C	-2.117128	-2.974987	-1.928848
H	-2.723529	-0.143348	-0.015169
H	-2.405600	-1.806060	0.547668
C	-4.287751	-1.574067	-0.501813

H	-2.017423	-0.777613	-3.653820
H	-2.532311	0.449764	-2.452767
C	-4.069098	-1.002187	-2.942286
H	-1.690564	-3.605807	-1.119442
H	-1.548588	-3.207740	-2.855822
C	-3.599703	-3.349036	-2.149516
H	-4.854620	-1.370413	0.432812
C	-4.869547	-0.727157	-1.652314
C	-4.397859	-3.071204	-0.858134
H	-4.482415	-0.389438	-3.772723
C	-4.173506	-2.499325	-3.303787
H	-3.676697	-4.427439	-2.408428
H	-4.816621	0.352829	-1.394098
H	-5.941717	-0.978828	-1.807192
H	-4.000209	-3.690947	-0.024378
H	-5.464546	-3.351636	-1.001362
H	-5.235961	-2.773332	-3.485808
H	-3.612641	-2.703494	-4.242300
C	3.344466	-0.285403	-0.475374
C	3.755582	-1.635084	-0.291646
C	3.916713	0.487164	-1.526908
C	4.703765	-2.188873	-1.171584
C	4.871947	-0.107389	-2.371806
C	5.253120	-1.431708	-2.198313
H	5.034556	-3.212657	-1.056652
H	5.328513	0.456198	-3.174670
H	5.987187	-1.872803	-2.860421
C	-1.458677	2.158783	0.661224
C	-1.664891	2.762456	-0.608103
C	-2.553692	1.998534	1.559374
C	-2.970842	3.127321	-0.984158
C	-3.843387	2.359331	1.128727
C	-4.047318	2.907535	-0.132315
H	-3.160885	3.602974	-1.937022
H	-4.699825	2.229296	1.776986
H	-5.045500	3.189209	-0.442020
C	0.270795	3.810261	2.291966
H	-0.738183	4.146418	1.984894
H	0.297932	3.780889	3.401786
H	0.990383	4.577827	1.935718
C	4.262458	1.115228	1.891783
H	4.912135	0.388979	1.366213
H	4.709473	2.123820	1.768637
H	4.276897	0.850187	2.970260
C	-2.366831	1.481070	2.983292
C	-3.091315	0.147946	3.202705
C	-2.824893	2.520244	4.016199
H	-1.297000	1.296956	3.190068
H	-2.685206	-0.620867	2.518773
H	-2.927254	-0.208498	4.242123
H	-4.183661	0.246097	3.030591

H	-2.326828	3.494744	3.830305
H	-3.924670	2.668404	3.979506
H	-2.552073	2.183767	5.039314
C	-0.496461	3.123423	-1.521666
C	-0.357332	4.646297	-1.638508
C	-0.622395	2.478984	-2.909041
H	0.456916	2.757379	-1.093483
H	-0.278814	5.100303	-0.627424
H	0.564755	4.902908	-2.202854
H	-1.229056	5.088571	-2.165725
H	-0.451825	1.386685	-2.830397
H	-1.615165	2.665896	-3.366585
H	0.143781	2.888693	-3.598530
C	3.228784	-2.488156	0.852323
C	4.355953	-2.902711	1.806646
C	2.480965	-3.718582	0.322493
H	2.514927	-1.906521	1.460886
H	4.894280	-2.004316	2.175742
H	3.931494	-3.434832	2.684847
H	5.082589	-3.576664	1.306072
H	1.670242	-3.403132	-0.368165
H	3.164497	-4.404472	-0.220345
H	2.026511	-4.280449	1.165808
C	3.526913	1.941516	-1.766287
C	2.943741	2.135383	-3.170900
C	4.720698	2.878317	-1.543431
H	2.739706	2.256051	-1.054384
H	2.114236	1.417689	-3.340022
H	2.548109	3.167982	-3.275251
H	3.713135	1.979265	-3.955755
H	5.152482	2.716927	-0.534490
H	5.514386	2.706064	-2.300813
H	4.390531	3.936798	-1.613784
Fe	0.407409	-0.125200	0.195415
N	0.083873	-1.451989	1.961887
C	0.373260	-0.952865	3.176239
C	-0.308153	-2.734410	1.889706
C	0.250294	-1.694222	4.345113
H	0.728422	0.070380	3.199639
C	-0.462942	-3.544398	3.007606
H	-0.488025	-3.117233	0.892819
C	-0.184864	-3.013352	4.263312
H	0.495099	-1.238105	5.297383
H	-0.787715	-4.571250	2.886160
H	-0.296090	-3.617338	5.157650

$L^{Me}Fe(py)(N_3Ad\text{-}\kappa N^1)$ (sextet, $C_{44}H_{61}FeN_6$)

N	2.421433	0.284067	0.412839
N	-0.137841	1.681009	1.028851
C	2.844081	1.082343	1.401480

C	0.698175	2.422728	1.754286
C	2.017642	2.014076	2.061805
H	2.518915	2.620921	2.813850
N	-0.612110	-1.081383	-1.306697
N	0.174837	-1.388623	-2.398083
N	1.339230	-1.214030	-2.520667
C	-2.036264	-1.442656	-1.561323
C	-2.842248	-1.196721	-0.276959
C	-2.644478	-0.573034	-2.685948
C	-2.178819	-2.935956	-1.949256
H	-2.756519	-0.136542	0.020191
H	-2.442508	-1.811266	0.550358
C	-4.331673	-1.550901	-0.480347
H	-2.081430	-0.710406	-3.635039
H	-2.579821	0.499531	-2.409781
C	-4.129051	-0.936043	-2.911900
H	-1.749178	-3.583090	-1.154398
H	-1.617998	-3.154020	-2.884507
C	-3.664883	-3.299098	-2.165227
H	-4.890416	-1.361545	0.462134
C	-4.918019	-0.680444	-1.610860
C	-4.451834	-3.040853	-0.862890
H	-4.545693	-0.306410	-3.727915
C	-4.243623	-2.425957	-3.299438
H	-3.749013	-4.372273	-2.442941
H	-4.857602	0.394425	-1.333584
H	-5.992617	-0.923983	-1.761847
H	-4.050923	-3.677515	-0.043576
H	-5.520949	-3.313538	-1.002945
H	-5.308801	-2.691586	-3.477927
H	-3.691150	-2.615854	-4.245891
C	3.356345	-0.300746	-0.487738
C	3.758119	-1.655998	-0.326533
C	3.930163	0.484222	-1.528993
C	4.700455	-2.202192	-1.217394
C	4.879331	-0.103205	-2.385555
C	5.252468	-1.432528	-2.233476
H	5.024123	-3.230041	-1.119705
H	5.336821	0.469750	-3.181247
H	5.981814	-1.868079	-2.904412
C	-1.430015	2.156327	0.683166
C	-1.639658	2.767841	-0.581872
C	-2.520164	2.001688	1.588385
C	-2.944286	3.149714	-0.945446
C	-3.809221	2.377995	1.169174
C	-4.016617	2.936281	-0.086844
H	-3.136455	3.633343	-1.893825
H	-4.662329	2.252377	1.822669
H	-5.014026	3.230379	-0.387354
C	0.316093	3.784921	2.318726
H	-0.688726	4.133449	2.011733

H	0.340868	3.747467	3.428348
H	1.044061	4.547720	1.969330
C	4.281859	1.054031	1.902901
H	4.924229	0.325323	1.371823
H	4.740548	2.058579	1.789926
H	4.290999	0.778649	2.978848
C	-2.328915	1.472633	3.007590
C	-3.062296	0.143523	3.221698
C	-2.772894	2.507761	4.050733
H	-1.259460	1.278428	3.206889
H	-2.662543	-0.624610	2.533185
H	-2.898705	-0.219473	4.258919
H	-4.154259	0.250121	3.052161
H	-2.270481	3.480517	3.867530
H	-3.872001	2.662715	4.023420
H	-2.494454	2.162875	5.069524
C	-0.474438	3.119810	-1.503064
C	-0.314321	4.641457	-1.607498
C	-0.622120	2.490146	-2.895173
H	0.477170	2.735478	-1.087094
H	-0.218099	5.084796	-0.593227
H	0.605091	4.890069	-2.179675
H	-1.185391	5.101105	-2.120778
H	-0.476134	1.393785	-2.827065
H	-1.612757	2.703159	-3.345809
H	0.149761	2.888470	-3.585077
C	3.226292	-2.523809	0.804117
C	4.351735	-2.964691	1.748648
C	2.466348	-3.738253	0.255106
H	2.518761	-1.946492	1.424297
H	4.899065	-2.077670	2.131695
H	3.924351	-3.507759	2.618690
H	5.071086	-3.636665	1.235072
H	1.656904	-3.403814	-0.428071
H	3.142606	-4.420688	-0.301065
H	2.008592	-4.310307	1.089770
C	3.547005	1.943943	-1.745886
C	2.959075	2.160813	-3.145157
C	4.746300	2.871352	-1.513886
H	2.764227	2.252474	-1.026507
H	2.127516	1.447445	-3.322188
H	2.564488	3.195454	-3.232098
H	3.725364	2.015157	-3.935074
H	5.179852	2.693908	-0.508315
H	5.536933	2.705261	-2.275816
H	4.421497	3.932398	-1.568906
Fe	0.423743	-0.127312	0.168661
N	0.090758	-1.469943	1.934778
C	0.387874	-0.993750	3.156054
C	-0.312416	-2.747223	1.842231
C	0.262991	-1.753920	4.312830

H	0.750958	0.026186	3.195322
C	-0.470010	-3.575252	2.946521
H	-0.499718	-3.110393	0.839246
C	-0.182892	-3.067980	4.210066
H	0.514469	-1.316144	5.271976
H	-0.803791	-4.597196	2.808906
H	-0.295771	-3.686291	5.094382

$L^{Me}Fe(py)(N_3Ad\text{-}\kappa N^3)$ (quartet, $C_{44}H_{61}FeN_6$)

N	0.506340	-0.936219	1.669286
N	2.970462	-0.120254	0.173724
C	1.433308	-1.295364	2.561646
C	3.539820	-0.497557	1.324805
C	2.803709	-0.953170	2.440562
H	3.410812	-1.211593	3.306469
N	-0.035099	0.217759	-1.574277
N	-1.251180	0.263180	-1.658245
N	-2.117369	0.069179	-2.558780
C	5.048009	-0.470886	1.526186
H	5.296258	0.194934	2.379790
H	5.412330	-1.495190	1.752466
H	5.607406	-0.099340	0.645640
C	1.103316	-2.122227	3.797460
H	1.709566	-3.052903	3.793779
H	1.348454	-1.539257	4.710378
H	0.040817	-2.424496	3.867454
C	-0.826946	-1.423116	1.747974
C	-1.189929	-2.602000	1.045052
C	-1.786854	-0.763044	2.564171
C	-2.468301	-3.153751	1.251132
C	-3.068705	-1.325884	2.703830
C	-3.395371	-2.519361	2.070365
H	-2.758795	-4.076971	0.768391
H	-3.822050	-0.843278	3.312313
H	-4.381045	-2.947022	2.201269
C	3.730979	0.041834	-1.013892
C	4.164118	1.335079	-1.411660
C	4.052168	-1.089583	-1.811488
C	4.898180	1.474018	-2.603445
C	4.799785	-0.904362	-2.989140
C	5.211991	0.364650	-3.380577
H	5.238375	2.446947	-2.933128
H	5.066485	-1.746785	-3.613633
H	5.782945	0.488868	-4.291819
C	3.615387	-2.497188	-1.420823
C	4.827642	-3.395568	-1.147152
C	2.708936	-3.112450	-2.492812
H	3.022806	-2.478721	-0.484719
H	5.481869	-2.929801	-0.380200
H	4.490066	-4.381455	-0.761822

H	5.421479	-3.563354	-2.070336
H	1.836436	-2.449468	-2.676136
H	3.253673	-3.261156	-3.448568
H	2.335983	-4.100551	-2.149468
C	3.874756	2.569384	-0.568851
C	3.004558	3.571453	-1.337215
C	5.170019	3.228491	-0.078747
H	3.314659	2.286425	0.340767
H	2.096896	3.065686	-1.729546
H	2.682185	4.391462	-0.660299
H	3.560348	4.015786	-2.189683
H	5.789534	2.488771	0.471499
H	5.762668	3.634689	-0.925236
H	4.931160	4.063117	0.614649
C	-0.219617	-3.293252	0.095648
C	-0.841659	-3.502947	-1.293564
C	0.262696	-4.621977	0.685573
H	0.678417	-2.661545	-0.059735
H	-1.193575	-2.535157	-1.705142
H	-0.089637	-3.922592	-1.991936
H	-1.696557	-4.209200	-1.257641
H	0.729487	-4.449076	1.678616
H	-0.580831	-5.334890	0.804044
H	1.025557	-5.079676	0.020149
C	-1.468126	0.541705	3.280167
C	-1.624363	0.406253	4.800271
C	-2.335784	1.685100	2.739374
H	-0.414573	0.825761	3.103780
H	-1.010699	-0.439497	5.175037
H	-1.274832	1.334905	5.300037
H	-2.683472	0.234074	5.085121
H	-2.247119	1.740867	1.634070
H	-3.404596	1.536641	3.001623
H	-1.998060	2.653748	3.165663
C	-3.515916	0.265681	-2.106882
C	-3.765257	1.724464	-1.658407
C	-4.433169	-0.051261	-3.297999
C	-3.865377	-0.686737	-0.941547
H	-3.513631	2.426757	-2.483742
H	-3.110511	1.982329	-0.797458
C	-5.242374	1.909421	-1.245582
H	-4.265024	-1.095857	-3.643439
H	-4.195031	0.618922	-4.154011
C	-5.915807	0.128314	-2.897418
H	-3.213031	-0.472467	-0.068559
H	-3.683574	-1.742844	-1.240190
C	-5.341618	-0.507341	-0.527124
H	-5.409740	2.960063	-0.923178
C	-6.153269	1.586951	-2.449701
C	-5.572728	0.952267	-0.078649
H	-6.567238	-0.103886	-3.767773

C	-6.251894	-0.827301	-1.731926
H	-5.579225	-1.196172	0.312314
H	-5.934155	2.282745	-3.289298
H	-7.219948	1.730571	-2.169333
H	-4.930318	1.185807	0.798815
H	-6.629822	1.089616	0.238341
H	-7.319891	-0.714772	-1.442595
H	-6.103510	-1.882574	-2.050515
Fe	0.982347	0.155263	0.030796
N	0.582613	2.204590	0.724879
C	1.133644	2.632643	1.874509
C	-0.207679	3.054123	0.049209
C	0.915278	3.904570	2.386768
H	1.767350	1.920435	2.392952
C	-0.482492	4.341982	0.493877
H	-0.623464	2.676261	-0.876490
C	0.088308	4.778260	1.685297
H	1.384860	4.196686	3.318916
H	-1.131007	4.984374	-0.090635
H	-0.105553	5.777907	2.059486

L^{Me}Fe(py)(N_3Ad-κ*N*^{3}) (sextet, $C_{44}H_{61}FeN_6$)

N	0.551531	-0.329982	1.977490
N	2.935376	-0.535941	0.201655
C	1.471755	-0.619841	2.906017
C	3.492496	-0.917944	1.355380
C	2.834922	-0.819783	2.605002
H	3.459919	-1.052471	3.465172
N	-0.212389	-0.129365	-1.411214
N	-1.439848	-0.058844	-1.435794
N	-2.252378	0.352714	-2.321010
C	4.890113	-1.517544	1.430797
H	5.538897	-0.870368	2.058076
H	4.836244	-2.525213	1.895007
H	5.382664	-1.638604	0.446938
C	1.115399	-0.770757	4.377794
H	1.365462	-1.797685	4.718483
H	1.699999	-0.041344	4.977617
H	0.044578	-0.592978	4.596807
C	-0.836736	-0.438132	2.252565
C	-1.482059	-1.699941	2.157600
C	-1.579692	0.711731	2.629980
C	-2.850210	-1.791816	2.473233
C	-2.943671	0.571696	2.944162
C	-3.567265	-0.668785	2.871795
H	-3.368929	-2.739627	2.416175
H	-3.534338	1.428603	3.240126
H	-4.618239	-0.758071	3.114885
C	3.577756	-0.761938	-1.043829
C	4.548762	0.157028	-1.528688

