Experimental Considerations. All manipulations were performed under an argon atmosphere by standard Schlenk techniques or in an M. Braun glovebox maintained at or below 1 ppm of O_2 and H_2O. Glassware was dried at 150 °C overnight. ^{1}H NMR data were recorded on a Bruker Avance 500 spectrometer (500 MHz) at 25 °C and referenced internally to residual protiated solvent (C_6HD_5 at δ 7.16 ppm). Peaks of these paramagnetic complexes are all singlets. Relative integrations of peaks and assignments are given. Solution magnetic susceptibilities were determined at 294 K using the Evans method.[1] Electronic spectra were recorded between 400 nm and 800 nm on a Cary 50 UV-visible spectrophotometer, using resealable quartz cuvettes of 1 mm optical path length. Elemental analyses were performed by the CENTC Elemental Analysis Facility at the University of Rochester. Infrared spectra (500-4000 cm^{-1}) were recorded on KBr pellets in a Shimadzu FTIR spectrophotometer (FTIR-8400S) at 1 cm^{-1} resolution.

Pentane, diethyl ether, and toluene were purified by passage through activated alumina and "deoxygenizer" columns obtained from Glass Contour Co. Tetrahydrofuran (THF) was distilled from a sodium benzophenone ketyl still into a resealable flask. Solvents were additionally passed through a plug of activated alumina in the glove box immediately before use to ensure that they were completely moisture-free. Deuterated benzene was dried over activated alumina in a bomb flask, and was filtered into a storage container with 3Å molecular sieves prior to use. Before use, an aliquot of each solvent was tested with a drop of sodium benzophenone ketyl in THF solution. Celite and alumina were dried overnight at 200 °C under vacuum.

LFeOPh was prepared as described in the literature.[2] UV-Vis properties for bis-phenoxide complex $[KLFe(OPh)_2]_2$ (**P**) are given at a specific concentration due to the influence of the equilibrium with LFeOPh as discussed below.

Synthesis and Characterization of D. In an argon-filled glove box, a resealable flask was charged with LFeOPh (0.200 g, 0.307 mmol) and dissolved in toluene (20 mL) producing a clear orange solution. This solution was degassed for 3 min to remove trace N_2 or diethyl ether that might be present in the headspace. Potassium graphite (KC_8) (0.0889 g, 0.658 mmol) was added to the stirring solution of LFeOPh, which immediately began to turn dark green. The reaction mixture was stirred at room temperature for 1.5 h, concentrated to 12 mL, and then filtered through Celite. The first ~20 drops were red-orange in color and discarded. (It is likely that the desired product reacts with trace water in the Celite to form the red-orange solution.) The remaining dark green filtrate was collected and dried under vacuum. To crystallize the product, 15 mL of pentane was added the dark green solid to create a dark green solution. This solution was placed in a freezer (-40 °C) overnight. Dark green crystals were obtained in two crops (0.1335 g, 63%). ^{1}H NMR (500 MHz, C_6D_6): δ 44 (s, 8H, *i*Pr methine), 22 (s, 4H, *o*-OPh), 20 (s, 4H, *m*-aryl), 2.2 (s, 24H, *i*Pr methyl), -5.3 (s, 24H, *i*Pr methyl), -7.3 (s, 36H, tBu), -13 (s, 6H, *m*- and *o*-OPh), -64 (s, 4H, *p*-aryl), -132 (s, 2H, α-H) ppm. μ_{eff} (Evans, C_6D_6): 6.5(3) μ_B per dimeric molecule. IR (KBr): 3049 (w), 2957 (s), 2867 (m), 1585 (m), 1560 (m), 1481 (s), 1423 (m), 1378 (m), 1358 (s), 1320 (m), 1285 (m), 1164 (w), 1096 (m), 1055 (w), 1019 (w), 993 (w), 934 (w), 890 (w), 846 (w), 801 (w), 766 (m), 754 (m), 698 (m), 584 (w) cm^{-1}. UV-vis (toluene): 444 nm (12 $mM^{-1}cm^{-1}$), 641 nm (7.2 $mM^{-1}cm^{-1}$), 732 nm

(6.5 $mM^{-1}cm^{-1}$). Elem. Anal. Calcd for $C_{82}H_{116}Fe_2K_2N_4O_2$: C, 71.38; H, 8.47; N, 4.06. Found: C, 71.50; H, 8.56; N, 4.06.

Synthesis and Characterization of M. In an argon-filled glove box, a resealable flask was charged with LFeOPh (0.1517 g, 0.233 mmol) and dissolved in diethyl ether (Et_2O) (40 mL) producing a clear orange solution. This solution was degassed for 1 min to remove trace N_2 that might be present. Potassium graphite (KC_8) (0.0388 g, 0.287 mmol) was added to the stirring solution of LFeOPh, which immediately began to turn dark green. The reaction mixture was stirred at room temperature for 1 h and then filtered through Celite. The first ~20 drops were red-orange in color and discarded. (It is likely that the desired product reacts with trace water in the Celite to form the red-orange solution.) The remaining dark green filtrate was collected and concentrated to 3 mL. To crystallize the product by vapor diffusion, the concentrated solution in diethyl ether was transferred to a 5 mL vial and placed in a 20 mL scintillation vial, and then 5 mL toluene was added to the outside vial. The vials were placed in the freezer (-40 °C) overnight. Dark green crystals of **M** were obtained in two crops and dried under vacuum for 6 h (0.1482 g, 92%). The diethyl ether molecules were not observed in ^{1}H NMR spectra of this dried solid in C_6D_6; these spectra appear the same as for **D**. μ_{eff} (Evans, Et_2O): 4.1(2) μ_B. Elem. Anal. Calcd. for $C_{49}H_{78}FeKN_2O_3$ (with 2•Et_2O): C, 70.22; H, 9.38; N, 3.34. Calcd for $C_{41}H_{58}FeKN_2O$ (without Et_2O): C, 71.38; H, 8.47; N, 4.06. Found: C, 71.52; H, 8.61; N, 3.96.

Independent Synthesis and Characterization of P. In an argon-filled glove box, a resealable flask was charged with LFeOPh (0.1060 g, 0.163 mmol) and dissolved in tetrahydrofuran (THF) (10 mL) producing a clear orange solution. Potassium phenoxide

(KOPh) (0.0215 g, 0.163 mmol) was added as a solution in THF (5 mL) to the stirring solution of LFeOPh. The solution turned red-orange upon addition of KOPh. The reaction mixture was stirred at room temperature for 2 h. The solvent was pumped off under vacuum and subsequent solid was redissolved in 3 mL of Et_2O. Pentane (12 mL) was added until a red-orange solid precipitated from solution and was allowed to settle. The powder was separated by filtration and dried under vacuum (103.8 mg, 81%). This complex can be crystallized by concentrating the Et_2O through vapor diffusion into toluene at -40 °C. ^{1}H NMR (500 MHz, C_6D_6): δ 22 (s, 8H, *i*Pr methine), 17 (s, 8H, *o*-OPh), 9.4 (s, 18H, tBu), 2.7 (s, 24H, *i*Pr methyl), -4.8 (s, 24H, *i*Pr methyl), -20 (s, 4H, *p*-aryl), -33 (s, 8H, *m*-OPh), -44 (s, 4H, *p*-OPh), -57 (s, 2H, α-H). The peak corresponding to *m*-aryl (4H) is likely hidden under the solvent peak at δ 7.16 ppm. Two peaks corresponding to an impurity of LFeOPh can also be observed at δ 42 (s, 18H, tBu) and -29 (s, 12H, *i*Pr methyl) ppm. IR (KBr): 3054 (w), 2962 (m), 2868 (m), 2371 (w), 2339 (w), 1586 (m), 1532 (m), 1481 (s), 1430 (m), 1382 (s), 1362 (s), 1317 (m), 1285 (s), 1216 (m), 1097 (m), 1022 (w), 990 (w), 935 (w), 828 (m), 756 (m), 693 (m), 566 (m) cm^{-1}. UV-vis (~3.0 mM in toluene): 462 nm (A = 0.70), 516 nm (A = 0.38). As described below, this compound is in a dynamic equilibrium at room temperature, and so true extinction coefficients were not derived. Elem. Anal. Calcd for $C_{94}H_{126}Fe_2K_2N_4O_4$: C, 72.10; H, 8.11; N, 3.58. Found: C, 72.56; H, 8.82; N, 3.21.