C	3.266568	-1.926277	-1.793564
C	5.228963	-0.138481	-2.724132
C	3.998195	-2.199227	-2.963952
C	4.965616	-1.311678	-3.422973
H	5.976042	0.538386	-3.117324
H	3.818926	-3.102164	-3.531970
H	5.510140	-1.530999	-4.332464
C	2.181262	-2.896616	-1.341649
C	2.799805	-4.198239	-0.823132
C	1.168894	-3.179014	-2.462608
H	1.600596	-2.457764	-0.504885
H	3.503777	-3.979133	0.007748
H	2.004287	-4.869551	-0.434621
H	3.350331	-4.726479	-1.630510
H	0.777599	-2.226592	-2.877373
H	1.626114	-3.765915	-3.286105
H	0.313253	-3.763422	-2.066282
C	4.865522	1.453896	-0.793090
C	4.518163	2.673253	-1.657290
C	6.333596	1.504113	-0.349887
H	4.256544	1.532727	0.129151
H	3.467413	2.606021	-2.009308
H	4.627283	3.604761	-1.061865
H	5.184749	2.742556	-2.542673
H	6.584339	0.608977	0.255742
H	7.018067	1.546486	-1.223096
H	6.509052	2.404815	0.276390
C	-0.727215	-2.955298	1.734008
C	-1.310100	-3.543162	0.443936
C	-0.716418	-3.999320	2.856989
H	0.333855	-2.720210	1.516613
H	-1.284378	-2.781287	-0.363020
H	-0.705081	-4.415902	0.118389
H	-2.358393	-3.879089	0.587931
H	-0.306479	-3.553162	3.787764
H	-1.738669	-4.381326	3.062061
H	-0.071173	-4.857417	2.571123
C	-0.934772	2.088162	2.708694
C	-0.993335	2.653276	4.133022
C	-1.579597	3.053601	1.705950
H	0.138415	2.023258	2.447252
H	-0.527547	1.939721	4.845459
H	-0.430446	3.609785	4.184075
H	-2.040187	2.845284	4.449208
H	-1.564757	2.610588	0.687820
H	-2.632384	3.275780	1.980408
H	-1.012558	4.008553	1.678483
C	-3.681819	0.209739	-1.968446
C	-4.021509	0.959462	-0.660075
C	-4.498689	0.823535	-3.116777
C	-4.073890	-1.277194	-1.814637

H	-3.740118	2.032182	-0.748606
H	-3.438213	0.536485	0.184100
C	-5.530089	0.837974	-0.351439
H	-4.265422	0.304512	-4.073308
H	-4.226167	1.894300	-3.250907
C	-6.011800	0.708845	-2.822434
H	-3.496258	-1.744520	-0.987218
H	-3.828137	-1.836168	-2.744632
C	-5.584102	-1.401741	-1.513337
H	-5.760389	1.376179	0.593712
C	-6.338229	1.457729	-1.511633
C	-5.907599	-0.652740	-0.202443
H	-6.589035	1.157196	-3.660046
C	-6.391779	-0.780087	-2.672761
H	-5.854495	-2.474564	-1.404809
H	-6.086482	2.535980	-1.616924
H	-7.427196	1.390689	-1.295600
H	-5.344228	-1.107559	0.639941
H	-6.990094	-0.748999	0.033746
H	-7.481551	-0.876810	-2.472532
H	-6.178524	-1.324104	-3.619138
Fe	1.043059	0.145173	0.092834
N	1.220851	2.306465	-0.186471
C	0.610185	2.904681	-1.225036
C	1.932315	3.070169	0.660686
C	0.689701	4.274683	-1.448373
H	0.043530	2.251844	-1.879750
C	2.056431	4.444442	0.511196
H	2.412177	2.551147	1.483737
C	1.423337	5.060668	-0.565719
H	0.178171	4.707634	-2.300020
H	2.640098	5.013589	1.225337
H	1.500705	6.132848	-0.712181

$L^{Me}Fe(py)(\eta^2\text{-}N_3Ad)$ (sextet, $C_{44}H_{61}FeN_6$)

N	-0.504671	1.925344	-0.862327
N	-2.612545	-0.158224	-0.618474
C	-1.531818	2.613811	-1.371294
C	-3.303242	0.767048	-1.290359
C	-2.834842	2.086931	-1.492834
H	-3.560722	2.763723	-1.939627
N	0.318865	-1.370258	0.538065
N	1.095607	-0.428838	0.296622
N	2.301494	-0.068121	0.222818
C	-4.655726	0.479628	-1.927643
H	-5.428259	1.133537	-1.470802
H	-4.605279	0.694945	-3.016189
H	-4.990580	-0.569961	-1.820527
C	-1.372373	4.038164	-1.882717
H	-1.626850	4.076832	-2.963010

H	-2.059757	4.710848	-1.327188
H	-0.348599	4.442360	-1.761956
C	0.837069	2.351170	-1.050827
C	1.528655	2.000736	-2.241587
C	1.506023	3.082648	-0.032367
C	2.873470	2.387452	-2.389252
C	2.854780	3.436241	-0.218186
C	3.528171	3.090560	-1.384262
H	3.425813	2.138283	-3.285606
H	3.392578	3.985309	0.543475
H	4.565710	3.371721	-1.511117
C	-3.072482	-1.497976	-0.511107
C	-4.042181	-1.851853	0.469021
C	-2.580554	-2.482951	-1.407867
C	-4.526997	-3.171897	0.502858
C	-3.128546	-3.778402	-1.365529
C	-4.085093	-4.117593	-0.415250
H	-5.261832	-3.472721	1.237981
H	-2.814194	-4.537528	-2.068791
H	-4.484161	-5.123460	-0.387290
C	-1.508611	-2.154629	-2.441087
C	-2.121064	-2.070710	-3.842401
C	-0.353349	-3.168605	-2.408532
H	-1.058231	-1.164594	-2.222313
H	-2.925962	-1.305352	-3.859430
H	-1.346449	-1.774056	-4.581093
H	-2.549466	-3.049107	-4.147871
H	0.031273	-3.282654	-1.374097
H	-0.673012	-4.163538	-2.781689
H	0.479718	-2.822065	-3.053478
C	-4.563731	-0.845157	1.487489
C	-4.181683	-1.261511	2.913622
C	-6.081819	-0.654769	1.367189
H	-4.110978	0.148992	1.311434
H	-3.090598	-1.454088	2.976552
H	-4.434716	-0.449033	3.627826
H	-4.720737	-2.182280	3.221592
H	-6.356521	-0.387252	0.326192
H	-6.629363	-1.577269	1.653300
H	-6.413262	0.169242	2.034621
C	0.853410	1.212099	-3.358269
C	1.568699	-0.120753	-3.602909
C	0.775289	2.038386	-4.647219
H	-0.190725	0.958234	-3.085851
H	1.612110	-0.699344	-2.657424
H	1.011302	-0.718410	-4.354740
H	2.602239	0.033721	-3.977188
H	0.261770	3.003280	-4.449630
H	1.787288	2.247081	-5.053895
H	0.193249	1.487403	-5.416648
C	0.799806	3.496465	1.250687

C	0.756832	5.022452	1.398113
C	1.452726	2.844873	2.476499
H	-0.253479	3.163281	1.228664
H	0.286466	5.479344	0.501679
H	0.149524	5.299918	2.286154
H	1.775603	5.445501	1.524220
H	1.520552	1.745873	2.335949
H	2.474854	3.243581	2.647414
H	0.840620	3.042252	3.382435
C	3.356051	-1.062668	0.521717
C	3.304576	-2.269595	-0.443620
C	4.698972	-0.337971	0.337406
C	3.258781	-1.571091	1.978683
H	3.373524	-1.920091	-1.496874
H	2.343380	-2.816194	-0.339992
C	4.470367	-3.238189	-0.143210
H	4.755385	0.543481	1.015086
H	4.787003	0.046554	-0.703711
C	5.874080	-1.295456	0.635880
H	2.296189	-2.100147	2.146553
H	3.287709	-0.712060	2.685386
C	4.425152	-2.538014	2.281675
H	4.423434	-4.103724	-0.839289
C	5.812229	-2.498039	-0.330277
C	4.358677	-3.740213	1.313596
H	6.837025	-0.757268	0.498410
C	5.766839	-1.798367	2.091569
H	4.345687	-2.899844	3.329817
H	5.909443	-2.146794	-1.381154
H	6.659903	-3.190176	-0.131755
H	3.401344	-4.288785	1.454008
H	5.184170	-4.452068	1.534537
H	6.614069	-2.481077	2.322073
H	5.830894	-0.940027	2.796036
Fe	-0.741605	0.152401	0.026933
N	-1.254203	0.693876	2.153248
C	-2.131327	1.675783	2.413481
C	-0.684750	0.063211	3.191333
C	-2.463810	2.067980	3.704459
H	-2.576332	2.158761	1.549632
C	-0.960170	0.390901	4.514198
H	0.005255	-0.732435	2.934023
C	-1.865510	1.414286	4.777956
H	-3.178021	2.868880	3.857469
H	-0.471050	-0.150360	5.315985
H	-2.101892	1.695485	5.798852

$L^{Me}Fe(N_3Ad\text{-}\kappa N^1)$ (quartet, $C_{39}H_{56}FeN_5$)

N	-2.244364	-0.449847	0.727391
N	0.217268	-1.886008	0.591072

C	-2.660562	-1.538913	1.397043
C	-0.551103	-2.902129	1.027960
C	-1.847989	-2.681591	1.531916
H	-2.312220	-3.531707	2.026974
N	0.354791	1.607689	-0.612128
N	-0.404038	2.308096	-1.549973
N	-1.542433	2.151891	-1.814266
Fe	-0.396553	-0.028621	0.152802
C	1.740899	2.117724	-0.509062
C	2.377973	1.465873	0.724649
C	2.569426	1.738089	-1.755216
C	1.777685	3.653410	-0.322508
H	2.358779	0.365289	0.608215
H	1.790134	1.715327	1.636348
C	3.839450	1.936292	0.899477
H	2.123161	2.190584	-2.667974
H	2.564413	0.635517	-1.895154
C	4.028279	2.220980	-1.596386
H	1.186027	3.945687	0.572663
H	1.324738	4.167130	-1.198710
C	3.235876	4.138437	-0.160616
H	4.285008	1.450768	1.794309
C	4.654214	1.551754	-0.353868
C	3.863550	3.468332	1.079691
H	4.612146	1.944229	-2.500992
C	4.046013	3.754967	-1.418610
H	3.248862	5.242656	-0.032459
H	4.660106	0.446738	-0.478763
H	5.710922	1.878008	-0.236618
H	3.296669	3.752495	1.993519
H	4.909997	3.820073	1.214761
H	5.094039	4.113984	-1.319858
H	3.610171	4.246462	-2.316113
C	-3.228164	0.495926	0.337627
C	-3.369807	1.700395	1.073622
C	-4.028570	0.263103	-0.814672
C	-4.349835	2.628528	0.678708
C	-4.990786	1.223225	-1.177084
C	-5.151785	2.388217	-0.432910
H	-4.493819	3.548340	1.230136
H	-5.619746	1.074972	-2.044985
H	-5.898165	3.115443	-0.725755
C	1.488349	-2.203558	0.045377
C	1.633923	-2.274796	-1.364865
C	2.626582	-2.338371	0.890928
C	2.920717	-2.435370	-1.908863
C	3.895374	-2.476860	0.298914
C	4.038200	-2.515978	-1.084435
H	3.064456	-2.503912	-2.978956
H	4.783482	-2.568806	0.910087
H	5.021985	-2.631173	-1.520896

C	-0.083493	-4.350728	1.079707
H	0.780754	-4.562940	0.419908
H	0.183646	-4.614143	2.123776
H	-0.900508	-5.026038	0.746243
C	-4.029903	-1.645239	2.054321
H	-4.614228	-0.704854	2.029157
H	-4.622745	-2.438810	1.554259
H	-3.906873	-1.918305	3.123978
C	2.505901	-2.391840	2.413890
C	3.218550	-1.214298	3.090589
C	3.043118	-3.724208	2.958306
H	1.443042	-2.330163	2.723270
H	2.692951	-0.268905	2.858275
H	3.197069	-1.336941	4.194631
H	4.277490	-1.136363	2.766678
H	2.597252	-4.578560	2.407755
H	4.148054	-3.780904	2.862414
H	2.780267	-3.829244	4.032635
C	0.420365	-2.250512	-2.293428
C	0.262101	-3.596260	-3.010767
C	0.492358	-1.099640	-3.304425
H	-0.514599	-2.095643	-1.715989
H	0.209085	-4.419559	-2.266487
H	-0.678753	-3.604715	-3.601832
H	1.113066	-3.786594	-3.698553
H	0.486076	-0.128797	-2.771929
H	1.402996	-1.164058	-3.935164
H	-0.393873	-1.123491	-3.973186
C	-2.491128	2.001066	2.283833
C	-3.326862	2.068439	3.567423
C	-1.690315	3.293810	2.082526
H	-1.744243	1.193641	2.435478
H	-3.886709	1.119412	3.707218
H	-2.662590	2.210473	4.446532
H	-4.050272	2.910292	3.532701
H	-1.134934	3.251334	1.123430
H	-2.354719	4.183300	2.070624
H	-0.953474	3.416669	2.904881
C	-3.858813	-0.988391	-1.673341
C	-3.410221	-0.631674	-3.095544
C	-5.147303	-1.820313	-1.703759
H	-3.067396	-1.645207	-1.258882
H	-2.470942	-0.043208	-3.061318
H	-3.212351	-1.558590	-3.675448
H	-4.185335	-0.041298	-3.627989
H	-5.485533	-2.043124	-0.670822
H	-5.960667	-1.284027	-2.236475
H	-4.963911	-2.784715	-2.223950

$L^{Me}Fe(N_3Ad\text{-}\kappa N^1)$ (sextet, $C_{39}H_{56}FeN_5$)

N	2.272172	0.466757	0.686785
N	-0.121805	1.908297	0.589692
C	2.738518	1.538361	1.342585
C	0.661566	2.930338	0.980417
C	1.963110	2.707338	1.468187
H	2.453723	3.557360	1.936510
N	-0.431197	-1.585843	-0.621853
N	0.327588	-2.331601	-1.503276
N	1.460118	-2.147580	-1.788089
Fe	0.422069	0.023903	0.112926
C	-1.828841	-2.060172	-0.503774
C	-2.438046	-1.392619	0.734763
C	-2.653469	-1.656696	-1.744218
C	-1.908697	-3.594873	-0.319550
H	-2.388071	-0.293638	0.618630
H	-1.851110	-1.659840	1.642010
C	-3.911167	-1.820586	0.919016
H	-2.225507	-2.122811	-2.658970
H	-2.615624	-0.555050	-1.885755
C	-4.124982	-2.096401	-1.576071
H	-1.320341	-3.906936	0.570707
H	-1.477726	-4.119936	-1.200166
C	-3.379161	-4.037798	-0.147929
H	-4.335904	-1.323261	1.817549
C	-4.722844	-1.410995	-0.328490
C	-3.978447	-3.351516	1.097604
H	-4.706445	-1.801448	-2.476455
C	-4.186600	-3.629368	-1.399767
H	-3.423214	-5.141358	-0.020985
H	-4.697757	-0.306262	-0.452178
H	-5.787743	-1.706661	-0.204437
H	-3.413623	-3.653254	2.007071
H	-5.033685	-3.672939	1.239624
H	-5.243987	-3.957609	-1.293944
H	-3.771712	-4.132382	-2.300812
C	3.178811	-0.573931	0.358626
C	3.212680	-1.748266	1.153364
C	4.023751	-0.454387	-0.778987
C	4.124623	-2.767043	0.824252
C	4.912190	-1.503686	-1.076790
C	4.963535	-2.643097	-0.279192
H	4.187782	-3.666481	1.422447
H	5.571299	-1.443531	-1.932811
H	5.656115	-3.439015	-0.521146
C	-1.382558	2.213975	0.013741
C	-1.506501	2.256880	-1.400041
C	-2.527920	2.400278	0.839561

C	-2.780128	2.447832	-1.965267
C	-3.784588	2.556578	0.226805
C	-3.906570	2.573928	-1.158909
H	-2.907108	2.503855	-3.038073
H	-4.678442	2.683203	0.823220
H	-4.880490	2.708097	-1.611760
C	0.200244	4.380488	1.012006
H	-0.657561	4.585279	0.341403
H	-0.074939	4.656310	2.050663
H	1.022109	5.049668	0.678176
C	4.119420	1.602919	1.977459
H	4.677313	0.646989	1.937012
H	4.725504	2.382538	1.471047
H	4.019990	1.875093	3.049682
C	-2.425819	2.487882	2.362441
C	-3.164962	1.336909	3.056225
C	-2.949303	3.840387	2.869790
H	-1.367734	2.417660	2.686715
H	-2.646537	0.379403	2.858546
H	-3.162331	1.487977	4.156945
H	-4.218607	1.263337	2.714302
H	-2.487851	4.675246	2.302501
H	-4.052586	3.909487	2.763713
H	-2.693685	3.967951	3.943426
C	-0.281913	2.176028	-2.310624
C	-0.046542	3.516921	-3.015116
C	-0.395914	1.038265	-3.333234
H	0.634538	1.967993	-1.720158
H	0.046969	4.329785	-2.263508
H	0.896530	3.479331	-3.601472
H	-0.883068	3.758800	-3.704589
H	-0.482666	0.066141	-2.810988
H	-1.272289	1.171792	-4.000386
H	0.515773	1.003133	-3.966171
C	2.298136	-1.916574	2.362523
C	3.110193	-1.952826	3.662151
C	1.420283	-3.167316	2.229399
H	1.601084	-1.056572	2.448408
H	3.723660	-1.031198	3.752648
H	2.426669	-2.000792	4.536651
H	3.782936	-2.836019	3.690766
H	0.895051	-3.159536	1.253128
H	2.024718	-4.095849	2.301256
H	0.655751	-3.182882	3.035357
C	3.985995	0.775299	-1.683898
C	3.551446	0.408065	-3.107804
C	5.341556	1.493518	-1.700061
H	3.241738	1.510793	-1.316162
H	2.563426	-0.094194	-3.086256
H	3.454056	1.327188	-3.724473
H	4.287279	-0.266387	-3.594100

H	5.669287	1.720352	-0.664606
H	6.120340	0.872760	-2.191155
H	5.256281	2.452399	-2.254640

$L^{Me}Fe(N_3Ad\text{-}\kappa N^3)$ (quartet, $C_{39}H_{56}FeN_5$)

N	0.803127	1.935304	0.105549
N	3.126801	0.136248	-0.051793
C	1.754744	2.852135	0.294349
C	3.775276	1.281123	0.225106
C	3.130813	2.529384	0.317581
H	3.793452	3.375584	0.484943
N	-0.227232	-1.103607	-0.429475
N	-1.440757	-1.246961	-0.397263
N	-2.211444	-2.235665	-0.516150
Fe	1.176582	0.030806	-0.231769
C	5.275887	1.320598	0.470891
H	5.759888	1.970479	-0.288653
H	5.475467	1.738298	1.480582
H	5.764710	0.328321	0.423874
C	1.433035	4.321923	0.513465
H	1.811477	4.640444	1.507814
H	1.928281	4.931223	-0.272020
H	0.350086	4.551414	0.476660
C	-0.574407	2.239514	0.220945
C	-1.217831	2.121134	1.479164
C	-1.319130	2.600317	-0.930300
C	-2.582130	2.448795	1.578892
C	-2.682073	2.917750	-0.786736
C	-3.299775	2.856240	0.458593
H	-3.098991	2.383289	2.527221
H	-3.275264	3.210150	-1.643113
H	-4.347374	3.110780	0.553346
C	3.778456	-1.118640	-0.028038
C	4.436573	-1.603929	-1.187896
C	3.709730	-1.916096	1.142041
C	5.060109	-2.864128	-1.137386
C	4.351109	-3.167868	1.150967
C	5.022304	-3.631933	0.023218
H	5.573492	-3.261967	-2.002857
H	4.328676	-3.794074	2.033181
H	5.507269	-4.599437	0.045106
C	2.960196	-1.441910	2.384041
C	3.913780	-1.274225	3.572506
C	1.805352	-2.389589	2.730827
H	2.500213	-0.446629	2.210985
H	4.741284	-0.584607	3.299603
H	3.369825	-0.837554	4.437293
H	4.345002	-2.249028	3.883688
H	1.123755	-2.492301	1.859565
H	2.179872	-3.395178	3.015855

H	1.219859	-1.979999	3.581214
C	4.461125	-0.802922	-2.485589
C	3.716766	-1.545020	-3.602166
C	5.897592	-0.470670	-2.909235
H	3.939480	0.168065	-2.356291
H	2.678547	-1.773820	-3.278863
H	3.664024	-0.909443	-4.511902
H	4.228817	-2.494583	-3.865613
H	6.428613	0.050579	-2.085060
H	6.462668	-1.388507	-3.175727
H	5.886156	0.202402	-3.793019
C	-0.466010	1.638247	2.715235
C	-1.064822	0.331497	3.250543
C	-0.437582	2.719397	3.801782
H	0.592650	1.413591	2.469210
H	-1.054947	-0.444318	2.455564
H	-0.460121	-0.041687	4.104352
H	-2.109451	0.477331	3.597460
H	-0.007889	3.658273	3.391525
H	-1.457046	2.928964	4.188689
H	0.199258	2.388688	4.649927
C	-0.677722	2.639124	-2.312437
C	-0.721768	4.053321	-2.903374
C	-1.340000	1.625474	-3.254383
H	0.394148	2.355844	-2.254930
H	-0.242979	4.772109	-2.204566
H	-0.164367	4.080945	-3.863973
H	-1.766208	4.378444	-3.094077
H	-1.295026	0.608217	-2.810014
H	-2.402284	1.886030	-3.446124
H	-0.802638	1.602208	-4.226413
C	-3.652573	-1.913193	-0.398864
C	-4.097353	-0.907915	-1.485526
C	-4.426347	-3.227104	-0.588222
C	-3.986083	-1.331337	0.993364
H	-3.855710	-1.304919	-2.496329
H	-3.550099	0.053754	-1.371369
C	-5.616263	-0.645283	-1.376001
H	-4.114804	-3.969644	0.180147
H	-4.193846	-3.668856	-1.582998
C	-5.947094	-2.976840	-0.477288
H	-3.436004	-0.378746	1.156215
H	-3.663303	-2.036765	1.790846
C	-5.504578	-1.069288	1.109701
H	-5.925870	0.079230	-2.160267
C	-6.380986	-1.972681	-1.567228
C	-5.938122	-0.065425	0.018861
H	-6.493312	-3.935057	-0.616197
C	-6.269550	-2.396298	0.916858
H	-5.733670	-0.649659	2.113331
H	-6.169778	-2.391199	-2.575842

H	-7.476882	-1.793247	-1.505127
H	-5.408241	0.899851	0.159499
H	-7.027763	0.140785	0.102993
H	-7.363891	-2.222587	1.013206
H	-5.977692	-3.121754	1.707808

$L^{Me}Fe(N_3Ad\text{-}\kappa N^3)$ (sextet, $C_{39}H_{56}FeN_5$)

N	0.711179	1.944597	-0.025588
N	3.061385	0.194163	-0.115837
C	1.653356	2.892914	0.058981
C	3.702218	1.364367	0.012037
C	3.033379	2.604614	0.037333
H	3.683662	3.474190	0.100185
N	-0.009042	-1.552632	-0.322618
N	-1.243718	-1.571888	-0.276258
N	-2.088626	-2.489369	-0.115327
Fe	1.105581	0.023232	-0.251611
C	5.214574	1.449720	0.148822
H	5.629927	2.049165	-0.688835
H	5.472672	1.945890	1.108421
H	5.721932	0.465539	0.137793
C	1.309295	4.368493	0.193727
H	1.730922	4.762573	1.142653
H	1.749575	4.931371	-0.656514
H	0.221575	4.576380	0.199641
C	-0.663821	2.242794	0.127426
C	-1.254188	2.195893	1.415741
C	-1.455394	2.538389	-1.011099
C	-2.615897	2.521776	1.552637
C	-2.818169	2.838855	-0.832176
C	-3.385391	2.845254	0.439043
H	-3.093625	2.506560	2.523335
H	-3.449701	3.069110	-1.680037
H	-4.435108	3.080168	0.559711
C	3.737476	-1.044431	-0.015439
C	4.283590	-1.652317	-1.174873
C	3.807247	-1.702657	1.238363
C	4.935521	-2.892581	-1.048510
C	4.471297	-2.939907	1.320882
C	5.032229	-3.523803	0.188510
H	5.367630	-3.380469	-1.912311
H	4.552653	-3.461603	2.265414
H	5.536988	-4.478041	0.268377
C	3.180250	-1.096445	2.490606
C	4.247415	-0.788782	3.547320
C	2.085089	-2.006919	3.059388
H	2.686122	-0.130659	2.255987
H	5.030390	-0.129838	3.114372
H	3.787246	-0.259813	4.409183
H	4.725405	-1.719198	3.919967

H	1.317185	-2.208257	2.282213
H	2.504879	-2.973011	3.410315
H	1.585711	-1.509674	3.917937
C	4.165059	-0.999052	-2.547819
C	3.339929	-1.871066	-3.501936
C	5.546789	-0.691421	-3.138301
H	3.632197	-0.028122	-2.475069
H	2.343539	-2.081657	-3.057280
H	3.183985	-1.338909	-4.464661
H	3.851202	-2.834330	-3.711467
H	6.133929	-0.068774	-2.430408
H	6.111780	-1.623404	-3.350479
H	5.436190	-0.124705	-4.087425
C	-0.449709	1.784657	2.644299
C	-1.011294	0.498988	3.263770
C	-0.394224	2.918228	3.674947
H	0.601974	1.560258	2.369498
H	-1.014496	-0.315357	2.507909
H	-0.374790	0.177530	4.115357
H	-2.046745	0.648269	3.635896
H	0.005358	3.841048	3.202425
H	-1.400338	3.133682	4.092254
H	0.280457	2.637561	4.511805
C	-0.861673	2.531427	-2.415563
C	-0.995684	3.905828	-3.082920
C	-1.499244	1.434204	-3.275586
H	0.224807	2.306622	-2.381122
H	-0.543885	4.688165	-2.436348
H	-0.459345	3.909143	-4.055838
H	-2.059678	4.162613	-3.269164
H	-1.344327	0.443941	-2.796881
H	-2.588447	1.605873	-3.407748
H	-1.021339	1.409550	-4.278167
C	-3.508157	-2.075794	-0.145450
C	-3.908742	-1.575688	-1.550442
C	-4.353942	-3.309834	0.204141
C	-3.796277	-0.964407	0.888317
H	-3.699574	-2.360393	-2.310878
H	-3.307989	-0.681833	-1.825372
C	-5.409293	-1.208470	-1.577230
H	-4.074796	-3.692853	1.211166
H	-4.157006	-4.128656	-0.523519
C	-5.858059	-2.952745	0.185850
H	-3.190845	-0.063679	0.656442
H	-3.505915	-1.302738	1.907619
C	-5.295018	-0.591785	0.867231
H	-5.686435	-0.849563	-2.592226
C	-6.248325	-2.454979	-1.222723
C	-5.682104	-0.094321	-0.543338
H	-6.457687	-3.853377	0.441023
C	-6.134199	-1.838807	1.219630

H	-5.488683	0.211542	1.611009
H	-6.071938	-3.257652	-1.972164
H	-7.331857	-2.205679	-1.252044
H	-5.095659	0.813019	-0.803012
H	-6.757144	0.189683	-0.564531
H	-7.216180	-1.581276	1.222417
H	-5.875162	-2.195183	2.240887

$L^{Me}Fe(\eta^2\text{-}N_3Ad)$ ($C_{39}H_{56}FeN_5$)

N	0.752037	2.109489	-0.104990
N	2.780543	0.038057	-0.126562
C	1.824485	2.909871	-0.103212
C	3.606635	1.090042	-0.089800
C	3.145285	2.420341	-0.130010
H	3.922599	3.180622	-0.136406
N	-0.171790	-1.408868	-0.237563
N	-0.971234	-0.441151	-0.186642
N	-2.177334	-0.098109	-0.133214
Fe	0.840127	0.159305	-0.191669
C	5.115871	0.933757	0.005136
H	5.594207	1.406226	-0.878855
H	5.483493	1.436930	0.924500
H	5.455156	-0.119631	0.044791
C	1.702480	4.425058	-0.062159
H	2.207142	4.813249	0.847887
H	2.192108	4.861178	-0.958607
H	0.656962	4.789900	-0.044868
C	-0.563049	2.613530	0.031931
C	-1.149201	2.702436	1.320503
C	-1.324195	2.928518	-1.123212
C	-2.478312	3.149031	1.433916
C	-2.650347	3.370225	-0.964018
C	-3.217343	3.480573	0.302190
H	-2.952336	3.233745	2.402869
H	-3.256134	3.622442	-1.824341
H	-4.240908	3.816744	0.406644
C	3.245063	-1.288416	0.033172
C	3.638673	-2.044140	-1.100606
C	3.246887	-1.878164	1.322428
C	4.081009	-3.366656	-0.915241
C	3.702188	-3.201504	1.464031
C	4.118452	-3.933664	0.355628
H	4.393499	-3.968336	-1.758583
H	3.730574	-3.675211	2.436499
H	4.461878	-4.952511	0.481050
C	2.767845	-1.108253	2.549756
C	3.907873	-0.913205	3.555802
C	1.564893	-1.798710	3.204744
H	2.422663	-0.091754	2.267301
H	4.767495	-0.411594	3.061702

H	3.567726	-0.270319	4.395654
H	4.248462	-1.884874	3.971657
H	0.746218	-1.920855	2.463959
H	1.840341	-2.796931	3.605061
H	1.182003	-1.179506	4.043511
C	3.574219	-1.460411	-2.508012
C	2.576984	-2.234626	-3.378485
C	4.962440	-1.423866	-3.158996
H	3.213307	-0.411149	-2.481147
H	1.578379	-2.247634	-2.891058
H	2.472637	-1.740760	-4.368200
H	2.911593	-3.280945	-3.541031
H	5.673066	-0.869168	-2.510167
H	5.355781	-2.448157	-3.329027
H	4.908668	-0.901932	-4.138246
C	-0.375199	2.311723	2.575834
C	-1.044195	1.135035	3.297421
C	-0.207640	3.512077	3.514632
H	0.649509	1.972698	2.317417
H	-1.125886	0.265510	2.611754
H	-0.431504	0.827709	4.171387
H	-2.058571	1.405257	3.658707
H	0.273600	4.353679	2.971688
H	-1.186988	3.852742	3.911877
H	0.442875	3.236076	4.371936
C	-0.742842	2.780260	-2.525230
C	-0.700653	4.130514	-3.250818
C	-1.522128	1.740448	-3.340834
H	0.304931	2.417025	-2.478826
H	-0.138228	4.871302	-2.643373
H	-0.183671	4.020630	-4.228001
H	-1.723544	4.520471	-3.436756
H	-1.530448	0.766292	-2.807860
H	-2.570073	2.064418	-3.513117
H	-1.034715	1.588441	-4.327489
C	-3.217665	-1.149540	-0.113535
C	-3.079930	-2.062516	1.126044
C	-4.569294	-0.421396	-0.046423
C	-3.179270	-2.015530	-1.392862
H	-3.100578	-1.450682	2.055127
H	-2.109042	-2.602725	1.111414
C	-4.230904	-3.093240	1.153952
H	-4.685821	0.252637	-0.924791
H	-4.615127	0.219145	0.863033
C	-5.729551	-1.441125	-0.019567
H	-2.211312	-2.555004	-1.473890
H	-3.271236	-1.369435	-2.294059
C	-4.330565	-3.046094	-1.368371
H	-4.122874	-3.747473	2.046225
C	-5.582692	-2.350318	1.219596
C	-4.179388	-3.954598	-0.127736

H	-6.699625	-0.900367	0.028873
C	-5.682233	-2.303256	-1.299464
H	-4.294253	-3.666479	-2.290132
H	-5.636173	-1.739630	2.147676
H	-6.418644	-3.083061	1.255627
H	-3.214896	-4.506433	-0.176123
H	-4.993894	-4.711739	-0.109700
H	-6.519494	-3.035387	-1.296732
H	-5.807856	-1.658484	-2.197023

L^{Me}Fe(py) (quartet, $C_{34}H_{46}FeN_3$)

N	1.461901	-0.829794	0.728141
N	-1.479946	-0.859774	0.687108
C	1.264506	-1.649714	1.771613
C	-1.295858	-1.718828	1.700651
C	-0.016553	-2.091172	2.165060
H	-0.020423	-2.797601	2.993351
C	2.740476	-0.313316	0.417201
C	3.603029	-1.026155	-0.454830
C	3.113975	0.963427	0.908067
C	4.849196	-0.463806	-0.786253
C	4.370546	1.486875	0.554318
C	5.227733	0.777159	-0.281782
H	5.532141	-0.983024	-1.445669
H	4.690640	2.452602	0.922761
H	6.189858	1.195936	-0.547537
C	-2.766629	-0.398358	0.327392
C	-3.277736	0.784615	0.919149
C	-3.499859	-1.066744	-0.685371
C	-4.543483	1.251523	0.521223
C	-4.761094	-0.565091	-1.054748
C	-5.276831	0.578885	-0.452154
H	-4.965640	2.146078	0.959867
H	-5.348576	-1.055431	-1.819792
H	-6.247921	0.953291	-0.749621
C	-2.458889	-2.357204	2.445989
H	-3.453781	-2.061114	2.059951
H	-2.388310	-3.462802	2.366983
H	-2.415501	-2.069548	3.517847
C	2.411039	-2.168655	2.626981
H	3.406287	-1.797360	2.314245
H	2.257191	-1.857067	3.681907
H	2.437007	-3.277966	2.579789
C	-2.943418	-2.301014	-1.386787
C	-2.740454	-2.038488	-2.883989
C	-3.842536	-3.521764	-1.156622
H	-1.945475	-2.566973	-0.979975
H	-2.084805	-1.153141	-3.028540
H	-2.249473	-2.913869	-3.360345
H	-3.708672	-1.856507	-3.396313

H	-3.982643	-3.690642	-0.067568
H	-4.837427	-3.385402	-1.630392
H	-3.369164	-4.428905	-1.589359
C	-2.481609	1.559275	1.965362
C	-3.225235	1.599753	3.305487
C	-2.149282	2.973595	1.474533
H	-1.507410	1.066294	2.164327
H	-3.460983	0.566659	3.639701
H	-2.587207	2.077027	4.079725
H	-4.170564	2.176605	3.224701
H	-1.590274	2.921227	0.516287
H	-3.069825	3.575443	1.322772
H	-1.508938	3.493171	2.218837
C	3.200888	-2.371520	-1.050208
C	4.172715	-3.479519	-0.625354
C	3.094722	-2.288700	-2.577835
H	2.198473	-2.677689	-0.685448
H	4.247607	-3.517311	0.482109
H	3.803192	-4.465168	-0.980581
H	5.185625	-3.312048	-1.048185
H	2.375801	-1.492416	-2.865960
H	4.080355	-2.068175	-3.039291
H	2.723069	-3.252838	-2.986007
C	2.187392	1.769595	1.814518
C	1.804814	3.109295	1.173343
C	2.817697	1.979549	3.196087
H	1.234049	1.227608	1.986284
H	1.323171	2.935517	0.188626
H	1.078865	3.646469	1.820006
H	2.693914	3.758613	1.030860
H	3.087546	0.998389	3.642495
H	3.730284	2.608832	3.130839
H	2.092420	2.480019	3.872762
Fe	-0.002001	-0.052094	-0.334495
N	-0.002720	1.084983	-1.930484
C	1.190699	1.600949	-2.367118
C	-1.118941	1.835019	-2.196955
C	1.303700	2.831048	-2.984934
H	2.061705	0.974275	-2.215019
C	-1.072529	3.071906	-2.809517
H	-2.067047	1.392886	-1.913623
C	0.158496	3.602989	-3.211799
H	2.282941	3.174945	-3.300068
H	-1.998582	3.608825	-2.984398
H	0.219783	4.566359	-3.704136