Details of Structure for M. The monomer of $[K(Et_2O)_2][LFeOPh]$ (**M**) has two Et_2O molecules associated with the potassium cation, which also interacts with the aryl group of the β-diketiminate ligand and the oxygen atom of the phenoxide. The potassium cation is 2.7256(11) and 2.7534(10) Å from the two Et_2O oxygen atoms, 2.6092(10) Å from the oxygen of the phenoxide ligand, and 3.036 Å from the centroid of the β-diketiminate aryl group. The Fe-N distances at 1.9130(10) and 1.9258(10) Å fall within the range (1.905(5) – 2.0049(12) Å) of Fe-N distances from previously reported three-coordinate iron(I) complexes with this ligand.[3]

The Fe-O bond is noticeably off the C_2 axis as demonstrated by the inequivalent N-Fe-O angles of 142.28(4)° and 116.80(4)° (25° difference). We attribute the difference to the binding of the oxygen of the potassium cation. The iron(II) analogue (LFeOTol) contains N-Fe-O angles that are less asymmetric at 140.20(8)° and 125.01(9)° (15° difference).[2]

Details of Structure for D. The crystal structure of $[KLFeOPh]_2$ (**D**) shows that the two crystallographically equivalent LFeOPh units are held together by potassium cations. Each potassium cation associates with the oxygen atom as well as one aryl group of the β-diketiminate ligand on the same LFeOPh unit. They lie 2.79 Å from the centroid of the β-diketiminate ligand aryl groups and 2.586(2) Å from the oxygen atom. The cation also associates with the phenoxide aryl group of the second monomer unit at a K^+-centroid distance of 2.85 Å. The potassium cation associates with one aryl group from each monomer unit, which contributes to the N-Fe-O angles being closer to the N-Fe-O angles in LFeOTol where the largest difference in angles between this iron(II) analogue and **D** is less than 3°.[2]

Table S1. Relevant bond lengths and angles for diiron(II) complex $[KLFe(OPh)_2]_2$ (**P**).

	$[KLFe(OPh)_2]_2$	
	Fe(1)	Fe(2)
Fe-N (Å)	2.025(3)	2.037(3)
	2.031(3)	2.050(3)
Fe-O (Å)	1.953(3)	1.990(2)
	1.995(2)	2.007(2)
K••O (Ar) (Å)	2.657(2)	2.640(2)
	2.674(3)	
	2.677(2)	
	2.818(2)	
K••O (THF) (Å)		2.602(3)
N-Fe-N (°)	94.08(11)	94.14(11)
N-Fe-O (°)	127.47(11)	115.68(10)
	111.50(10)	130.98(10)
	113.55(11)	116.01(10)
Fe-O-C (°)	119.66(10)	111.81(10)
O-Fe-O (°)	92.96(10)	90.00(9)

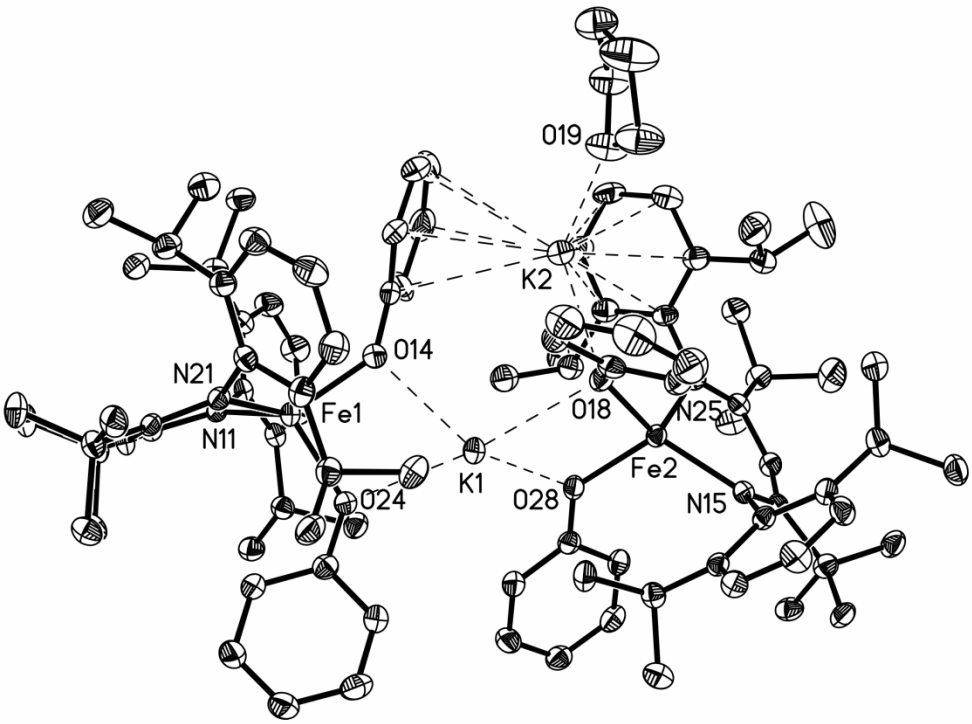
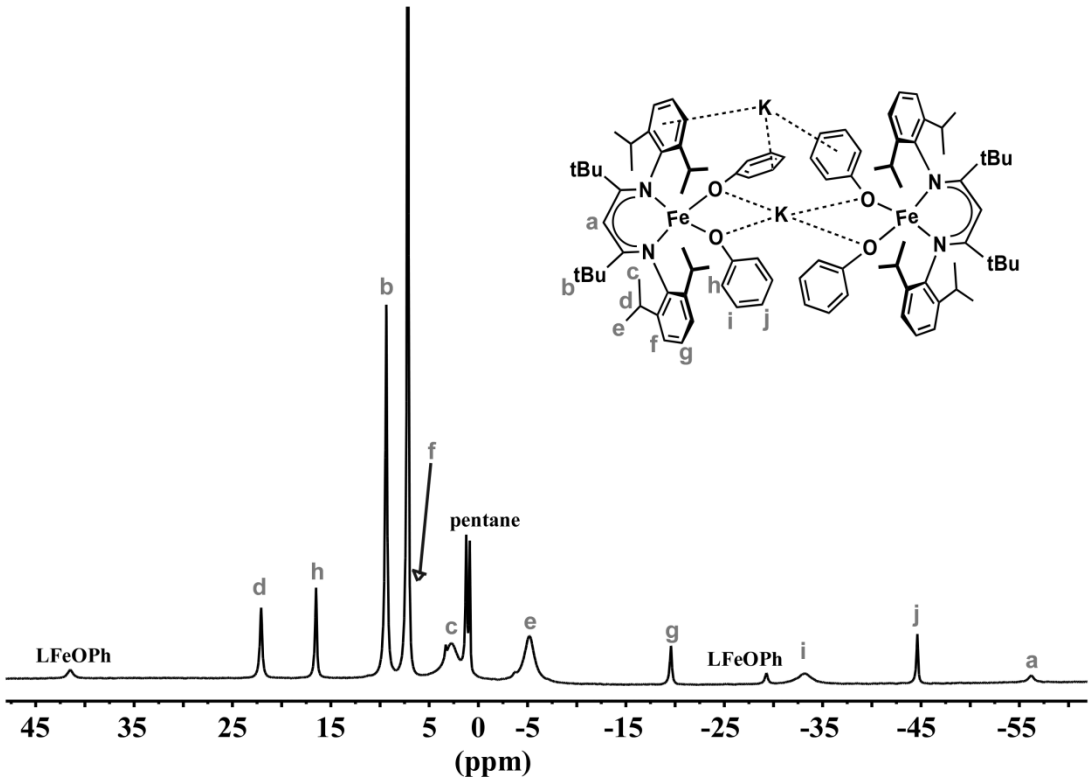
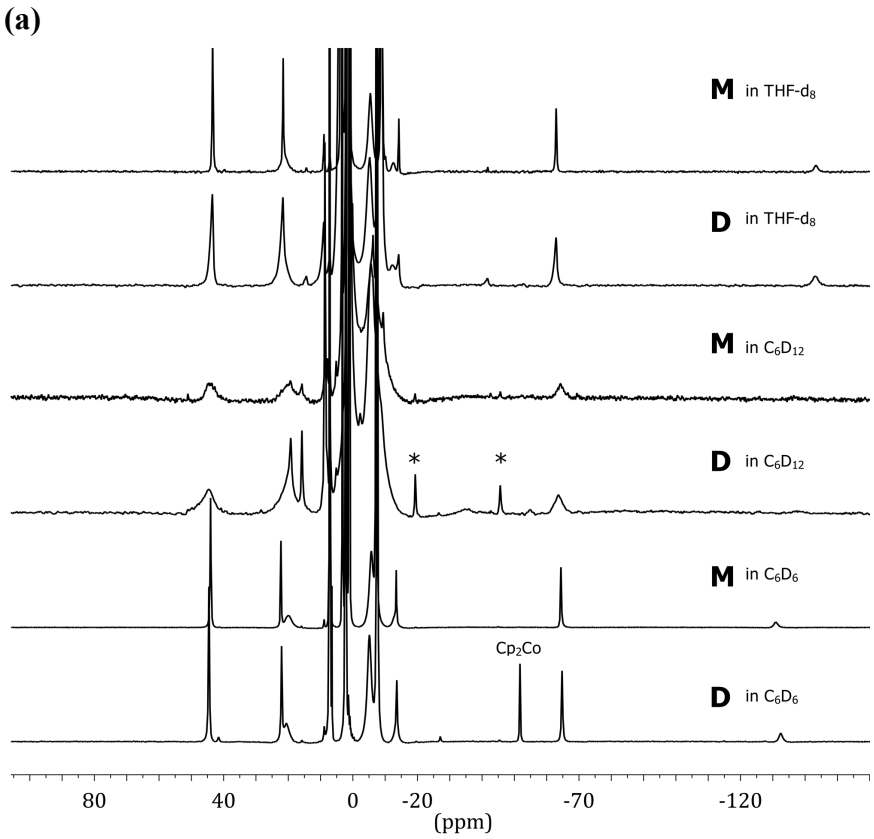