L^{Me}Fe(py) (sextet, $C_{34}H_{46}FeN_3$)

N	1.457476	-1.111603	0.182203
N	-1.473323	-1.090083	0.219206
C	1.266521	-2.382288	0.560398

C	-1.288254	-2.346583	0.644823
C	-0.014164	-2.942934	0.739648
H	-0.018472	-3.986163	1.046895
C	2.746054	-0.532085	0.127145
C	3.473638	-0.541489	-1.089825
C	3.265057	0.133639	1.266231
C	4.737392	0.074996	-1.130937
C	4.532946	0.736948	1.182160
C	5.261021	0.701743	-0.003704
H	5.320862	0.079427	-2.042200
H	4.960230	1.246607	2.035703
H	6.233762	1.174013	-0.052874
C	-2.744317	-0.470368	0.244634
C	-3.110290	0.325564	1.359221
C	-3.609554	-0.576525	-0.874340
C	-4.367771	0.955587	1.361425
C	-4.855352	0.075689	-0.833801
C	-5.230457	0.826682	0.276648
H	-4.682948	1.557354	2.203682
H	-5.540449	0.011302	-1.668866
H	-6.192614	1.322376	0.291709
C	-2.445405	-3.238123	1.068151
H	-3.436376	-2.748595	1.000840
H	-2.473685	-4.141334	0.422467
H	-2.302716	-3.554811	2.123132
C	2.425791	-3.326161	0.839537
H	3.422365	-2.869870	0.680784
H	2.378425	-3.670068	1.894531
H	2.355155	-4.209320	0.169730
C	-3.207934	-1.358314	-2.120520
C	-3.099954	-0.432772	-3.338515
C	-4.180727	-2.513044	-2.390023
H	-2.205839	-1.817081	-1.989564
H	-2.385762	0.391629	-3.126672
H	-2.722026	-1.000687	-4.215394
H	-4.086307	0.004515	-3.601184
H	-4.255415	-3.165575	-1.494375
H	-5.193529	-2.136523	-2.645482
H	-3.812055	-3.129775	-3.237343
C	-2.170778	0.509556	2.547384
C	-2.779303	-0.079165	3.825131
C	-1.800491	1.985308	2.740838
H	-1.214044	-0.027941	2.380415
H	-3.036439	-1.148189	3.664415
H	-2.045672	-0.020600	4.657435
H	-3.696427	0.470704	4.124506
H	-1.362140	2.394186	1.805874
H	-2.688257	2.592100	3.016966
H	-1.044775	2.084171	3.548649
C	2.909537	-1.190551	-2.349200
C	3.800970	-2.344332	-2.824274

C	2.709265	-0.153238	-3.460855
H	1.909531	-1.629566	-2.150613
H	3.937079	-3.081678	-2.004538
H	3.323655	-2.864682	-3.681972
H	4.797959	-1.977477	-3.147241
H	2.057541	0.670371	-3.098517
H	3.678702	0.274628	-3.792678
H	2.214950	-0.625184	-4.336740
C	2.472370	0.220676	2.566764
C	2.139609	1.676613	2.914148
C	3.219261	-0.466064	3.716148
H	1.498735	-0.303290	2.471353
H	1.576140	2.146094	2.079443
H	1.504207	1.714096	3.824492
H	3.060483	2.266908	3.104640
H	3.458470	-1.515285	3.439475
H	4.162758	0.066452	3.959266
H	2.581774	-0.484486	4.625866
Fe	-0.003227	0.130093	-0.272665
N	-0.005008	1.983304	-0.842075
C	1.179604	2.732276	-0.960490
C	-1.189502	2.671866	-1.161058
C	1.200878	4.034817	-1.365407
H	2.097493	2.212405	-0.704984
C	-1.207730	3.973884	-1.568044
H	-2.109531	2.104355	-1.064652
C	-0.002444	4.716515	-1.692682
H	2.159330	4.540911	-1.429612
H	-2.165944	4.431520	-1.794578
H	-0.001215	5.748373	-2.018781

$L^{Me}Fe(py)_2$ ($C_{39}H_{51}FeN_4$)

N	1.559820	-0.093289	-1.110082
N	-1.405185	-0.430583	-1.109626
C	1.364169	-0.239067	-2.429269
C	-1.178240	-0.608439	-2.412475
C	0.088095	-0.385396	-3.013276
H	0.092412	-0.461834	-4.099676
C	-2.258650	-1.080393	-3.375599
H	-2.429615	-0.303881	-4.150855
H	-1.928503	-2.016396	-3.874043
H	-3.230609	-1.291535	-2.889155
C	2.522348	-0.230391	-3.415656
H	2.544260	-1.188530	-3.976021
H	2.388245	0.603045	-4.137427
H	3.509662	-0.091979	-2.932767
C	2.827500	-0.335622	-0.516393
C	3.268675	-1.669366	-0.290587
C	3.651373	0.755525	-0.131112
C	4.525266	-1.880416	0.306701

C	4.893608	0.495683	0.475156
C	5.323565	-0.808558	0.688684
H	4.892701	-2.882516	0.484118
H	5.541199	1.307510	0.779365
H	6.285143	-0.990330	1.151386
C	-2.650073	-0.761009	-0.510916
C	-3.715506	0.180783	-0.506810
C	-2.839121	-2.046673	0.062886
C	-4.956854	-0.194989	0.037295
C	-4.110581	-2.392023	0.557329
C	-5.152897	-1.471980	0.550257
H	-5.786280	0.499735	0.054802
H	-4.302438	-3.379123	0.955390
H	-6.120495	-1.750475	0.947706
C	-1.708793	-3.067829	0.122401
C	-1.951700	-4.200527	-0.879685
C	-1.517139	-3.627566	1.541245
H	-0.747722	-2.588916	-0.154041
H	-2.060641	-3.785419	-1.903923
H	-1.088710	-4.900215	-0.880707
H	-2.871294	-4.768297	-0.622820
H	-1.357493	-2.801973	2.263626
H	-2.392508	-4.225637	1.867913
H	-0.629897	-4.291720	1.575229
C	-3.550018	1.582944	-1.078131
C	-3.742247	2.646102	0.010996
C	-4.505667	1.826548	-2.253165
H	-2.527418	1.715188	-1.478676
H	-3.088357	2.425178	0.880449
H	-3.471323	3.648467	-0.384002
H	-4.795842	2.678504	0.360150
H	-4.369754	1.042603	-3.027145
H	-5.565024	1.820501	-1.920774
H	-4.289970	2.812286	-2.718058
C	2.419032	-2.876668	-0.673026
C	2.078935	-3.727812	0.555788
C	3.114723	-3.723717	-1.745706
H	1.450885	-2.555159	-1.104220
H	1.570064	-3.103779	1.320240
H	1.396595	-4.554009	0.264040
H	2.989687	-4.174594	1.006345
H	3.379017	-3.092821	-2.619852
H	4.040998	-4.191943	-1.350866
H	2.433729	-4.529769	-2.093419
C	3.236965	2.197929	-0.382776
C	4.209447	2.899631	-1.338694
C	3.105695	2.972193	0.934655
H	2.249392	2.229132	-0.877244
H	4.293383	2.325020	-2.285677
H	3.832904	3.915976	-1.583070
H	5.219224	2.998605	-0.887694

H	2.449966	2.417746	1.639173
H	4.095924	3.120651	1.414590
H	2.653277	3.969134	0.745366
Fe	0.025676	0.243347	0.158864
N	-0.227668	2.412452	0.275054
C	-0.342729	3.088997	1.431793
C	-0.277637	3.120277	-0.870132
C	-0.507833	4.468092	1.489907
H	-0.298951	2.492277	2.335988
C	-0.438168	4.498486	-0.901556
H	-0.178978	2.546023	-1.785571
C	-0.556689	5.191306	0.301830
H	-0.593730	4.958492	2.453052
H	-0.469451	5.013705	-1.854837
H	-0.683388	6.268653	0.312049
H	-2.139005	0.191992	2.225458
C	-1.256824	-0.054370	2.807568
C	-1.344658	-0.211207	4.173960
N	-0.089680	-0.208346	2.092987
C	-0.202206	-0.544705	4.919717
H	-2.308678	-0.081262	4.655356
C	1.018010	-0.539361	2.839265
C	0.997172	-0.704156	4.207763
H	-0.247355	-0.684986	5.992927
H	1.936078	-0.684950	2.281098
H	1.918029	-0.970559	4.716553

$L^{Me}Fe(py)_2$ (sextet, $C_{39}H_{51}FeN_4$)

N	1.563014	-0.035593	-1.066872
N	-1.366482	-0.401123	-1.120686
C	1.390559	-0.065786	-2.397263
C	-1.128545	-0.510866	-2.426526
C	0.129396	-0.206916	-3.006855
H	0.142773	-0.208190	-4.094944
C	-2.183100	-0.982427	-3.417547
H	-2.384408	-0.177743	-4.155907
H	-1.809903	-1.877897	-3.958281
H	-3.147094	-1.259210	-2.948556
C	2.559039	0.055623	-3.363266
H	2.616127	-0.853643	-3.997808
H	2.407301	0.939612	-4.018324
H	3.537206	0.183997	-2.859703
C	2.840108	-0.244023	-0.481518
C	3.357500	-1.562132	-0.347991
C	3.598618	0.863199	-0.016670
C	4.624131	-1.742170	0.237911
C	4.854822	0.633766	0.573103
C	5.359772	-0.655331	0.696021
H	5.047963	-2.731699	0.347120
H	5.454938	1.458255	0.935065

H	6.330618	-0.813294	1.147983
C	-2.593706	-0.825937	-0.545912
C	-3.705682	0.059469	-0.498502
C	-2.716882	-2.145791	-0.035687
C	-4.926149	-0.404722	0.023930
C	-3.969163	-2.578739	0.438517
C	-5.056819	-1.713387	0.474069
H	-5.789897	0.245255	0.072691
H	-4.110833	-3.592556	0.787372
H	-6.008944	-2.059644	0.855294
C	-1.536264	-3.110105	-0.024113
C	-1.722708	-4.203662	-1.080335
C	-1.315563	-3.727466	1.366058
H	-0.600658	-2.570391	-0.275116
H	-1.853516	-3.745361	-2.083363
H	-0.825604	-4.858103	-1.114215
H	-2.612202	-4.828910	-0.852622
H	-1.191570	-2.930112	2.125780
H	-2.161789	-4.379502	1.664889
H	-0.399284	-4.351623	1.367991
C	-3.612544	1.493639	-1.003887
C	-3.863054	2.495180	0.130941
C	-4.576889	1.740679	-2.171115
H	-2.597204	1.697577	-1.392823
H	-3.202923	2.268943	0.993993
H	-3.640802	3.526755	-0.216659
H	-4.918500	2.458773	0.474073
H	-4.397645	1.002271	-2.980151
H	-5.635209	1.662640	-1.844530
H	-4.413013	2.757142	-2.588594
C	2.576224	-2.785521	-0.814518
C	2.285590	-3.734100	0.354110
C	3.316633	-3.518380	-1.939936
H	1.591679	-2.488812	-1.226668
H	1.763953	-3.185446	1.166402
H	1.632231	-4.564577	0.012224
H	3.219509	-4.173649	0.762620
H	3.541006	-2.816850	-2.770389
H	4.269727	-3.957026	-1.576209
H	2.682370	-4.337948	-2.340410
C	3.099383	2.292731	-0.166346
C	4.027067	3.116424	-1.067783
C	2.924824	2.962534	1.202134
H	2.110300	2.300245	-0.658921
H	4.144610	2.615273	-2.052186
H	3.589787	4.122833	-1.242208
H	5.029338	3.244126	-0.607343
H	2.284276	2.332346	1.855362
H	3.903448	3.115146	1.703902
H	2.435232	3.952310	1.080277
Fe	0.016925	0.377180	0.156162

N	-0.384549	2.478785	0.327816
C	-0.500805	3.124593	1.514805
C	-0.418833	3.240724	-0.799389
C	-0.665935	4.493263	1.617770
H	-0.454910	2.497017	2.397308
C	-0.573935	4.614725	-0.775814
H	-0.315355	2.706172	-1.737782
C	-0.706040	5.271273	0.451605
H	-0.760045	4.944859	2.598901
H	-0.594362	5.162797	-1.711380
H	-0.830695	6.346858	0.500360
H	-2.149625	0.237240	2.260915
C	-1.301194	-0.175439	2.798163
C	-1.443905	-0.638563	4.082063
N	-0.102354	-0.204222	2.105811
C	-0.334680	-1.185142	4.768229
H	-2.419934	-0.584889	4.553810
C	0.978120	-0.726902	2.792076
C	0.896706	-1.211817	4.073652
H	-0.423978	-1.563649	5.778686
H	1.920309	-0.741877	2.254518
H	1.791157	-1.612452	4.539749

L^{Me}Fe(NAd) (2) (quartet, $C_{39}H_{56}FeN_3$)

N	0.152251	-2.177863	-0.161348
N	-2.323717	-0.698742	-0.163768
C	-0.669037	-3.229877	-0.233306
C	-2.856955	-1.924820	-0.238446
C	-2.071103	-3.093296	-0.299730
H	-2.626128	-4.025082	-0.377665
N	0.588321	1.026195	-0.005867
C	1.566056	2.056723	0.003152
C	1.482932	2.898538	-1.287535
C	1.366158	2.979625	1.223902
C	2.966383	1.411255	0.091563
H	0.476969	3.366607	-1.372440
H	1.617479	2.249143	-2.180271
C	2.568516	3.997670	-1.276619
H	1.418662	2.390354	2.165740
H	0.357267	3.447763	1.186465
C	2.450537	4.080285	1.242027
H	3.132626	0.731358	-0.772766
H	3.048224	0.791839	1.012016
C	4.057914	2.503735	0.105935
H	2.498810	4.598538	-2.209299
C	2.355364	4.916051	-0.053278
C	3.962824	3.339206	-1.189315
H	2.295625	4.740597	2.122805
C	3.845351	3.422923	1.328413
H	5.060241	2.026982	0.168566

H	1.359606	5.407640	-0.115970
H	3.122779	5.721027	-0.043764
H	4.131499	2.687508	-2.074841
H	4.753931	4.120903	-1.196763
H	4.634281	4.206330	1.357267
H	3.929619	2.832119	2.267093
C	1.551039	-2.307767	-0.009634
C	2.385889	-2.336352	-1.155390
C	2.118584	-2.278177	1.289224
C	3.781255	-2.365096	-0.979023
C	3.518659	-2.310119	1.420516
C	4.338356	-2.353784	0.296480
H	4.446069	-2.386577	-1.832422
H	3.982782	-2.291693	2.397765
H	5.414141	-2.371701	0.414646
C	-3.113603	0.462386	-0.006064
C	-3.378613	0.956933	1.295600
C	-3.554133	1.178371	-1.147525
C	-4.137998	2.132746	1.434611
C	-4.308649	2.351475	-0.964376
C	-4.602489	2.816659	0.314499
H	-4.365369	2.531163	2.414657
H	-4.664514	2.918223	-1.814694
H	-5.181861	3.722580	0.438333
C	-4.359257	-2.153672	-0.259653
H	-4.953216	-1.219878	-0.214944
H	-4.640744	-2.683646	-1.194204
H	-4.651395	-2.778896	0.610534
C	-0.152427	-4.658561	-0.245737
H	0.951533	-4.732491	-0.192990
H	-0.567599	-5.210565	0.623951
H	-0.477201	-5.162423	-1.180656
C	-3.205524	0.716952	-2.558522
C	-2.324433	1.750223	-3.271206
C	-4.469302	0.411766	-3.371737
H	-2.618220	-0.224490	-2.529913
H	-1.414292	1.953778	-2.666878
H	-2.002729	1.358642	-4.259854
H	-2.870717	2.703756	-3.430810
H	-5.097013	-0.330568	-2.834037
H	-5.068437	1.329929	-3.547103
H	-4.191457	-0.019075	-4.357344
C	-2.844135	0.250678	2.537988
C	-3.989278	-0.229530	3.437057
C	-1.873747	1.152452	3.310316
H	-2.266401	-0.655185	2.259034
H	-4.681296	-0.876288	2.856109
H	-3.584000	-0.826649	4.281755
H	-4.560725	0.626191	3.854229
H	-1.048925	1.480160	2.642373
H	-2.389765	2.049658	3.712252

H	-1.428452	0.592419	4.160050
C	1.803701	-2.322025	-2.565075
C	2.207154	-3.579732	-3.344410
C	2.212318	-1.050669	-3.317852
H	0.694423	-2.319999	-2.531894
H	1.914797	-4.488776	-2.776509
H	1.685831	-3.602121	-4.325218
H	3.301663	-3.606850	-3.528991
H	1.874149	-0.155644	-2.755269
H	3.313021	-0.997480	-3.454067
H	1.731125	-1.029123	-4.318928
C	1.244351	-2.206694	2.537954
C	1.496901	-0.911818	3.318575
C	1.451236	-3.438105	3.427691
H	0.168296	-2.197974	2.266223
H	1.300415	-0.035592	2.666863
H	0.810434	-0.852319	4.189887
H	2.542179	-0.859659	3.689136
H	1.271477	-4.364322	2.840697
H	2.480893	-3.468056	3.842140
H	0.732309	-3.420004	4.274536
Fe	-0.420980	-0.333022	-0.129006