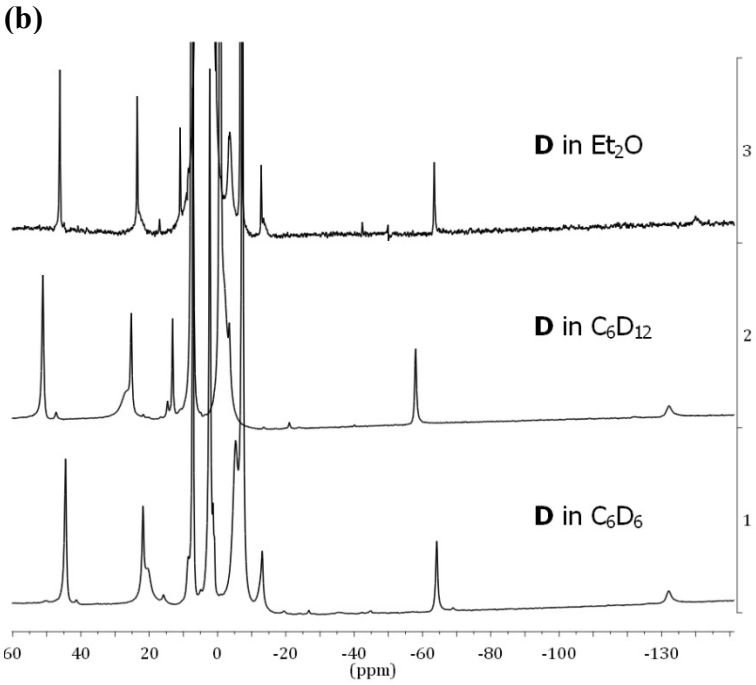
Figure S-1. ^{1}H NMR spectrum of the bis-phenoxide complex $[KLFe(OPh)_2]_2$. The *m*-aryl proton is presumably under the solvent peak. Two peaks not belonging to the product are assigned to the tBu (18 H) and one of the *i*Pr methyl (12 H) resonances of LFeOPh, which match the literature.[2]



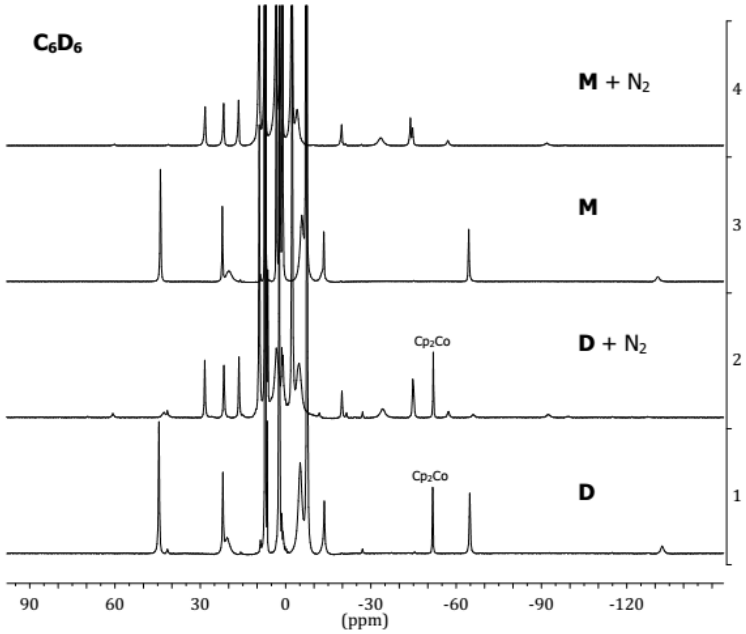
Details of NMR spectra and related experiments. The ^{1}H NMR spectra of **M** and **D** are shown in Figure S2a. These show that when dissolved in the same solvent, **M** (crystallized from Et_2O) and **D** give practically identical spectra. Adding Et_2O (20 equivalents) to a sample of **D** in C_6D_6 does not change the chemical shifts of the peaks, presumably because the equilibrium is not shifted enough toward the monomer. However, the ^{1}H NMR spectra in neat Et_2O (C_6D_6 capillary to reference and lock) and in THF-d_8 show a spectrum with the peaks shifted from the spectrum in C_6D_6. The most noticeable difference in chemical shift is for the α-H peak. In Et_2O it is shifted to δ -142 ppm (10 ppm further upfield than the spectrum in C_6D_6 as seen in Figure S2b).