L^{Me}Fe(NAd) (2) (sextet, $C_{39}H_{56}FeN_3$)

N	0.138874	-2.138568	-0.193585
N	-2.397869	-0.613578	-0.204388
C	-0.702013	-3.167102	-0.256298
C	-2.904070	-1.854711	-0.251283
C	-2.108384	-3.013453	-0.330770
H	-2.664322	-3.945689	-0.403816
N	0.972980	0.805390	-0.194350
C	1.863083	1.913817	-0.097825
C	1.809078	2.756500	-1.391646
C	1.471619	2.814429	1.095056
C	3.305211	1.403735	0.109521
H	0.774300	3.129160	-1.561992
H	2.079422	2.132243	-2.270488
C	2.783404	3.951594	-1.292432
H	1.494554	2.232621	2.041562
H	0.431239	3.188134	0.966413
C	2.444456	4.009530	1.204864
H	3.604491	0.747203	-0.737870
H	3.363900	0.788129	1.034834
C	4.283132	2.594629	0.214880
H	2.737309	4.547980	-2.229458
C	2.383721	4.840368	-0.094953
C	4.220552	3.425108	-1.085581
H	2.153997	4.647544	2.067651
C	3.881373	3.482812	1.412632
H	5.317043	2.214400	0.364047

H	1.356051	5.239009	-0.243666
H	3.070547	5.712127	-0.021928
H	4.523744	2.797273	-1.952251
H	4.933161	4.277052	-1.027489
H	4.589028	4.335509	1.508109
H	3.938571	2.896707	2.356271
C	1.533647	-2.302433	-0.022834
C	2.382501	-2.372046	-1.157000
C	2.084424	-2.307598	1.284059
C	3.772129	-2.469895	-0.961387
C	3.479456	-2.407654	1.434028
C	4.311525	-2.487020	0.321373
H	4.446493	-2.528972	-1.805483
H	3.930339	-2.420047	2.417541
H	5.383278	-2.559835	0.454226
C	-3.215713	0.516300	0.027994
C	-3.418356	0.972755	1.354821
C	-3.757713	1.235620	-1.067217
C	-4.214326	2.112878	1.567493
C	-4.544922	2.372922	-0.810482
C	-4.775257	2.799792	0.494428
H	-4.396632	2.480784	2.568654
H	-4.977764	2.940647	-1.623643
H	-5.381912	3.677940	0.674817
C	-4.403434	-2.116462	-0.219867
H	-5.018570	-1.197524	-0.162278
H	-4.705296	-2.659736	-1.140430
H	-4.652685	-2.740776	0.664315
C	-0.219796	-4.610615	-0.243304
H	0.881578	-4.712110	-0.184153
H	-0.652027	-5.138546	0.633056
H	-0.552234	-5.121693	-1.171637
C	-3.488243	0.813426	-2.507539
C	-2.700554	1.894433	-3.257753
C	-4.791477	0.470644	-3.239781
H	-2.863180	-0.103375	-2.536996
H	-1.759607	2.125056	-2.713007
H	-2.432696	1.533746	-4.273849
H	-3.294458	2.827107	-3.360635
H	-5.351690	-0.305638	-2.676305
H	-5.436993	1.366456	-3.356372
H	-4.564442	0.068333	-4.250151
C	-2.781921	0.262465	2.545938
C	-3.850765	-0.286770	3.497844
C	-1.806046	1.187474	3.282998
H	-2.184244	-0.610952	2.211380
H	-4.548740	-0.949099	2.942131
H	-3.371625	-0.885233	4.301974
H	-4.431301	0.534050	3.969138
H	-1.032760	1.559939	2.577896
H	-2.333142	2.055612	3.731607

H	-1.293556	0.630065	4.095540
C	1.821801	-2.344373	-2.574829
C	2.142475	-3.645336	-3.320616
C	2.335503	-1.125283	-3.349162
H	0.715421	-2.257845	-2.557441
H	1.767391	-4.517091	-2.743210
H	1.643370	-3.647196	-4.313154
H	3.235671	-3.761398	-3.477034
H	2.088429	-0.197378	-2.794314
H	3.434665	-1.173572	-3.498434
H	1.846584	-1.073034	-4.345351
C	1.198202	-2.210696	2.522214
C	1.519111	-0.953247	3.337577
C	1.317559	-3.472730	3.384457
H	0.129003	-2.127965	2.236443
H	1.402181	-0.053666	2.699648
H	0.815953	-0.864428	4.192795
H	2.554922	-0.981182	3.736059
H	1.085234	-4.372016	2.774658
H	2.339589	-3.577671	3.805731
H	0.593131	-3.428214	4.225613
Fe	-0.450940	-0.201865	-0.270413

[L^{Me}Fe(N$_3$Ad)]‡ (quartet, $C_{39}H_{56}FeN_5$, transition state for N_2 elimination)

N	-2.275565	-0.528076	0.696845
N	0.324822	-1.924060	0.570298
C	-2.604535	-1.624879	1.390612
C	-0.440554	-2.924772	1.029477
C	-1.738238	-2.725888	1.538116
H	-2.170494	-3.586782	2.043564
N	0.298717	1.549057	-0.484094
N	-0.550496	2.288724	-1.626026
N	-1.673909	2.192518	-1.820490
C	1.653925	2.124416	-0.446070
C	2.365679	1.507021	0.766805
C	2.458889	1.780302	-1.718608
C	1.625831	3.660138	-0.260852
H	2.395759	0.406611	0.651584
H	1.799810	1.728988	1.699424
C	3.808200	2.046395	0.890708
H	1.963761	2.207335	-2.618043
H	2.502945	0.678769	-1.855190
C	3.897466	2.332441	-1.610248
H	1.056310	3.926447	0.655918
H	1.117904	4.151916	-1.118687
C	3.064363	4.213971	-0.150840
H	4.306175	1.584374	1.770445
C	4.596781	1.697318	-0.389285
C	3.765814	3.578285	1.067896
H	4.462660	2.081113	-2.533953

C	3.847837	3.865917	-1.435548
H	3.029450	5.317950	-0.024610
H	4.650980	0.593451	-0.512847
H	5.640171	2.073754	-0.308925
H	3.218146	3.838047	2.000511
H	4.798432	3.979653	1.166001
H	4.880262	4.274917	-1.373724
H	3.358104	4.333239	-2.318055
C	-3.245296	0.440349	0.341564
C	-3.361388	1.631109	1.102241
C	-4.086666	0.223301	-0.782246
C	-4.358804	2.562110	0.760588
C	-5.060653	1.188219	-1.097082
C	-5.197862	2.339937	-0.327516
H	-4.488633	3.469049	1.336266
H	-5.719748	1.052115	-1.944377
H	-5.956144	3.069717	-0.580721
C	1.596643	-2.163189	-0.003105
C	1.718570	-2.187676	-1.416426
C	2.750258	-2.299203	0.820356
C	2.999903	-2.290467	-1.986329
C	4.011885	-2.387785	0.203816
C	4.132784	-2.371091	-1.182548
H	3.126671	-2.321013	-3.060329
H	4.911812	-2.481628	0.797086
H	5.111727	-2.445848	-1.638253
C	0.025068	-4.373251	1.033157
H	1.002385	-4.530009	0.537618
H	0.103993	-4.736417	2.079615
H	-0.713423	-5.001431	0.490881
C	-3.962806	-1.786921	2.056264
H	-4.619719	-0.901525	1.949216
H	-4.491358	-2.660318	1.619609
H	-3.822588	-1.961999	3.144036
C	2.654746	-2.396527	2.343352
C	3.379640	-1.239047	3.042874
C	3.198758	-3.743907	2.840601
H	1.597334	-2.343145	2.672321
H	2.862674	-0.283570	2.833819
H	3.361071	-1.385967	4.143990
H	4.438227	-1.162356	2.717997
H	2.711472	-4.582973	2.302410
H	4.296560	-3.814407	2.688763
H	2.987454	-3.862499	3.924855
C	0.485745	-2.198779	-2.320752
C	0.371425	-3.537797	-3.058857
C	0.483750	-1.029126	-3.311928
H	-0.443549	-2.095615	-1.722489
H	0.370416	-4.375046	-2.328187
H	-0.580307	-3.578026	-3.630880
H	1.215394	-3.678526	-3.766944

H	0.444855	-0.069406	-2.761978
H	1.382230	-1.041806	-3.963010
H	-0.416854	-1.080588	-3.960046
C	-2.444661	1.908600	2.288567
C	-3.231673	1.886531	3.603534
C	-1.697702	3.237821	2.118532
H	-1.664457	1.122630	2.370376
H	-3.744232	0.908285	3.722944
H	-2.540835	2.022815	4.462838
H	-3.992373	2.695421	3.629013
H	-1.220724	3.280229	1.118310
H	-2.384612	4.104158	2.220470
H	-0.902615	3.328326	2.889240
C	-3.947107	-1.018423	-1.659609
C	-3.552726	-0.644985	-3.093655
C	-5.233322	-1.853717	-1.646213
H	-3.138584	-1.677849	-1.282809
H	-2.612991	-0.054848	-3.087712
H	-3.375358	-1.564946	-3.690940
H	-4.348479	-0.050526	-3.589874
H	-5.520420	-2.097181	-0.601847
H	-6.071953	-1.309873	-2.129805
H	-5.072163	-2.807577	-2.192516
Fe	-0.397589	-0.088202	0.213610

[L^{Me}Fe(N$_3$Ad)]‡ (sextet, $C_{39}H_{56}FeN_5$, transition state for N_2 elimination)

N	2.315568	0.456094	0.701291
N	-0.227570	1.936704	0.568801
C	2.679748	1.544151	1.395770
C	0.570051	2.916537	1.009513
C	1.856552	2.675695	1.532942
H	2.315435	3.523726	2.036621
N	-0.473818	-1.497215	-0.482445
N	0.450147	-2.341452	-1.618053
N	1.546488	-2.111423	-1.808130
C	-1.824041	-2.054941	-0.431485
C	-2.547491	-1.377797	0.743232
C	-2.608131	-1.762062	-1.729267
C	-1.811060	-3.580389	-0.176320
H	-2.569178	-0.283248	0.579874
H	-1.995454	-1.564640	1.691596
C	-3.995650	-1.899368	0.870932
H	-2.103421	-2.234120	-2.600504
H	-2.639533	-0.667055	-1.917313
C	-4.052814	-2.297105	-1.616042
H	-1.256051	-3.808504	0.759676
H	-1.294940	-4.113619	-1.003836
C	-3.255722	-4.117497	-0.061746
H	-4.500662	-1.393259	1.722174
C	-4.763128	-1.601539	-0.434771

C	-3.968727	-3.422100	1.117155
H	-4.603222	-2.083468	-2.557971
C	-4.018694	-3.821537	-1.371644
H	-3.231807	-5.214901	0.114440
H	-4.805236	-0.503571	-0.608629
H	-5.810921	-1.965117	-0.352453
H	-3.436356	-3.644029	2.068211
H	-5.005996	-3.810475	1.218378
H	-5.055335	-4.219097	-1.305881
H	-3.521039	-4.332163	-2.225253
C	3.257304	-0.536993	0.339803
C	3.324359	-1.743461	1.081466
C	4.115280	-0.332531	-0.774325
C	4.289548	-2.704770	0.731392
C	5.056785	-1.326707	-1.096914
C	5.145430	-2.495250	-0.345949
H	4.381341	-3.625409	1.292467
H	5.727560	-1.200938	-1.936610
H	5.878808	-3.247914	-0.605460
C	-1.489080	2.210422	-0.012795
C	-1.609435	2.207759	-1.426758
C	-2.635918	2.418078	0.805513
C	-2.883110	2.367967	-2.000726
C	-3.891232	2.555696	0.185047
C	-4.011259	2.520300	-1.200849
H	-3.007505	2.387498	-3.075148
H	-4.786282	2.703304	0.774739
H	-4.984695	2.636126	-1.659774
C	0.163394	4.382311	0.978038
H	-0.804310	4.566750	0.473100
H	0.094032	4.771868	2.015613
H	0.929824	4.967561	0.426630
C	4.036299	1.653901	2.075113
H	4.658037	0.742400	1.976974
H	4.603537	2.505008	1.643174
H	3.891722	1.836596	3.161072
C	-2.539238	2.530904	2.327137
C	-3.319087	1.416686	3.037296
C	-3.021480	3.907845	2.806642
H	-1.486327	2.431963	2.659973
H	-2.858111	0.433888	2.824011
H	-3.281049	1.565348	4.137675
H	-4.383545	1.397725	2.723124
H	-2.495426	4.716912	2.259175
H	-4.114623	4.027002	2.651668
H	-2.806674	4.029746	3.889835
C	-0.377601	2.132959	-2.329167
C	-0.166766	3.463777	-3.060082
C	-0.458205	0.972034	-3.327885
H	0.540169	1.958263	-1.729572
H	-0.096969	4.293783	-2.324561

H	0.781134	3.435183	-3.639148
H	-1.003524	3.672561	-3.760038
H	-0.527839	0.010370	-2.785292
H	-1.331505	1.072649	-4.004877
H	0.461097	0.941780	-3.950437
C	2.390169	-2.006104	2.257653
C	3.170006	-2.043912	3.576596
C	1.588606	-3.298586	2.056504
H	1.643478	-1.189765	2.352839
H	3.724643	-1.091656	3.716991
H	2.468977	-2.165581	4.429823
H	3.893895	-2.886141	3.590545
H	1.105846	-3.294650	1.057994
H	2.239660	-4.194737	2.132454
H	0.793393	-3.376630	2.828446
C	4.026631	0.925430	-1.635204
C	3.633235	0.586047	-3.078038
C	5.341002	1.715126	-1.599488
H	3.237712	1.606881	-1.256389
H	2.676437	0.024491	-3.089098
H	3.488811	1.520016	-3.662330
H	4.414820	-0.024576	-3.577151
H	5.629913	1.930779	-0.549687
H	6.163482	1.150540	-2.087064
H	5.216756	2.683020	-2.130536
Fe	0.430082	0.054104	0.244066

[L^{Me}Fe(py)(N$_3$Ad)]‡ (quartet, $C_{44}H_{61}FeN_6$, transition state for N_2 elimination)

N	2.393588	0.339762	0.411340
N	-0.192099	1.724910	0.976377
C	2.805549	1.191453	1.359226
C	0.633485	2.506794	1.671048
C	1.962964	2.134867	1.984066
H	2.456321	2.780324	2.708854
N	-0.554121	-1.144897	-1.172758
N	0.339235	-1.484262	-2.480506
N	1.476556	-1.418358	-2.584890
C	-1.948705	-1.531347	-1.495683
C	-2.815999	-1.278509	-0.249576
C	-2.528128	-0.690931	-2.657931
C	-2.050430	-3.033823	-1.859737
H	-2.762223	-0.211598	0.033477
H	-2.443243	-1.871417	0.606089
C	-4.288861	-1.663832	-0.508829
H	-1.927143	-0.828658	-3.582845
H	-2.497333	0.385771	-2.393882
C	-3.994583	-1.086832	-2.939483
H	-1.644192	-3.657800	-1.034326
H	-1.448202	-3.262218	-2.765614
C	-3.519442	-3.427599	-2.131846

H	-4.890247	-1.468927	0.405867
C	-4.842665	-0.824192	-1.677961
C	-4.365805	-3.161972	-0.869094
H	-4.388017	-0.479378	-3.783383
C	-4.064706	-2.585003	-3.305054
H	-3.572745	-4.506752	-2.393619
H	-4.813909	0.256194	-1.417474
H	-5.905202	-1.090836	-1.869788
H	-3.988953	-3.776888	-0.022226
H	-5.422876	-3.457020	-1.049495
H	-5.116124	-2.874010	-3.524183
H	-3.468566	-2.780230	-4.223517
C	3.336735	-0.277713	-0.458937
C	3.758769	-1.616605	-0.227640
C	3.903010	0.461901	-1.537081
C	4.712346	-2.193174	-1.086869
C	4.864896	-0.153692	-2.359131
C	5.256998	-1.467822	-2.138761
H	5.051019	-3.209699	-0.936038
H	5.318032	0.385172	-3.180678
H	5.995649	-1.925691	-2.784169
C	-1.489518	2.166303	0.607417
C	-1.699325	2.741043	-0.674557
C	-2.584873	2.009654	1.505094
C	-3.009465	3.075213	-1.064293
C	-3.878471	2.339802	1.061755
C	-4.086041	2.855812	-0.212328
H	-3.202859	3.525945	-2.028567
H	-4.735176	2.211148	1.709946
H	-5.087393	3.113768	-0.532283
C	0.225233	3.877949	2.193704
H	-0.790368	4.192354	1.885333
H	0.259765	3.877723	3.303712
H	0.932438	4.645080	1.812644
C	4.245685	1.214240	1.854893
H	4.901715	0.477587	1.352157
H	4.682648	2.222610	1.698403
H	4.264419	0.984474	2.941376
C	-2.393822	1.532176	2.942330
C	-3.097844	0.194030	3.195181
C	-2.870330	2.590913	3.946543
H	-1.321644	1.370719	3.156121
H	-2.675560	-0.586683	2.534872
H	-2.933390	-0.130950	4.244801
H	-4.190717	0.269560	3.015246
H	-2.385304	3.567243	3.736894
H	-3.971982	2.722225	3.902507
H	-2.596276	2.285019	4.978892
C	-0.532479	3.102723	-1.590136
C	-0.424342	4.624609	-1.746799
C	-0.635668	2.418968	-2.960300

H	0.425909	2.769110	-1.146678
H	-0.363837	5.107067	-0.747719
H	0.496936	4.885346	-2.310627
H	-1.300474	5.034265	-2.292694
H	-0.437950	1.333632	-2.851567
H	-1.630971	2.568616	-3.426170
H	0.123277	2.829334	-3.657321
C	3.237381	-2.433381	0.944780
C	4.366889	-2.807960	1.912750
C	2.497016	-3.685495	0.457098
H	2.520098	-1.835714	1.533191
H	4.900005	-1.894039	2.250064
H	3.945444	-3.311516	2.809058
H	5.097372	-3.494848	1.435939
H	1.684767	-3.398418	-0.244169
H	3.184895	-4.385330	-0.061962
H	2.045362	-4.220836	1.318982
C	3.500471	1.903274	-1.828471
C	2.918864	2.042608	-3.240223
C	4.685400	2.858044	-1.636616
H	2.708481	2.235377	-1.129834
H	2.091043	1.317332	-3.383430
H	2.521459	3.069754	-3.383843
H	3.689665	1.859264	-4.017730
H	5.117270	2.735522	-0.622306
H	5.481680	2.666966	-2.386738
H	4.345811	3.910440	-1.743770
Fe	0.389796	-0.112773	0.213410
N	0.092332	-1.374340	2.027271
C	0.380406	-0.842190	3.227655
C	-0.299106	-2.658354	1.989429
C	0.256239	-1.551208	4.416446
H	0.734072	0.181950	3.222799
C	-0.455241	-3.437296	3.129197
H	-0.475723	-3.065214	1.001430
C	-0.178914	-2.872144	4.370466
H	0.499777	-1.069121	5.356246
H	-0.779868	-4.467218	3.035791
H	-0.291426	-3.451287	5.280982

[L^{Me}Fe(py)(N$_3$Ad)]‡ (sextet, $C_{44}H_{61}FeN_6$, transition state for N_2 elimination)

N	2.422099	0.293210	0.403627
N	-0.122653	1.728849	0.972297
C	2.852345	1.128613	1.360702
C	0.715890	2.496798	1.662338
C	2.036323	2.093775	1.981712
H	2.542396	2.725972	2.709351
N	-0.655693	-1.108659	-1.157269
N	0.286505	-1.498993	-2.500205
N	1.413991	-1.355566	-2.550727

C	-2.044236	-1.479904	-1.478871
C	-2.910443	-1.211968	-0.234002
C	-2.609369	-0.636527	-2.645573
C	-2.164485	-2.982276	-1.837828
H	-2.843732	-0.144580	0.046348
H	-2.545052	-1.807655	0.623923
C	-4.387477	-1.578625	-0.495494
H	-2.007484	-0.788472	-3.567731
H	-2.561934	0.441499	-2.387890
C	-4.080658	-1.013195	-2.927864
H	-1.768196	-3.608855	-1.009606
H	-1.563539	-3.221243	-2.741688
C	-3.638147	-3.357507	-2.111622
H	-4.988302	-1.373083	0.417216
C	-4.927112	-0.734786	-1.668439
C	-4.483436	-3.076721	-0.851437
H	-4.464459	-0.403392	-3.774488
C	-4.170316	-2.511568	-3.288498
H	-3.705174	-4.436695	-2.370074
H	-4.883502	0.346061	-1.411090
H	-5.992942	-0.987062	-1.861420
H	-4.116482	-3.693978	-0.001929
H	-5.543962	-3.358283	-1.033107
H	-5.225176	-2.787177	-3.508340
H	-3.575447	-2.717902	-4.205356
C	3.352893	-0.340062	-0.466869
C	3.729863	-1.694589	-0.251565
C	3.942420	0.393641	-1.536233
C	4.663761	-2.292150	-1.117893
C	4.884934	-0.242676	-2.364803
C	5.233569	-1.571789	-2.160178
H	4.966781	-3.321757	-0.980442
H	5.354433	0.290765	-3.180718
H	5.956769	-2.045969	-2.811273
C	-1.413092	2.190657	0.604466
C	-1.617631	2.755188	-0.682770
C	-2.505951	2.068127	1.510359
C	-2.921467	3.119574	-1.066532
C	-3.793827	2.427345	1.072770
C	-3.997170	2.936356	-0.204877
H	-3.110294	3.565219	-2.034035
H	-4.649075	2.325842	1.727666
H	-4.993886	3.216603	-0.520527
C	0.339917	3.881831	2.172079
H	-0.666523	4.218225	1.856707
H	0.370820	3.890096	3.282134
H	1.067356	4.627852	1.787270
C	4.288220	1.101898	1.867892
H	4.921351	0.341044	1.371793
H	4.761500	2.093995	1.713068
H	4.290461	0.873440	2.954832

C	-2.317651	1.594084	2.949279
C	-3.053784	0.275677	3.213766
C	-2.761173	2.669914	3.950415
H	-1.248488	1.405596	3.157519
H	-2.655685	-0.518475	2.554465
H	-2.890507	-0.048259	4.263896
H	-4.145580	0.377996	3.040631
H	-2.254067	3.632915	3.731813
H	-3.859560	2.827915	3.912964
H	-2.487640	2.363250	4.982669
C	-0.448466	3.073283	-1.611573
C	-0.295202	4.589697	-1.781862
C	-0.585056	2.382265	-2.975078
H	0.503243	2.712931	-1.174281
H	-0.208090	5.077699	-0.787463
H	0.626895	4.817528	-2.358405
H	-1.164843	5.021917	-2.320721
H	-0.438011	1.290122	-2.856673
H	-1.573097	2.573537	-3.441134
H	0.191304	2.751224	-3.676230
C	3.178923	-2.507031	0.910541
C	4.294843	-2.944006	1.868146
C	2.383671	-3.718211	0.406893
H	2.489860	-1.888933	1.511659
H	4.869666	-2.059018	2.214221
H	3.855213	-3.439681	2.760104
H	4.991757	-3.656853	1.379412
H	1.576746	-3.384607	-0.279765
H	3.037850	-4.434630	-0.132802
H	1.918357	-4.251144	1.263048
C	3.579773	1.848247	-1.815109
C	2.999210	2.014661	-3.224395
C	4.790859	2.768243	-1.617491
H	2.798323	2.197059	-1.112609
H	2.159082	1.305339	-3.375089
H	2.617874	3.049691	-3.355379
H	3.766189	1.826767	-4.004686
H	5.218914	2.627040	-0.603891
H	5.581497	2.559816	-2.368942
H	4.480760	3.830365	-1.717851
Fe	0.423154	-0.129492	0.207362
N	0.079874	-1.378328	2.041251
C	0.388782	-0.859931	3.241987
C	-0.382484	-2.637754	2.001725
C	0.219552	-1.559296	4.431079
H	0.793305	0.145495	3.237101
C	-0.587988	-3.405635	3.141486
H	-0.577895	-3.032659	1.012330
C	-0.287084	-2.854627	4.383402
H	0.482501	-1.090074	5.372183
H	-0.969327	-4.415969	3.048077

H	-0.436385	-3.425481	5.293909

$L^{Me}FeNNFeL^{Me}$ (septet, $C_{58}H_{82}Fe_2N_6$)

Fe	2.070945	-0.457611	1.006601
N	3.596547	-1.513333	0.376250
N	0.725643	0.275417	0.090204
C	4.459055	-1.843718	2.609630
H	5.305674	-2.257461	3.153582
C	3.541470	-1.836574	-1.000021
C	4.489980	-2.057874	1.212222
N	2.346054	-0.712854	2.920713
C	3.469527	-1.245733	3.421064
C	1.070815	1.092026	3.978099
C	1.267407	-0.290997	3.733766
C	3.760029	-1.254203	4.912330
H	2.985126	-0.740077	5.514693
H	4.724245	-0.738060	5.105764
H	3.835096	-2.302468	5.270913
C	0.430313	-2.719248	3.855023
H	1.331049	-2.914051	3.237915
C	5.620901	-2.946286	0.720377
H	5.612686	-3.109675	-0.374948
H	5.548537	-3.942011	1.206992
H	6.596697	-2.486385	0.984415
C	0.328990	-1.240359	4.216529
C	4.293978	-1.086317	-1.939330
C	-0.011160	1.495152	4.781546
H	-0.175626	2.541356	5.003593
C	2.654043	-2.850284	-1.443546
C	-0.742942	-0.793286	5.010493
H	-1.473757	-1.491480	5.396677
C	-0.902423	0.559315	5.296751
H	-1.736526	0.887156	5.903719
C	2.002798	2.144623	3.388434
H	2.759014	1.670707	2.727850
C	1.764264	-3.612147	-0.465904
H	1.872634	-3.207478	0.562210
C	4.197647	-1.413535	-3.304437
H	4.759640	-0.861761	-4.046337
C	3.364309	-2.442428	-3.733731
H	3.298969	-2.678927	-4.787979
C	2.779740	2.866648	4.494752
H	3.509336	3.574873	4.047168
H	3.342389	2.128587	5.105870
H	2.096098	3.436547	5.159101
C	5.170779	0.082632	-1.505291
H	5.148421	0.200562	-0.401899
C	0.567823	-3.591856	5.108475
H	0.757222	-4.647002	4.816824
H	-0.354101	-3.559663	5.726261

H	1.424668	-3.243191	5.723163
C	2.167286	-5.088845	-0.397943
H	3.239403	-5.176133	-0.119319
H	2.007071	-5.593589	-1.374206
H	1.564312	-5.612237	0.374685
C	0.280883	-3.462770	-0.827927
H	0.015693	-2.388309	-0.923265
H	-0.351547	-3.909031	-0.031724
H	0.046113	-3.977523	-1.782111
C	-0.767437	-3.158574	3.004239
H	-0.639974	-4.214500	2.683186
H	-0.834506	-2.527229	2.092733
H	-1.718450	-3.073758	3.571256
C	1.232908	3.144394	2.513553
H	0.615510	2.604926	1.764363
H	1.945302	3.800103	1.968963
H	0.568259	3.787902	3.126739
C	4.650624	1.401748	-2.089905
H	3.591151	1.556387	-1.792347
H	4.715879	1.405142	-3.198528
H	5.247628	2.253162	-1.698956
C	6.638272	-0.149705	-1.885754
H	7.271538	0.661211	-1.466707
H	6.772606	-0.164487	-2.987771
H	6.992068	-1.115859	-1.467327
Fe	-1.691334	1.233690	-1.330713
N	-3.050245	2.537549	-0.788144
N	-0.214123	0.703018	-0.480171
C	-4.381173	2.173178	-2.772073
H	-5.260848	2.538073	-3.298227
C	-2.881526	3.028584	0.527916
C	-4.150161	2.775789	-1.513801
N	-2.611638	0.532261	-2.900835
C	-3.697414	1.121399	-3.421099
C	-2.594616	-1.911367	-3.134015
C	-2.039683	-0.642313	-3.444654
C	-4.283682	0.691151	-4.755084
H	-3.699131	-0.105427	-5.256483
H	-5.317544	0.315394	-4.603378
H	-4.314839	1.561055	-5.444886
C	-0.173936	0.785425	-4.480518
H	-0.699060	1.602674	-3.942767
C	-5.238936	3.726544	-1.043903
H	-5.039923	4.172743	-0.050019
H	-5.344707	4.559216	-1.771143
H	-6.204170	3.181153	-0.977859
C	-0.852314	-0.553825	-4.215014
C	-3.231438	2.206433	1.629477
C	-1.998279	-3.064894	-3.675368
H	-2.398517	-4.046928	-3.460626
C	-2.275910	4.292501	0.745143

C	-0.291963	-1.731829	-4.741339
H	0.601638	-1.695139	-5.350455
C	-0.865570	-2.971800	-4.478623
H	-0.415274	-3.869799	-4.881684
C	-3.786741	-2.053396	-2.192373
H	-4.149150	-1.058791	-1.861427
C	-2.096144	4.742225	2.066237
H	-1.638783	5.702202	2.266176
C	-1.786839	5.151025	-0.415625
H	-2.014260	4.663562	-1.386473
C	-3.044907	2.699212	2.933660
H	-3.321982	2.105075	3.794480
C	-2.486157	3.955614	3.146286
H	-2.337359	4.314898	4.156441
C	-4.970383	-2.734954	-2.889494
H	-5.860634	-2.721253	-2.225016
H	-5.226788	-2.191307	-3.823457
H	-4.737640	-3.791007	-3.140925
C	-3.800157	0.805160	1.427231
H	-3.816572	0.538872	0.349571
C	-0.227259	1.137959	-5.971078
H	0.200975	2.149324	-6.138357
H	0.347451	0.406204	-6.577506
H	-1.281920	1.145252	-6.320962
C	-2.493635	6.511962	-0.439026
H	-3.594946	6.369076	-0.459468
H	-2.226615	7.121373	0.449810
H	-2.201079	7.075502	-1.350641
C	-0.263310	5.320464	-0.365373
H	0.228807	4.324114	-0.362343
H	0.087671	5.876964	-1.260516
H	0.050777	5.878356	0.542049
C	1.272327	0.790329	-3.964739
H	1.692597	1.817063	-4.021564
H	1.304427	0.460348	-2.904751
H	1.917249	0.117576	-4.567483
C	-3.389901	-2.804461	-0.915704
H	-2.545750	-2.281806	-0.417486
H	-4.245312	-2.830223	-0.207245
H	-3.084640	-3.848400	-1.139590
C	-2.929989	-0.255186	2.114404
H	-1.873099	-0.154223	1.787804
H	-2.976242	-0.159272	3.218612
H	-3.283779	-1.271967	1.842249
C	-5.249807	0.728299	1.917436
H	-5.674894	-0.273032	1.691369
H	-5.312404	0.900517	3.012854
H	-5.866291	1.492467	1.397168
C	2.596727	-3.152778	-2.816039
H	1.946119	-3.935427	-3.183394

$L^{Me}Fe$ (quartet, $C_{29}H_{41}FeN_2$, iron(I)–β-diketiminate fragment)

Fe	-0.007418	-0.198309	-0.720221
N	-1.573508	-0.295047	0.385272
N	1.529556	-0.375222	0.414516
C	-1.320444	-0.321254	1.709077
C	-0.040471	-0.579758	2.263453
H	-0.057469	-0.723878	3.343210
C	1.265403	-0.596715	1.715083
C	-2.833529	0.070731	-0.144812
C	-3.057507	1.411119	-0.549850
C	-4.317283	1.764233	-1.066699
H	-4.525487	2.782352	-1.368300
C	-5.323126	0.812080	-1.204175
H	-6.285559	1.099592	-1.607696
C	-5.093988	-0.510144	-0.834637
H	-5.891659	-1.228898	-0.968762
C	-3.851945	-0.905230	-0.304823
C	-1.970709	2.474493	-0.418383
H	-1.033664	2.032913	-0.020258
C	-1.612504	3.075317	-1.783266
H	-1.304092	2.269334	-2.483001
H	-0.764588	3.784502	-1.676139
H	-2.471956	3.624478	-2.221808
C	-2.386915	3.566567	0.573443
H	-2.639534	3.110474	1.554758
H	-3.266971	4.133043	0.202282
H	-1.548198	4.278746	0.728228
C	-3.621531	-2.367952	0.061123
H	-2.602100	-2.511578	0.475533
C	-3.711781	-3.264564	-1.179742
H	-2.994931	-2.915096	-1.953417
H	-4.735954	-3.256493	-1.609035
H	-3.450504	-4.310927	-0.912835
C	-4.601326	-2.833294	1.146144
H	-4.343219	-3.863062	1.473559
H	-5.646599	-2.836987	0.771773
H	-4.540109	-2.164457	2.030169
C	2.830049	-0.106098	-0.072320
C	3.623938	-1.160650	-0.591240
C	4.912412	-0.867346	-1.073942
H	5.545277	-1.649973	-1.471338
C	5.400789	0.436070	-1.054801
H	6.394694	0.644550	-1.429482
C	4.613178	1.474164	-0.565184
H	5.017963	2.477693	-0.573094
C	3.317517	1.225975	-0.076945
C	3.109376	-2.595599	-0.638651
H	2.083944	-2.657660	-0.217938
C	3.013360	-3.098428	-2.084228
H	2.379361	-2.410660	-2.683873

H	2.547152	-4.106663	-2.105937
H	4.016721	-3.165182	-2.555388
C	3.982698	-3.527499	0.210821
H	4.045442	-3.147174	1.252370
H	5.009290	-3.608480	-0.204432
H	3.535401	-4.544000	0.240868
C	2.468043	2.387266	0.431280
H	1.471558	2.030381	0.763932
C	2.202699	3.408792	-0.681043
H	1.741653	2.904055	-1.556946
H	3.141043	3.906225	-1.004896
H	1.498254	4.188439	-0.319835
C	3.117243	3.053670	1.649838
H	3.301877	2.297247	2.442363
H	2.439705	3.830835	2.063712
H	4.081107	3.534559	1.380156
C	-2.417394	-0.088509	2.737618
H	-2.540836	-0.997791	3.363265
H	-2.136413	0.763304	3.392765
H	-3.402697	0.151612	2.293430
C	2.379213	-0.857006	2.716811
H	2.375616	-0.062501	3.492841
H	2.216348	-1.840440	3.206542
H	3.387895	-0.877092	2.260194