We note that the changes in ^{1}H NMR spectra are relatively subtle; thus, the main evidence for a different solution structure are in the very different reactivities toward N_2 in C_6D_6 and C_6D_{12} (where N_2 reacts rapidly) versus in diethyl ether and THF (where the reaction is not seen). The spectra for these reactions are shown in Figures S2c-S2e.

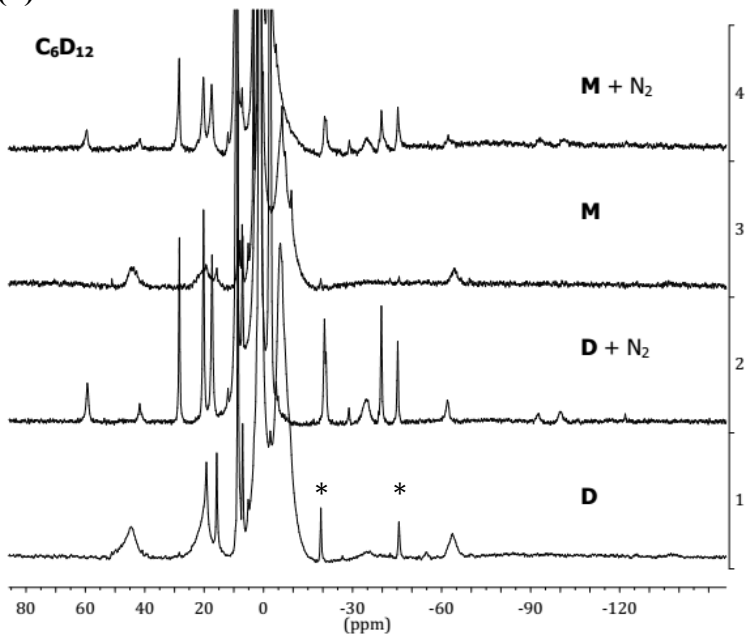




(c)



(d)



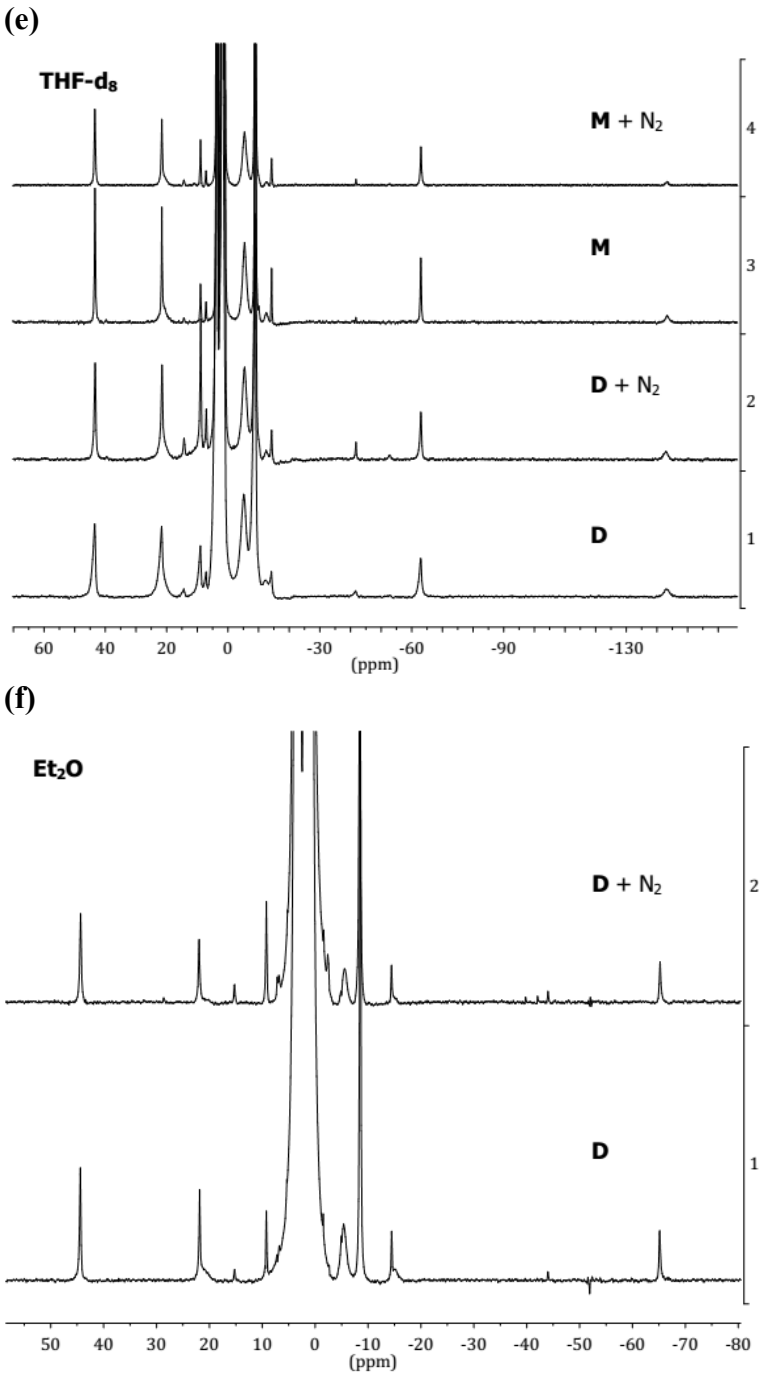


Figure S-2. ^{1}H NMR spectra of isolated **M** and isolated **D** after dissolving in the indicated solvents. The starred peaks are from **N** and **P** due to reaction with trace N_2.

These spectra show that, no matter whether one starts with **M** or with **D** in the solid state, dissolving in C_6D_{12} or C_6D_6 gives a solution that reacts with N_2, while dissolving in Et_2O or THF gives a solution that does not react with N_2.

Evans Method Measurements. The solution magnetic moment has been probed in different solvents to determine the spin states of **M** and **D**. In diethyl ether solution with benzene as the reporter, the magnetic moment of **M** is 4.1(2) μ_B, which compares well to the spin-only moment of 3.9 μ_B for $S = 3/2$. In benzene, where **D** dominates, the magnetic moment is calculated as $\mu_{eff} = 6.5(3)$ μ_B for a dimer or 4.6(2) μ_B per monomer, consistent with two uncoupled high-spin $S = 3/2$ metal centers. Thus, both **M** and **D** have high-spin iron(I). The experimental values are somewhat elevated from the spin-only values, probably from spin-orbit coupling.

Decomposition. D is very susceptible to oxidation. After two days at room temperature under Ar, solutions in C_6D_6 show a new set of paramagnetic peaks in the ^{1}H NMR spectrum, concomitant with a gradual color change to brown. ^{1}H NMR spectra indicate that this decomposition corresponds to the formation of **P**. In this case, the oxidant is likely to be trace oxygen in the glove box atmosphere. Very brief exposure of **D** to air results in an immediate color change from dark green to red-orange. The ^{1}H NMR spectrum shows disappearance of the starting material and growth of peaks corresponding to **P**. Prolonged exposure of **D** to air results in decomposition of all of the iron complexes.

Computational Details. The calculations were performed using ORCA version 2.8, 2.9, and 3.0.[4] The ligands were not truncated, which made them prohibitively expensive to optimize with a triple-zeta basis set; thus we used the Ahlrichs split-valence basis set with polarization functions (def2-SVP). The geometries were optimized, starting from the crystallographic coordinates, using the pure functional BP86[5] accelerated with the resolution of identity (RI) approximation.[6] Scalar relativistic corrections were introduced according to the ZORA approximation,[7] and a van der Waals correction was applied (VDW10).[8] All computations on iron(I) complexes assumed high-spin configurations and little coupling between metals: thus we used a quartet spin state on monomers, and a septet spin state on dimers. Point calculations on the optimized structures using a triple-zeta basis set def2-TZVP, and using both BP86 and B3LYP, confirmed that the quartet was lower in energy than the doublet state, by 14 kcal/mol (BP86/def2-TZVP) or 20 kcal/mol (B3LYP/def2-TZVP).

Enthalpies and free energies were calculated by means of numerical frequency calculations (NumFreq) on the optimized geometries. None of the frequencies were negative, except for a small negative freqency of -13 cm^{-1} in **D-N_2**, which is a local minimum on the way to **D-N_2-bridge**.

Sample Input File

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Table S-2. Optimized Coordinates

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H	12.636261	5.814788	10.504618

M-N_2 (filename mon2)

Fe	11.316598	3.311496	2.642754
K	11.783302	3.519673	6.232244
O	10.270500	4.120147	4.145071
N	12.892286	4.518889	2.381068
N	10.667581	3.164584	0.773852
C	14.541018	5.699596	0.750001
C	13.352725	4.740886	1.135514
C	12.741643	4.144843	-0.003308
H	13.297018	4.334263	-0.914740
C	11.514700	3.475881	-0.234607
C	11.205433	3.117751	-1.734641
C	15.350106	6.325988	1.909837
H	16.135716	6.970960	1.474171
H	15.850982	5.577389	2.540864
H	14.740731	6.955700	2.571859
C	15.565382	4.939618	-0.140339
H	16.435647	5.590275	-0.344863
H	15.149278	4.636456	-1.115346
H	15.930430	4.026544	0.360782
C	13.931466	6.871992	-0.070180
H	14.716629	7.607208	-0.329991
H	13.150553	7.392797	0.510361
H	13.466319	6.520783	-1.006641
C	12.467328	3.196972	-2.633939
H	12.207866	2.823876	-3.641426
H	13.292583	2.573360	-2.246044
H	12.837679	4.229605	-2.764527

C	10.158004	4.085187	-2.336313
H	10.039526	3.884600	-3.418011
H	10.474657	5.136508	-2.215685
H	9.171855	3.960222	-1.862896
C	10.682772	1.668495	-1.845288
H	10.596986	1.378277	-2.908708
H	9.686012	1.562911	-1.394777
H	11.367364	0.958298	-1.348853
C	13.464675	4.972553	3.593757
C	14.457424	4.171375	4.254889
C	15.028343	4.645068	5.454999
H	15.820354	4.056381	5.936939
C	14.621865	5.860072	6.032310
H	15.097753	6.226817	6.949837
C	13.599189	6.600539	5.416610
H	13.272582	7.546491	5.868970
C	12.998178	6.180153	4.212473
C	14.924440	2.832626	3.683765
H	14.234750	2.577749	2.859993
C	14.853934	1.703708	4.733667
H	15.038933	0.725959	4.255556
H	13.862246	1.634429	5.210071
H	15.613264	1.841047	5.527268
C	16.355542	2.904934	3.110808
H	16.438811	3.650202	2.304355
H	16.654958	1.924979	2.696175
H	17.085063	3.177816	3.896954
C	11.898788	7.037391	3.589513
H	11.522583	6.482070	2.711048
C	10.719620	7.240284	4.562248
H	10.277832	6.269537	4.829268
H	9.930128	7.853114	4.092006
H	11.039321	7.764518	5.483129
C	12.423662	8.411419	3.118388
H	13.272023	8.323683	2.420279
H	12.760834	9.022792	3.976878
H	11.620204	8.971359	2.605491
C	9.266039	2.936330	0.640700
C	8.399047	4.066827	0.472659
C	7.008489	3.859510	0.430284
H	6.343427	4.723720	0.313059
C	6.453395	2.578336	0.554626
H	5.365896	2.438909	0.516756
C	7.302669	1.482521	0.748630
H	6.870360	0.481387	0.872658
C	8.702818	1.631544	0.808908
C	8.941264	5.496472	0.453516
H	10.010847	5.452595	0.179431

C	8.857975	6.091797	1.873766
H	9.272157	7.117135	1.890413
H	9.417929	5.477060	2.596626
H	7.807965	6.138632	2.217339
C	8.230632	6.422442	-0.553048
H	8.185386	5.987085	-1.566015
H	8.764709	7.388020	-0.618995
H	7.195181	6.649254	-0.237652
C	9.552051	0.404353	1.136534
H	10.611586	0.709562	1.063719
C	9.278517	-0.038343	2.589859
H	9.405762	0.802763	3.286951
H	9.972315	-0.841738	2.894703
H	8.240671	-0.405909	2.698954
C	9.315611	-0.788222	0.185622
H	9.462848	-0.522384	-0.873798
H	8.289414	-1.187558	0.290053
H	10.012550	-1.610432	0.431367
C	9.097961	3.814860	4.695969
C	8.773464	4.253359	6.017658
H	9.458888	4.924192	6.554600
C	7.569943	3.868971	6.632912
H	7.349826	4.227059	7.648186
C	6.641301	3.055331	5.959345
H	5.704735	2.755946	6.445001
C	6.924817	2.662787	4.635727
H	6.204789	2.056999	4.069733
C	8.118049	3.043283	4.011838
H	8.319831	2.757438	2.976116
C	9.999312	0.563051	6.113320
H	9.357438	-0.234179	5.702367
H	10.173464	1.273595	5.287873
H	9.434349	1.081089	6.908082
C	11.302208	-0.028688	6.626915
H	11.108053	-0.788758	7.416107
H	11.856662	-0.517766	5.798391
O	12.112215	1.024756	7.182503
C	13.298304	0.567271	7.830831
H	13.944349	0.025206	7.104788
H	13.029335	-0.154079	8.635183
C	14.034084	1.766841	8.415555
H	14.925223	1.436810	8.977184
H	13.380155	2.332519	9.102984
H	14.376801	2.452088	7.618853
C	10.109878	2.777721	9.421778
H	9.642003	2.300693	10.300827
H	10.774960	2.040124	8.937648
H	9.312136	3.041911	8.705253

C	10.886038	4.015222	9.848796
H	10.216403	4.750197	10.348949
H	11.675232	3.740049	10.582713
O	11.472765	4.623294	8.691012
C	12.181763	5.842741	8.944110
H	11.564586	6.509210	9.585814
H	12.282956	6.336570	7.959427
C	13.563052	5.616417	9.558987
H	14.097315	6.578077	9.662335
H	14.166195	4.956187	8.911163
H	13.502040	5.159187	10.562311
N	11.858050	1.691808	3.202293
N	12.230208	0.628513	3.458285

D (filename K3)