$L^{Me}Fe(\mu\text{-}N_3Ad)FeL^{Me}$ (septet, $C_{68}H_{97}Fe_2N_7$)

Fe	-2.224127	0.132111	0.312739
Fe	1.554716	-0.740415	0.247451
N	-3.889874	-0.884114	0.324012
N	-3.019035	1.818195	0.789865
C	-4.909087	-0.522271	1.116918
C	-5.013931	0.767907	1.658416
H	-5.889867	0.950530	2.276797
C	-4.221249	1.897595	1.372688
C	-3.974775	-2.050404	-0.484442
C	-4.722300	-2.025017	-1.696553
C	-4.886195	-3.218164	-2.423742
H	-5.462371	-3.234575	-3.339278
C	-4.322856	-4.407602	-1.979914
H	-4.465145	-5.317137	-2.549316
C	-3.581113	-4.434942	-0.805674
H	-3.171950	-5.382994	-0.483368
C	-3.383450	-3.266038	-0.046112
C	-5.366093	-0.746647	-2.223203
H	-5.102560	0.114759	-1.577995
C	-4.863155	-0.410307	-3.633886
H	-5.238676	0.586740	-3.944701
H	-5.213082	-1.155182	-4.378734
H	-3.755541	-0.389032	-3.651307
C	-6.895767	-0.853766	-2.211593

H	-7.346302	0.119791	-2.500777
H	-7.255399	-1.112259	-1.195035
H	-7.249700	-1.631118	-2.921405
C	-2.595378	-3.352141	1.254172
H	-2.485704	-2.345747	1.705773
C	-1.175597	-3.878203	1.010497
H	-0.619316	-3.162747	0.372830
H	-1.177707	-4.872099	0.518410
H	-0.635610	-3.988075	1.973045
C	-3.328012	-4.223471	2.281611
H	-4.351184	-3.830349	2.456776
H	-2.784654	-4.209364	3.249867
H	-3.401535	-5.276097	1.935473
C	-2.304363	2.989850	0.407990
C	-1.543951	3.724053	1.363860
C	-0.927200	4.925234	0.968739
H	-0.336313	5.501264	1.668438
C	-1.066384	5.407328	-0.326308
H	-0.597567	6.341795	-0.606725
C	-1.804832	4.695196	-1.262556
H	-1.904655	5.112336	-2.254792
C	-2.404762	3.466862	-0.927502
C	-1.384571	3.256084	2.804094
H	-1.988902	2.346489	2.978813
C	0.077234	2.898445	3.103744
H	0.424904	2.092016	2.425176
H	0.169769	2.538198	4.148857
H	0.742485	3.778710	2.979507
C	-1.897652	4.304995	3.801363
H	-1.911536	3.875946	4.826137
H	-2.931506	4.613540	3.543173
H	-1.249243	5.206096	3.811571
C	-3.208672	2.710831	-1.978504
H	-3.340938	1.658009	-1.655497
C	-4.600007	3.333274	-2.130477
H	-5.194094	2.772351	-2.881475
H	-4.523859	4.393029	-2.455553
H	-5.144001	3.293832	-1.164319
C	-2.492216	2.651186	-3.337679
H	-2.979901	1.901394	-3.993608
H	-1.432250	2.359122	-3.204021
H	-2.528612	3.628907	-3.861853
N	1.982265	-1.657155	2.000405
N	2.193684	-2.303218	-0.848770
C	2.200239	-2.974240	2.102703
C	2.167603	-3.849495	0.997148
H	2.202945	-4.908428	1.244356
C	2.190407	-3.556130	-0.377798
C	2.149237	-0.798085	3.116605
C	3.394705	-0.144036	3.314134
C	3.576833	0.634879	4.471648

H	4.525998	1.109401	4.678855
C	2.540280	0.813128	5.381911
H	2.693784	1.427952	6.259466
C	1.311189	0.195571	5.176824
H	0.528803	0.351438	5.907830
C	1.094385	-0.625964	4.056291
C	4.553053	-0.334652	2.336485
H	4.169045	-0.717486	1.366076
C	5.278585	0.982396	2.019416
H	4.546034	1.782840	1.798434
H	5.934745	0.848841	1.132820
H	5.916398	1.311136	2.866503
C	5.545083	-1.369453	2.875592
H	5.035889	-2.340883	3.037896
H	5.983969	-1.031018	3.838637
H	6.365110	-1.529988	2.143190
C	-0.245278	-1.341098	3.905315
H	-0.231815	-1.988770	3.010576
C	-1.391145	-0.349042	3.693483
H	-1.236801	0.186756	2.737173
H	-1.452231	0.384145	4.524760
H	-2.362289	-0.884165	3.629290
C	-0.535432	-2.252096	5.106224
H	-1.437145	-2.868311	4.905473
H	-0.718189	-1.658829	6.026728
H	0.316672	-2.938511	5.288114
C	2.464100	-2.020860	-2.210555
C	1.388854	-1.718480	-3.085974
C	1.666739	-1.435127	-4.434568
H	0.866176	-1.224294	-5.131173
C	2.975724	-1.425973	-4.905316
H	3.171949	-1.200421	-5.945643
C	4.032199	-1.725983	-4.050872
H	5.035292	-1.730938	-4.456317
C	3.801942	-2.035552	-2.697736
C	-0.059624	-1.761370	-2.609141
H	-0.097793	-1.837633	-1.504458
C	-0.820497	-0.482161	-2.971515
H	-0.203091	0.404146	-2.735257
H	-1.756118	-0.421220	-2.376439
H	-1.083166	-0.453701	-4.050026
C	-0.780263	-2.993084	-3.165470
H	-0.270368	-3.919180	-2.826905
H	-0.798097	-2.976854	-4.275987
H	-1.826036	-3.019219	-2.795426
C	4.985328	-2.418962	-1.808884
H	4.648548	-2.619462	-0.771665
C	6.017534	-1.289127	-1.706256
H	5.551583	-0.385293	-1.274372
H	6.446967	-1.036119	-2.697969
H	6.846738	-1.592310	-1.031763

C	5.653112	-3.704752	-2.314859
H	4.900431	-4.510226	-2.437012
H	6.415032	-4.050611	-1.584062
H	6.153532	-3.538539	-3.292298
N	-0.429421	0.444122	0.183707
N	0.219111	1.422948	-0.298094
N	1.478551	1.137899	-0.574721
C	2.276722	2.234737	-1.132371
C	1.651814	2.789172	-2.432385
H	0.639607	3.200711	-2.229384
H	1.537688	1.975228	-3.181575
C	3.665285	1.675111	-1.458489
H	3.577347	0.843871	-2.192102
H	4.121947	1.258385	-0.538998
C	2.420014	3.385978	-0.113894
H	2.846574	3.009845	0.839091
H	1.423219	3.807085	0.128104
C	2.544833	3.905880	-3.018533
H	2.084632	4.299081	-3.950970
C	4.574495	2.779971	-2.038211
H	5.577344	2.356119	-2.263085
C	3.318099	4.501117	-0.691521
H	3.415145	5.322604	0.051115
C	2.681374	5.048504	-1.988072
H	3.311336	5.864257	-2.405877
H	1.681472	5.482051	-1.767290
C	3.942113	3.329881	-3.334694
H	4.591325	4.121237	-3.769665
H	3.856570	2.517524	-4.089904
C	4.713794	3.921512	-1.007979
H	5.186664	3.538084	-0.077274
H	5.374755	4.719739	-1.411510
C	-4.850932	3.222416	1.778767
H	-5.855945	3.314219	1.314697
H	-4.966957	3.254299	2.882636
H	-4.271890	4.112715	1.467821
C	-6.028539	-1.477622	1.498352
H	-6.027613	-1.623642	2.599254
H	-7.007846	-1.048353	1.200231
H	-5.939056	-2.476585	1.029017
C	2.489824	-3.660337	3.431017
H	1.662918	-4.361128	3.672629
H	3.433428	-4.241091	3.353768
H	2.608855	-2.962688	4.282006
C	2.200870	-4.771501	-1.291545
H	3.091899	-5.396745	-1.073164
H	1.288350	-5.377589	-1.107739
H	2.216034	-4.516021	-2.369217

$L^{Me}Fe(\mu\text{-}N_2)(\mu\text{-}N_3Ad)FeL^{Me}$ (septet, $C_{66}H_{95}Fe_2N_9$)

H	-0.072611	0.117882	-6.829888

C	-0.116784	0.044512	-5.745480
C	-0.090034	-1.271136	-5.228262
C	-0.331850	1.256718	-5.068275
N	-0.411522	1.342157	-3.735449
N	0.002636	-1.535050	-3.924944
N	-1.068548	0.019717	-0.910289
N	-0.726383	0.177946	0.180338
C	-0.232704	0.073611	4.861925
N	-0.502011	-1.339146	2.908077
N	-0.094022	1.734183	3.084802
C	-0.327957	1.401284	4.354661
C	-0.399919	-1.175745	4.236332
H	-0.191297	0.022961	5.949163
C	-1.185115	-2.469611	2.365224
C	-2.502337	-4.824276	1.543838
C	-0.450470	-3.541612	1.786330
C	-2.601955	-2.578380	2.474482
C	-3.233963	-3.770380	2.071681
C	-1.128211	-4.711411	1.393916
H	-4.306336	-3.886131	2.155293
H	-0.590782	-5.552480	0.976674
H	-3.006424	-5.731448	1.236177
C	-0.313353	3.065744	2.610362
C	-0.851986	5.699712	1.835556
C	0.664837	4.096927	2.779861
C	-1.573491	3.424032	2.056411
C	-1.793591	4.764303	1.677206
C	0.336630	5.408103	2.374133
H	-2.747616	5.071047	1.269979
H	1.044128	6.216223	2.503167
H	-1.063935	6.719921	1.539523
C	0.044349	-2.860499	-3.422919
C	0.059038	-5.544139	-2.600115
C	1.251515	-3.610942	-3.474935
C	-1.136907	-3.447393	-2.900518
C	-1.112280	-4.799085	-2.512147
C	1.232342	-4.956107	-3.062999
H	-2.004812	-5.285247	-2.141464
H	2.130987	-5.557662	-3.096800
H	0.061827	-6.581484	-2.291146
C	-1.061909	2.430764	-3.098898
C	-2.314193	4.677524	-1.972101
C	-0.292042	3.396421	-2.403759
C	-2.477441	2.559473	-3.159764
C	-3.079765	3.705291	-2.607984
C	-0.937387	4.520055	-1.855801
H	-4.152759	3.838867	-2.645954
H	-0.373876	5.283091	-1.335160
H	-2.795109	5.546850	-1.542445
C	-0.443618	-2.362904	5.187452
H	0.508451	-2.414544	5.757203

H	-0.570760	-3.333430	4.669060
H	-1.282063	-2.243227	5.904705
C	-0.790257	2.408038	5.400357
H	-0.063158	2.440250	6.238659
H	-1.772191	2.088008	5.809030
H	-0.921710	3.435819	5.011109
C	-0.226610	-2.364651	-6.277021
H	0.623420	-2.306551	-6.988969
H	-1.172569	-2.219178	-6.840705
H	-0.252358	-3.388480	-5.855963
C	-0.444082	2.486318	-5.954429
H	0.484974	2.596843	-6.552861
H	-0.579450	3.425162	-5.381085
H	-1.302357	2.373108	-6.648799
C	1.055383	-3.478900	1.614063
H	1.414303	-2.473403	1.880718
C	1.757107	-4.476450	2.544471
H	2.859108	-4.394269	2.440083
H	1.461506	-5.520540	2.308613
H	1.496139	-4.258958	3.601423
C	1.457343	-3.710397	0.152762
H	2.545843	-3.555216	0.020223
H	0.918521	-2.997938	-0.507350
H	1.231822	-4.747793	-0.164222
C	2.027880	3.861279	3.422067
H	2.190520	2.776386	3.555552
C	2.111453	4.513393	4.809115
H	3.090626	4.279399	5.279354
H	1.318520	4.133684	5.476262
H	2.007733	5.617214	4.738912
C	3.173053	4.403979	2.546806
H	4.147468	4.016726	2.912473
H	3.222315	5.512623	2.577019
H	3.044415	4.099029	1.491577
C	-2.724410	2.434850	1.957833
H	-2.363637	1.411797	2.175229
C	-3.804601	2.776260	2.992346
H	-3.374894	2.753984	4.014767
H	-4.630905	2.039394	2.952140
H	-4.230197	3.785344	2.807012
C	-3.321264	2.397417	0.544965
H	-2.518500	2.230460	-0.200112
H	-3.850884	3.340274	0.298209
H	-4.057473	1.574124	0.459321
C	1.215838	3.249092	-2.252546
H	1.563337	2.295017	-2.700395
C	-3.360708	1.468719	-3.759671
H	-2.744692	0.633308	-4.148299
C	1.616357	3.205509	-0.773889
H	2.694543	2.954783	-0.682148
H	1.031520	2.428448	-0.238140

H	1.435555	4.184656	-0.283848
C	1.955036	4.371273	-2.990107
H	3.051850	4.202732	-2.936634
H	1.728905	5.363058	-2.544487
H	1.657302	4.381534	-4.060507
C	-4.180905	1.999525	-4.941975
H	-3.514433	2.479659	-5.687546
H	-4.935206	2.742736	-4.608128
H	-4.712245	1.161063	-5.440916
C	-4.277126	0.854953	-2.693723
H	-3.670007	0.463710	-1.851438
H	-4.850982	0.007945	-3.126378
H	-4.996553	1.603034	-2.299104
C	-3.466942	-1.427094	2.966219
H	-2.839872	-0.551294	3.219146
C	-4.230875	-1.802101	4.241900
H	-3.525746	-2.158643	5.020382
H	-4.978734	-2.599011	4.045926
H	-4.763092	-0.911352	4.639009
C	-4.434796	-0.978835	1.863212
H	-3.863935	-0.713530	0.948929
H	-5.012873	-0.093566	2.193689
H	-5.160378	-1.778692	1.606978
C	2.560143	-2.998252	-3.967285
H	2.406207	-1.942507	-4.272053
C	3.614719	-2.973245	-2.853972
H	4.538631	-2.473010	-3.214976
H	3.876875	-3.999586	-2.521044
H	3.235325	-2.400708	-1.984661
C	3.095635	-3.740653	-5.199224
H	3.968322	-3.196771	-5.619708
H	2.315140	-3.800770	-5.984930
H	3.418031	-4.771123	-4.940158
C	-2.436641	-2.657372	-2.795264
H	-2.255679	-1.585160	-3.016488
C	-3.019212	-2.709922	-1.375730
H	-2.244927	-2.428314	-0.631981
H	-3.398074	-3.723541	-1.129765
H	-3.866072	-1.997557	-1.286473
C	-3.456860	-3.155131	-3.823709
H	-3.031531	-3.077822	-4.847197
H	-4.375329	-2.531640	-3.782291
H	-3.735568	-4.212676	-3.629269
Fe	0.189520	-0.119232	-2.496528
Fe	0.233639	0.154631	1.743769
N	1.738535	-0.187455	-1.358835
N	2.171924	-0.175016	0.922877
N	2.400524	-0.230891	-0.365382
C	3.428446	-0.222675	1.736297
C	4.246466	1.059702	1.509729
H	3.613121	1.930348	1.739338

H	4.547471	1.148161	0.442383
C	3.034976	-0.314121	3.221501
H	2.454745	-1.237933	3.420509
H	2.382881	0.535276	3.500196
C	4.318232	-1.438279	1.387492
H	4.619368	-1.413603	0.317030
H	3.763885	-2.379615	1.552763
C	4.292174	-0.317464	4.117777
H	3.987683	-0.380030	5.185211
C	5.585177	-1.448039	2.273858
H	6.215353	-2.325773	2.012372
C	5.507653	1.067453	2.400511
H	6.079251	2.005223	2.228411
C	5.091931	0.981014	3.884646
H	5.994759	0.993704	4.533925
H	4.473897	1.861883	4.161949
C	5.170149	-1.535480	3.758548
H	6.073902	-1.558054	4.406351
H	4.606888	-2.477302	3.941129
C	6.387059	-0.149222	2.040862
H	7.307316	-0.152139	2.665453
H	6.707547	-0.086187	0.977642

$L^{Me}Fe(\mu$-AdNNNNNNAd)FeL^{Me} (1) (septet, $C_{78}H_{112}Fe_2N_{10}$)

Fe	2.338943	0.041510	0.285559
N	1.075071	1.781812	0.383559
N	-0.540192	0.350681	-0.129919
N	-0.164089	1.567487	0.109547
N	3.394154	-0.459456	1.939254
N	3.973180	0.143594	-1.000762
C	4.596561	0.130847	2.052419
C	5.357070	0.558791	0.948739
H	6.328293	0.978686	1.205083
C	5.168153	0.337569	-0.444736
C	2.860159	-1.267513	2.989280
C	1.854708	-0.755979	3.858980
C	1.415914	-1.539728	4.943943
H	0.662363	-1.172402	5.627751
C	1.948306	-2.797518	5.179541
H	1.600607	-3.382219	6.021595
C	2.927813	-3.305989	4.341068
H	3.322847	-4.289391	4.558457
C	3.392531	-2.568030	3.235885
C	1.278462	0.638635	3.697949
H	1.705110	1.116990	2.799792
C	1.653109	1.522908	4.896966
H	2.757292	1.570359	5.004047
H	1.217852	1.130408	5.839773
H	1.279220	2.557123	4.754192
C	-0.244537	0.588457	3.505085