Fe	12.791777	2.233041	5.151217
K	16.171749	2.407958	3.567547
O	14.300411	3.449043	5.186071
N	11.930479	1.141099	6.469892
N	11.938479	1.545324	3.580407
C	10.435688	-0.860070	7.171824
C	10.964595	0.227853	6.176451
C	10.445928	0.133514	4.857706
H	9.594038	-0.535955	4.767067
C	10.839656	0.732068	3.642442
C	9.846226	0.624767	2.439082
C	8.887670	-0.961656	7.092624
H	8.420887	0.018494	7.299526
H	8.520979	-1.681741	7.847245
H	8.523446	-1.311239	6.112107
C	11.067009	-2.211558	6.736678
H	12.168683	-2.168297	6.818157
H	10.817411	-2.453419	5.688909
H	10.709176	-3.037152	7.381651
C	10.770586	-0.651588	8.666356
H	10.341615	0.280377	9.068980
H	11.850971	-0.634459	8.869153
H	10.340409	-1.493009	9.240983
C	10.498946	0.657030	1.036342
H	11.175044	-0.199432	0.871541
H	11.073640	1.574766	0.849683
H	9.702520	0.605404	0.270791
C	8.902002	1.851532	2.568297
H	9.476353	2.792577	2.522050
H	8.367544	1.829512	3.534846
H	8.153919	1.862102	1.752290
C	8.994655	-0.667607	2.494840
H	9.634321	-1.568513	2.537492

H	8.369760	-0.737875	1.585950
H	8.305706	-0.691195	3.356736
C	12.382904	1.532258	7.754109
C	11.627648	2.475554	8.521641
C	12.183565	2.967547	9.717820
H	11.622815	3.704261	10.305799
C	13.446904	2.547705	10.170108
H	13.862373	2.952208	11.101405
C	14.158721	1.582619	9.435862
H	15.125057	1.217238	9.810498
C	13.637342	1.050286	8.242576
C	10.280677	2.974086	8.001459
H	9.863726	2.169527	7.366464
C	10.475960	4.204537	7.089351
H	9.514765	4.529294	6.650711
H	11.166885	3.957616	6.257641
H	10.910575	5.050919	7.652197
C	9.260029	3.258563	9.116360
H	9.148415	2.393842	9.796028
H	8.269997	3.481057	8.678779
H	9.547313	4.134582	9.727427
C	14.377748	-0.036069	7.473540
H	13.675384	-0.397575	6.703249
C	15.593897	0.540895	6.728854
H	15.275278	1.441846	6.170090
H	16.002090	-0.184601	6.007318
H	16.413330	0.778439	7.434331
C	14.780020	-1.235776	8.348947
H	13.907191	-1.666617	8.870237
H	15.523540	-0.949851	9.114918
H	15.235136	-2.030464	7.729443
C	12.823638	1.672369	2.488835
C	13.573488	0.528553	2.023988
C	14.558489	0.724081	1.037390
H	15.136473	-0.135625	0.676534
C	14.815310	1.997562	0.485684
H	15.585883	2.121347	-0.285418
C	14.038162	3.093924	0.902389
H	14.198158	4.076269	0.437646
C	13.033473	2.956045	1.881085
C	13.302749	-0.857103	2.613433
H	12.208570	-0.931410	2.763014
C	13.929229	-1.002473	4.013252
H	13.649630	-0.144283	4.651108
H	15.030189	-1.044196	3.946612
H	13.579889	-1.923404	4.513878
C	13.721618	-2.021270	1.702337
H	13.291272	-1.925511	0.688704

H	13.376762	-2.979219	2.131521
H	14.821571	-2.091210	1.600727
C	12.130905	4.138606	2.224247
H	11.467883	3.793892	3.041287
C	12.916533	5.350074	2.755197
H	13.484954	5.066431	3.652405
H	12.231496	6.173564	3.027543
H	13.625568	5.741660	2.001227
C	11.254911	4.534116	1.016011
H	10.672081	3.678928	0.631776
H	11.875192	4.916774	0.183562
H	10.542924	5.331569	1.298548
C	14.500492	4.539786	5.939325
C	15.312808	5.609893	5.465906
H	15.741610	5.560617	4.457620
C	15.586521	6.718775	6.283911
H	16.224443	7.519014	5.888611
C	15.065529	6.808859	7.589507
H	15.280344	7.682021	8.217034
C	14.246178	5.763175	8.063478
H	13.813516	5.802226	9.071986
C	13.968166	4.651475	7.254004
H	13.326783	3.845883	7.619791
Fe	19.938905	1.903880	5.652449
K	16.805769	3.405231	7.585594
O	18.436018	3.121555	5.399451
N	21.104014	1.016778	4.389101
N	20.807412	1.270210	7.271868
C	23.079395	-0.550033	3.719904
C	22.176673	0.255519	4.723419
C	22.534677	0.079969	6.082956
H	23.443501	-0.502638	6.226527
C	21.941919	0.515382	7.286872
C	22.779609	0.184153	8.577011
C	24.570117	-0.178363	3.953111
H	24.731223	0.902214	3.786126
H	25.212797	-0.732312	3.243578
H	24.921893	-0.416699	4.970738
C	22.861119	-2.060904	4.012254
H	21.804438	-2.337253	3.842329
H	23.111001	-2.324404	5.054019
H	23.488056	-2.678770	3.341400
C	22.825302	-0.347509	2.208283
H	23.010632	0.686308	1.878806
H	21.804675	-0.616115	1.899742
H	23.522111	-1.002240	1.652187
C	22.111478	0.482621	9.938807
H	21.201254	-0.112770	10.113684

H	21.847931	1.542195	10.063396
H	22.829583	0.228626	10.740503
C	24.071726	1.045605	8.508328
H	23.821784	2.122294	8.507951
H	24.654787	0.837906	7.594860
H	24.717949	0.846297	9.384584
C	23.167331	-1.319404	8.603996
H	22.266950	-1.960470	8.603134
H	23.741157	-1.542893	9.522404
H	23.792634	-1.620501	7.747137
C	20.683912	1.336838	3.072892
C	21.270028	2.440943	2.377810
C	20.755964	2.785819	1.115029
H	21.189507	3.635214	0.574151
C	19.686132	2.080985	0.536978
H	19.293138	2.379497	-0.442649
C	19.134452	0.980781	1.216144
H	18.319757	0.409627	0.749993
C	19.637490	0.575573	2.467610
C	22.422702	3.219164	3.009931
H	22.952913	2.514051	3.678054
C	21.895151	4.361908	3.902278
H	22.727927	4.888038	4.403802
H	21.229669	3.949802	4.683598
H	21.311367	5.094845	3.316577
C	23.444026	3.740345	1.984127
H	23.796051	2.936812	1.311291
H	24.323443	4.161525	2.504147
H	23.022713	4.547764	1.356617
C	19.106669	-0.680034	3.152503
H	19.759762	-0.866174	4.024745
C	17.690086	-0.452343	3.701626
H	17.721347	0.379830	4.432441
H	17.313695	-1.344703	4.232714
H	16.977580	-0.226317	2.883071
C	19.153782	-1.921436	2.241619
H	20.168959	-2.089089	1.840981
H	18.466462	-1.824837	1.380609
H	18.855688	-2.825171	2.804420
C	19.926005	1.490821	8.351868
C	19.051979	0.440420	8.805666
C	18.078815	0.749288	9.772978
H	17.403152	-0.038681	10.126777
C	17.979616	2.037951	10.338984
H	17.224370	2.247114	11.107179
C	18.916815	3.024984	9.973024
H	18.905459	3.994388	10.489741
C	19.911655	2.767747	9.007950

C	19.262591	-0.984493	8.289979
H	20.355239	-1.096069	8.163996
C	18.657320	-1.213295	6.892956
H	18.889954	-0.356388	6.232421
H	17.562018	-1.322436	6.951461
H	19.071856	-2.125702	6.427882
C	18.807435	-2.074392	9.273218
H	19.243989	-1.929501	10.278288
H	19.119342	-3.068450	8.904792
H	17.706705	-2.100537	9.378554
C	21.020214	3.778792	8.718466
H	21.834437	3.202884	8.239098
C	20.582335	4.839825	7.696956
H	20.263638	4.346257	6.763544
H	21.407569	5.531878	7.449491
H	19.741945	5.444156	8.091286
C	21.581550	4.433804	9.994706
H	21.871532	3.681951	10.750436
H	20.848299	5.116346	10.463886
H	22.475564	5.036146	9.750872
C	18.525691	4.198396	4.582726
C	18.529299	5.525259	5.091118
H	18.497681	5.686133	6.172717
C	18.562160	6.630518	4.229680
H	18.571210	7.640792	4.659373
C	18.575100	6.462618	2.832122
H	18.597594	7.332127	2.164911
C	18.574542	5.156540	2.312155
H	18.617960	4.983834	1.229493
C	18.559643	4.047578	3.171050
H	18.647560	3.037281	2.757260

D-constrained (filename K3-constr)

Fe	12.373632	2.481959	4.863415
K	15.054391	3.161197	2.478127
O	13.914862	3.657764	4.846848
N	11.921170	0.924730	5.861365
N	11.022767	2.415178	3.526480
C	10.666412	-1.316627	6.138319
C	10.858940	0.124956	5.563118
C	9.929757	0.519023	4.564554
H	9.052852	-0.119721	4.500043
C	9.945022	1.575340	3.628881
C	8.612058	1.898511	2.883312
C	9.164147	-1.626779	6.376586
H	8.703744	-0.867755	7.034752
H	9.062044	-2.612102	6.866834
H	8.576964	-1.673776	5.443876

C	11.222990	-2.295626	5.067867
H	12.302000	-2.123562	4.904234
H	10.707889	-2.156548	4.100803
H	11.090414	-3.346702	5.389047
C	11.382322	-1.614257	7.475980
H	11.040497	-0.952417	8.289140
H	12.475675	-1.523159	7.410404
H	11.156142	-2.655021	7.773402
C	8.787506	2.484213	1.461998
H	9.307458	1.781843	0.787736
H	9.347337	3.430218	1.452127
H	7.789726	2.687088	1.030514
C	7.884903	2.948131	3.767813
H	8.512612	3.845093	3.903824
H	7.673273	2.530965	4.768584
H	6.927885	3.259880	3.306963
C	7.702084	0.654618	2.737654
H	8.225133	-0.166944	2.214216
H	6.807505	0.918959	2.144944
H	7.340124	0.272915	3.707979
C	12.733655	0.889273	7.019640
C	12.235615	1.432736	8.250063
C	13.113668	1.536793	9.344163
H	12.751123	1.970321	10.284091
C	14.444065	1.088458	9.265205
H	15.111514	1.170192	10.131845
C	14.901626	0.498497	8.073725
H	15.916860	0.077895	8.037832
C	14.069792	0.384033	6.943394
C	10.789381	1.922536	8.336908
H	10.203687	1.318554	7.617972
C	10.672089	3.391118	7.875398
H	9.616349	3.717654	7.861294
H	11.078532	3.504703	6.849478
H	11.237277	4.064812	8.545787
C	10.157745	1.724005	9.725319
H	10.271422	0.683189	10.079866
H	9.078438	1.958036	9.688688
H	10.606848	2.391030	10.484831
C	14.562274	-0.304976	5.673624
H	13.675958	-0.409393	5.022658
C	15.577394	0.560899	4.902746
H	15.162317	1.578798	4.777991
H	15.791913	0.131813	3.906669
H	16.555132	0.624335	5.415668
C	15.131418	-1.709986	5.944663
H	14.399191	-2.349390	6.468333
H	16.046763	-1.665590	6.562240

H	15.404445	-2.205200	4.995108
C	11.528133	2.998382	2.346536
C	11.996137	2.159757	1.267416
C	12.603503	2.766381	0.151851
H	12.950729	2.138274	-0.678138
C	12.767332	4.165228	0.065750
H	13.230215	4.615385	-0.821301
C	12.286806	4.975740	1.110500
H	12.375348	6.067530	1.029181
C	11.656439	4.425766	2.244141
C	11.880442	0.638030	1.373220
H	10.945393	0.421152	1.923498
C	13.023131	0.065937	2.239010
H	13.068846	0.594364	3.212132
H	13.999314	0.167815	1.723200
H	12.869077	-1.007125	2.452619
C	11.794353	-0.085115	0.020134
H	10.995579	0.336714	-0.616727
H	11.576634	-1.156931	0.177109
H	12.743898	-0.028925	-0.545395
C	11.056740	5.347543	3.303005
H	10.707185	4.692294	4.124528
C	12.091231	6.320748	3.897741
H	12.945144	5.766206	4.314809
H	11.640817	6.920072	4.709757
H	12.470869	7.028515	3.136499
C	9.841457	6.115614	2.739245
H	9.084071	5.434021	2.314958
H	10.150719	6.811489	1.936590
H	9.356165	6.712083	3.533817
C	14.480571	4.385082	5.811842
C	15.438383	5.393281	5.490104
H	15.679293	5.580640	4.436513
C	16.071023	6.142030	6.496830
H	16.806983	6.905897	6.213804
C	15.768754	5.926658	7.857305
H	16.262782	6.515016	8.638960
C	14.810117	4.946060	8.189025
H	14.551249	4.756655	9.238996
C	14.179417	4.188254	7.189580
H	13.445984	3.419824	7.452182
Fe	20.420991	1.494313	5.870127
K	16.948307	2.740006	7.118840
O	18.722790	2.175988	5.234894
N	21.792911	0.464310	5.035193
N	21.198222	1.644361	7.620508
C	24.083950	-0.775792	4.984015
C	22.938298	0.069106	5.645166

C	23.184672	0.424991	6.996366
H	24.154341	0.093548	7.369536
C	22.416453	1.127565	7.950698
C	23.123119	1.322229	9.338454
C	25.386445	0.070891	4.991496
H	25.250469	0.991830	4.395692
H	26.219794	-0.504645	4.545434
H	25.691286	0.371860	6.008162
C	24.285158	-2.067017	5.825221
H	23.355375	-2.664650	5.839058
H	24.560168	-1.855309	6.872165
H	25.087373	-2.689424	5.385226
C	23.872233	-1.239007	3.524360
H	23.783809	-0.401790	2.815794
H	22.979977	-1.871272	3.400966
H	24.751021	-1.839466	3.222733
C	22.308668	2.042769	10.435648
H	21.405642	1.488432	10.735384
H	21.996351	3.054681	10.136105
H	22.947937	2.146306	11.332325
C	24.396419	2.181266	9.099953
H	24.121422	3.169054	8.686676
H	25.095947	1.706199	8.391567
H	24.935058	2.345635	10.052860
C	23.522956	-0.060131	9.920504
H	22.628153	-0.686955	10.085943
H	24.032884	0.069189	10.893895
H	24.204677	-0.620322	9.258822
C	21.419814	0.218037	3.689240
C	21.812669	1.132177	2.663377
C	21.402420	0.880874	1.342972
H	21.692986	1.580195	0.549104
C	20.636411	-0.250417	1.016448
H	20.345274	-0.439281	-0.024546
C	20.237250	-1.130604	2.034578
H	19.622257	-2.005393	1.783815
C	20.607285	-0.912771	3.374968
C	22.644734	2.364518	3.007661
H	23.112504	2.171750	3.991202
C	21.727634	3.593319	3.179973
H	22.312257	4.499680	3.424004
H	21.016652	3.412951	4.005965
H	21.136419	3.786662	2.265397
C	23.774950	2.635983	1.998456
H	24.407767	1.742164	1.849197
H	24.421462	3.457036	2.359043
H	23.383394	2.940216	1.009859
C	20.098545	-1.839430	4.475084