H	-0.496422	-0.010482	2.607005
H	-0.647503	1.607238	3.359686
H	-0.756992	0.149551	4.385524
C	4.434206	-3.206770	2.328133
H	4.664442	-2.541978	1.474616
C	5.755211	-3.440082	3.071545
H	6.119259	-2.491311	3.515214
H	6.527308	-3.810278	2.363616
H	5.634957	-4.187965	3.883533
C	3.903927	-4.522900	1.743303
H	2.906057	-4.357603	1.285537
H	3.804679	-5.305131	2.524568
H	4.598986	-4.906986	0.970063
C	3.838376	-0.244326	-2.370075
C	3.816452	0.734605	-3.414233
C	3.779702	0.304706	-4.754811
H	3.792666	1.015716	-5.569309
C	3.745635	-1.042795	-5.075647
H	3.721160	-1.350083	-6.113404
C	3.780590	-1.998243	-4.073022
H	3.806663	-3.038154	-4.368521
C	3.832797	-1.626956	-2.716045
C	3.877336	2.234038	-3.143549
H	3.786903	2.422928	-2.056996
C	5.216445	2.828388	-3.600695
H	6.064552	2.311406	-3.115248
H	5.268799	3.902768	-3.322234
H	5.337359	2.742945	-4.701563
C	2.725779	2.979970	-3.839457
H	1.753886	2.529727	-3.560020
H	2.820387	2.952949	-4.944346
H	2.725700	4.048824	-3.536430
C	4.001105	-2.720739	-1.670807
H	3.953863	-2.286260	-0.654636
C	5.374116	-3.389739	-1.819181
H	6.178722	-2.626841	-1.770056
H	5.453235	-3.930361	-2.786084
H	5.542973	-4.115909	-0.999168
C	2.876440	-3.762147	-1.748862
H	1.912656	-3.276712	-1.515638
H	3.043007	-4.572396	-1.012642
H	2.809767	-4.237190	-2.748226
C	1.388473	3.221968	0.589268
C	2.875735	3.338714	0.962619
H	3.509619	2.883371	0.174589
H	3.084707	2.783496	1.902267
C	0.541593	3.849876	1.718071
H	0.711714	3.312217	2.666632
H	-0.541523	3.777138	1.480849
C	1.123530	4.013011	-0.704532
H	0.051909	3.945738	-0.995284

H	1.710695	3.569071	-1.519064
C	3.269391	4.820262	1.149859
H	4.346951	4.887833	1.414761
C	0.922757	5.334969	1.914177
H	0.308357	5.771853	2.731228
C	1.513914	5.494812	-0.528519
H	1.325613	6.044207	-1.476510
C	2.419036	5.434551	2.283023
H	2.703198	6.498500	2.438468
H	2.611714	4.896228	3.237300
C	0.664248	6.109063	0.603887
H	-0.415378	6.058847	0.339416
H	0.924792	7.182043	0.736768
C	3.011122	5.589252	-0.163863
H	3.307542	6.654623	-0.046031
H	3.629442	5.160157	-0.983336
N	-1.242153	-1.959705	-0.613512
C	-1.648499	-3.259494	-1.245510
C	-3.186467	-3.325372	-1.277827
H	-3.613063	-3.268909	-0.257268
H	-3.590231	-2.458324	-1.845826
C	-1.137467	-3.341436	-2.702540
H	-1.536107	-2.499886	-3.290972
H	-0.031095	-3.279402	-2.740162
C	-1.097320	-4.482031	-0.476861
H	0.013574	-4.460232	-0.445916
H	-1.449126	-4.476712	0.563962
C	-3.660675	-4.639914	-1.939048
H	-4.771921	-4.673174	-1.943927
C	-1.595263	-4.652797	-3.376258
H	-1.214214	-4.688027	-4.420138
C	-1.567591	-5.796288	-1.136771
H	-1.172032	-6.662674	-0.563227
C	-3.137372	-4.704546	-3.388799
H	-3.483818	-5.641072	-3.878576
H	-3.542438	-3.852068	-3.977645
C	-1.042634	-5.855534	-2.585366
H	0.069691	-5.834004	-2.588536
H	-1.359031	-6.806714	-3.067099
C	-3.111611	-5.843594	-1.143212
H	-3.460623	-6.794419	-1.602612
H	-3.498957	-5.818274	-0.101538
N	0.468214	-0.625787	-0.176022
N	0.040895	-1.806839	-0.493181
Fe	-2.320232	-0.307160	-0.188584
N	-3.386179	0.967917	-1.292095
N	-3.796489	-0.661796	1.118081
C	-4.612987	0.511238	-1.565944
C	-5.314898	-0.395426	-0.731534
H	-6.287866	-0.710506	-1.102377
C	-5.016051	-0.790625	0.591681

C	-2.775177	2.026344	-2.041318
C	-1.789106	1.731706	-3.029934
C	-1.221368	2.780371	-3.777976
H	-0.498929	2.580607	-4.557320
C	-1.597355	4.095771	-3.566449
H	-1.146629	4.887407	-4.151300
C	-2.579239	4.395324	-2.636981
H	-2.873191	5.430735	-2.529528
C	-3.194191	3.383722	-1.873447
C	-1.419683	0.306672	-3.401232
H	-1.818402	-0.381672	-2.634709
C	-2.064146	-0.068989	-4.744034
H	-3.170222	-0.047100	-4.654086
H	-1.757668	0.637133	-5.544848
H	-1.762005	-1.089126	-5.057873
C	0.106104	0.101027	-3.458817
H	0.601133	0.572557	-2.586067
H	0.353359	-0.978994	-3.454058
H	0.538594	0.534124	-4.384796
C	-4.304505	3.792609	-0.916421
H	-4.688207	2.912707	-0.369733
C	-5.498499	4.394221	-1.672160
H	-5.831115	3.715298	-2.482426
H	-6.349976	4.545303	-0.974637
H	-5.238098	5.374842	-2.123689
C	-3.785106	4.789699	0.126048
H	-2.896195	4.370578	0.641294
H	-3.494398	5.755138	-0.337606
H	-4.581637	5.003412	0.868619
C	-3.607594	-0.584393	2.538051
C	-3.134029	-1.708657	3.276273
C	-3.244244	-1.712645	4.680326
H	-2.936202	-2.571347	5.261652
C	-3.772431	-0.626760	5.358552
H	-3.862430	-0.653907	6.436991
C	-4.162502	0.503379	4.659413
H	-4.552078	1.339786	5.224465
C	-4.046529	0.566221	3.257186
C	-2.535840	-2.923409	2.600956
H	-2.447362	-2.715851	1.526612
C	-3.445267	-4.147257	2.772944
H	-4.450086	-3.935985	2.349405
H	-3.023764	-5.023200	2.238474
H	-3.555159	-4.417695	3.844092
C	-1.110901	-3.210590	3.108931
H	-0.439522	-2.370857	2.840415
H	-1.082762	-3.358785	4.207357
H	-0.699204	-4.130034	2.646578
C	-4.367511	1.878959	2.563141
H	-4.145484	1.790904	1.482971
C	-5.853556	2.231184	2.700076

H	-6.482551	1.394278	2.336035
H	-6.118646	2.446332	3.756705
H	-6.089020	3.127314	2.087157
C	-3.483140	3.016843	3.105954
H	-2.449836	2.901282	2.724846
H	-3.864299	4.004058	2.785729
H	-3.450909	3.041211	4.213446
C	6.464821	0.307322	-1.240760
H	6.973643	1.291164	-1.164046
H	7.138264	-0.468318	-0.818295

$L^{Me}Fe(N_3Ad–\kappa N^1N^3)$ triazametallocyclobutene core (quartet, $C_{39}H_{56}FeN_5$)

N	-2.061024	-1.265871	-0.369404
N	-1.796639	1.629722	-0.322639
C	-3.316450	-0.960251	-0.714793
C	-3.097513	1.571018	-0.612952
C	-3.776114	0.361049	-0.858013
H	-4.820430	0.463272	-1.143376
N	0.831263	-1.194541	0.141743
N	1.639069	-0.186872	0.084019
N	1.047053	0.968103	-0.089432
Fe	-0.614105	0.058201	-0.101991
C	-3.972634	2.814037	-0.689739
H	-4.397892	2.906096	-1.711568
H	-4.806507	2.725595	0.038707
H	-3.438426	3.756660	-0.462040
C	-4.372947	-2.027351	-0.965697
H	-5.213898	-1.891536	-0.252900
H	-4.761351	-1.928677	-2.001577
H	-4.003974	-3.064621	-0.848012
C	-1.672156	-2.602863	-0.108571
C	-1.737573	-3.106577	1.215254
C	-1.162065	-3.411544	-1.157983
C	-1.335977	-4.432353	1.459177
C	-0.773871	-4.732529	-0.869978
C	-0.864821	-5.235643	0.424665
H	-1.382255	-4.849237	2.456645
H	-0.392432	-5.378967	-1.649378
H	-0.559199	-6.253627	0.629617
C	-1.164251	2.852105	0.014167
C	-0.651937	3.696610	-1.006191
C	-0.976918	3.186686	1.379171
C	-0.012678	4.894611	-0.638525
C	-0.335828	4.396324	1.701741
C	0.135069	5.241525	0.701278
H	0.383350	5.563475	-1.391266
H	-0.191016	4.687091	2.733897
H	0.630405	6.166676	0.966696
C	-1.450139	2.261546	2.496312

C	-2.525898	2.938637	3.352977
C	-0.273745	1.786723	3.358923
H	-1.915673	1.344897	2.077922
H	-3.366658	3.274909	2.708869
H	-2.926855	2.218663	4.098151
H	-2.115126	3.815607	3.896323
H	0.485846	1.283308	2.723597
H	0.206501	2.635109	3.890057
H	-0.628431	1.056771	4.116855
C	-0.756538	3.322262	-2.481337
C	0.633434	3.131488	-3.101957
C	-1.566747	4.363800	-3.263611
H	-1.286243	2.354728	-2.602862
H	1.206124	2.371434	-2.529700
H	0.536240	2.773193	-4.149065
H	1.206462	4.082612	-3.107998
H	-2.563229	4.505023	-2.794947
H	-1.043415	5.342604	-3.293612
H	-1.722054	4.017383	-4.307687
C	-2.225165	-2.240193	2.372258
C	-1.122748	-2.044680	3.420085
C	-3.492194	-2.827141	3.005132
H	-2.495982	-1.224375	2.016769
H	-0.221529	-1.601207	2.944742
H	-1.472666	-1.350943	4.213872
H	-0.842333	-3.007791	3.895962
H	-4.274917	-2.964870	2.228610
H	-3.286009	-3.806387	3.486288
H	-3.888166	-2.132634	3.776617
C	-1.023265	-2.878696	-2.580773
C	-1.918254	-3.659215	-3.551110
C	0.439334	-2.902977	-3.045394
H	-1.348585	-1.818760	-2.634581
H	-2.972370	-3.633643	-3.202712
H	-1.876909	-3.197847	-4.560892
H	-1.593907	-4.717937	-3.634781
H	1.078124	-2.338723	-2.334145
H	0.821533	-3.942523	-3.122765
H	0.528519	-2.422048	-4.042880
C	3.130214	-0.297076	0.137687
C	3.553192	-1.733606	0.503596
C	3.711312	0.067575	-1.238817
C	3.676946	0.678604	1.195580
H	3.161919	-2.456299	-0.247087
H	3.130098	-2.019314	1.492475
C	5.094159	-1.832657	0.551863
H	3.409197	1.099046	-1.526608
H	3.312498	-0.620911	-2.016753
C	5.253938	-0.024636	-1.200114
H	3.251587	0.436200	2.194822
H	3.378667	1.723453	0.955920

C	5.218960	0.588702	1.247263
H	5.392614	-2.870345	0.816329
C	5.673212	-1.465081	-0.832274
C	5.637359	-0.851998	1.614266
H	5.667899	0.240122	-2.197258
C	5.798922	0.955187	-0.137120
H	5.607746	1.295195	2.012445
H	5.300905	-2.177127	-1.601374
H	6.782333	-1.545910	-0.814427
H	5.238697	-1.119484	2.617558
H	6.745927	-0.924465	1.667446
H	6.909752	0.907337	-0.109228
H	5.518411	1.998228	-0.402631

$L^{Me}Fe(N_3Ad–\kappa N^1N^3)$ triazametallocyclobutene core (sextet, $C_{39}H_{56}FeN_5$)

N	-1.875297	-1.421807	-0.613682
N	-1.781119	1.522028	-0.614846
C	-3.035679	-1.191869	-1.235103
C	-2.956050	1.366449	-1.231442
C	-3.482037	0.102824	-1.579345
H	-4.422109	0.132900	-2.125161
N	0.904443	-0.028147	0.964151
N	1.768662	-0.051494	-0.032850
N	1.317954	-0.043010	-1.246559
Fe	-0.512876	0.008184	-0.387177
C	-3.836245	2.549286	-1.604265
H	-4.004433	2.555632	-2.702080
H	-4.817284	2.458379	-1.091774
H	-3.403271	3.531152	-1.330133
C	-3.984420	-2.317176	-1.617776
H	-4.960358	-2.169619	-1.108757
H	-4.147964	-2.307597	-2.716274
H	-3.612766	-3.324935	-1.347601
C	-1.522084	-2.700373	-0.117733
C	-1.961034	-3.106259	1.169130
C	-0.720782	-3.567753	-0.904756
C	-1.636126	-4.397838	1.622729
C	-0.427632	-4.853854	-0.416082
C	-0.883807	-5.262210	0.833374
H	-1.965983	-4.742287	2.594004
H	0.159428	-5.547880	-1.003006
H	-0.646299	-6.254107	1.195960
C	-1.347395	2.774364	-0.115955
C	-0.504364	3.597549	-0.906800
C	-1.747971	3.197455	1.177710
C	-0.130775	4.861180	-0.414400
C	-1.343502	4.465214	1.634488
C	-0.549725	5.288508	0.841767
H	0.490727	5.522556	-1.003570

H	-1.642771	4.822758	2.610924
H	-0.250589	6.262590	1.207026
C	-2.598196	2.309254	2.079990
C	-3.953097	2.961718	2.378816
C	-1.854176	1.965713	3.376288
H	-2.817555	1.341229	1.584418
H	-4.471577	3.213692	1.429385
H	-4.596452	2.257133	2.948025
H	-3.830373	3.888471	2.978043
H	-0.892506	1.461990	3.139354
H	-1.646239	2.875537	3.977457
H	-2.466076	1.275490	3.993871
C	-0.011941	3.150504	-2.278731
C	1.521528	3.163172	-2.353704
C	-0.619443	4.017751	-3.387190
H	-0.326449	2.105439	-2.482752
H	1.952484	2.613763	-1.491437
H	1.859761	2.666149	-3.287920
H	1.918732	4.199946	-2.346511
H	-1.728109	3.981323	-3.334822
H	-0.291161	5.074750	-3.294786
H	-0.307400	3.636143	-4.382790
C	-2.767922	-2.174949	2.067812
C	-2.017950	-1.880083	3.372603
C	-4.160582	-2.750422	2.351138
H	-2.927150	-1.193887	1.574991
H	-1.027929	-1.428870	3.146925
H	-2.596521	-1.160585	3.988997
H	-1.865852	-2.803276	3.970104
H	-4.683178	-2.969867	1.395954
H	-4.096614	-3.684367	2.948338
H	-4.768553	-2.012178	2.916561
C	-0.190017	-3.144133	-2.269814
C	-0.840498	-3.966169	-3.388252
C	1.340439	-3.250620	-2.332871
H	-0.438167	-2.080636	-2.469954
H	-1.945206	-3.861317	-3.344729
H	-0.496904	-3.599408	-4.379033
H	-0.579114	-5.041957	-3.299168
H	1.797594	-2.734012	-1.463781
H	1.673154	-4.309861	-2.329554
H	1.716130	-2.769711	-3.261194
C	3.248075	-0.086371	0.284946
C	3.559085	-1.346773	1.112115
C	4.085842	-0.109704	-1.009269
C	3.618898	1.161643	1.106027
H	3.283184	-2.258879	0.538536
H	2.961693	-1.356337	2.050520
C	5.063356	-1.388573	1.465343
H	3.869802	0.790931	-1.625985
H	3.826830	-1.002207	-1.621320

C	5.591008	-0.144685	-0.664135
H	3.022479	1.203603	2.044271
H	3.386426	2.083172	0.528246
C	5.123480	1.133495	1.459147
H	5.280533	-2.301071	2.061990
C	5.896045	-1.411546	0.164886
C	5.430779	-0.133547	2.287843
H	6.187855	-0.161230	-1.601859
C	5.956089	1.110350	0.158625
H	5.383953	2.037547	2.051302
H	5.651438	-2.321084	-0.426783
H	6.980486	-1.455268	0.407939
H	4.850096	-0.117371	3.236328
H	6.509020	-0.158577	2.559498
H	7.041423	1.103654	0.401526
H	5.754909	2.027546	-0.437570