H	20.572351	-1.509304	5.418960
C	18.577068	-1.654282	4.640245
H	18.358739	-0.604486	4.906938
H	18.174945	-2.303111	5.438475
H	18.036503	-1.891685	3.704521
C	20.471122	-3.315422	4.243548
H	21.563789	-3.443848	4.144328
H	20.002149	-3.717755	3.326064
H	20.130499	-3.939070	5.090934
C	20.200022	2.101093	8.506965
C	19.397087	1.160089	9.240400
C	18.338059	1.638334	10.034077
H	17.717519	0.921991	10.588405
C	18.064557	3.018022	10.142621
H	17.239548	3.372680	10.772760
C	18.882640	3.936828	9.455643
H	18.689378	5.011908	9.565408
C	19.959186	3.509152	8.653489
C	19.666036	-0.335475	9.101219
H	20.698004	-0.444105	8.721159
C	18.739767	-0.933379	8.025252
H	18.836955	-0.351762	7.088087
H	17.683871	-0.909767	8.355479
H	19.002411	-1.982713	7.799057
C	19.571270	-1.107054	10.428166
H	20.219228	-0.659127	11.203151
H	19.886182	-2.156592	10.283499
H	18.538238	-1.129098	10.823125
C	20.872682	4.516654	7.960382
H	21.777280	3.954663	7.658348
C	20.223495	5.046288	6.666804
H	20.019511	4.200956	5.987224
H	20.887237	5.755978	6.140059
H	19.268211	5.563162	6.886291
C	21.307610	5.670236	8.883689
H	21.746475	5.295812	9.825978
H	20.459624	6.329785	9.147245
H	22.064727	6.298510	8.379869
C	18.481386	2.656507	4.012660
C	18.230391	4.049132	3.806154
H	18.249079	4.721245	4.670826
C	18.030684	4.567513	2.515332
H	17.890622	5.650043	2.388468
C	18.042631	3.720421	1.384498
H	17.934563	4.133588	0.373921
C	18.251612	2.335285	1.581276
H	18.299269	1.654899	0.721138
C	18.449497	1.809332	2.866407

H	18.662323	0.744455	3.002595

D-N_2 (filename K4-3)

Fe	12.846305	1.830237	5.411847
K	16.250793	3.017641	3.672940
O	13.449469	3.713468	5.368958
N	11.480363	0.970815	6.587735
N	12.085484	1.202056	3.689912
C	9.202554	-0.213878	6.997724
C	10.333461	0.451989	6.126079
C	10.056101	0.412567	4.728812
H	9.058277	0.049164	4.498792
C	10.841387	0.677820	3.586924
C	10.102366	0.448851	2.216833
C	7.861919	0.539372	6.775383
H	7.933933	1.590310	7.103995
H	7.063643	0.055684	7.368261
H	7.540961	0.536771	5.720031
C	9.033943	-1.683577	6.512803
H	9.974896	-2.250460	6.622992
H	8.733023	-1.748212	5.454191
H	8.259039	-2.189939	7.117672
C	9.438759	-0.267113	8.524487
H	9.433526	0.727536	8.991832
H	10.384610	-0.755129	8.800033
H	8.618310	-0.851371	8.980797
C	11.006235	0.178855	0.990159
H	11.630808	-0.719915	1.115418
H	11.679739	1.011034	0.754586
H	10.360093	0.018597	0.107528
C	9.289661	1.747699	1.959424
H	9.951072	2.627810	1.903272
H	8.561789	1.924905	2.770976
H	8.735860	1.673213	1.004368
C	9.108709	-0.743716	2.284535
H	9.603243	-1.666429	2.636515
H	8.703916	-0.938850	1.275174
H	8.241351	-0.552995	2.939123
C	11.842234	1.225624	7.938602
C	11.269531	2.350550	8.614000
C	11.752449	2.683520	9.892414
H	11.332981	3.552891	10.412781
C	12.771894	1.941176	10.504752
H	13.135521	2.219290	11.501813
C	13.323604	0.838247	9.834721
H	14.116198	0.259243	10.323178
C	12.881513	0.455569	8.553374
C	10.191960	3.214371	7.958271

H	9.742115	2.621589	7.143380
C	10.803375	4.468377	7.300535
H	10.011249	5.094533	6.849563
H	11.514615	4.191255	6.505521
H	11.348653	5.079400	8.042910
C	9.057159	3.599255	8.927567
H	8.636094	2.717794	9.444093
H	8.237841	4.094938	8.375564
H	9.401308	4.309866	9.701438
C	13.489037	-0.762306	7.856193
H	13.444851	-0.556257	6.772243
C	14.963922	-1.006368	8.222739
H	15.562601	-0.083358	8.145427
H	15.409576	-1.746972	7.535473
H	15.076417	-1.404275	9.249072
C	12.666875	-2.044457	8.097177
H	11.647126	-1.945358	7.693850
H	12.590339	-2.275191	9.176316
H	13.142232	-2.907439	7.594707
C	13.129999	1.070577	2.742121
C	13.887039	-0.149624	2.735107
C	14.917199	-0.296167	1.790814
H	15.490768	-1.231139	1.762924
C	15.245185	0.737443	0.894523
H	16.046949	0.597319	0.159151
C	14.543111	1.952648	0.954694
H	14.798831	2.757987	0.252331
C	13.482595	2.147430	1.867860
C	13.570950	-1.266203	3.732869
H	12.982771	-0.802470	4.546111
C	14.829593	-1.874568	4.379182
H	15.455776	-1.098079	4.846778
H	15.450694	-2.426418	3.649036
H	14.535444	-2.592187	5.166930
C	12.693921	-2.370964	3.109382
H	11.721155	-1.972505	2.779864
H	12.494074	-3.169082	3.847705
H	13.192106	-2.829711	2.234469
C	12.701411	3.463127	1.855651
H	11.884745	3.349149	2.593211
C	13.562423	4.655906	2.320681
H	13.839386	4.523227	3.380798
H	12.988914	5.598769	2.259002
H	14.460404	4.781957	1.683609
C	12.086941	3.765604	0.471241
H	11.478778	2.928511	0.089024
H	12.873654	3.974983	-0.277403
H	11.437666	4.658424	0.526506

C	14.113164	4.373353	6.308633
C	14.797198	5.590429	6.003210
H	14.775468	5.967037	4.972539
C	15.451125	6.325388	7.004042
H	15.954378	7.260981	6.729861
C	15.464251	5.888399	8.344380
H	15.957482	6.482350	9.122902
C	14.804000	4.682565	8.662826
H	14.767903	4.322024	9.700303
C	14.163665	3.928653	7.667116
H	13.648265	2.999829	7.929653
Fe	20.292301	2.195027	5.489211
K	17.180368	2.886786	7.540858
O	18.784863	3.422426	5.452491
N	21.300950	1.261485	4.148567
N	21.140467	1.402164	7.034791
C	23.148595	-0.374913	3.313709
C	22.307423	0.385538	4.399434
C	22.690512	0.097612	5.732989
H	23.552599	-0.563994	5.810366
C	22.197438	0.546154	6.977706
C	23.072568	0.140047	8.217223
C	24.636574	0.048793	3.453256
H	24.747124	1.133977	3.276031
H	25.257736	-0.483594	2.708170
H	25.047927	-0.171129	4.453018
C	23.005265	-1.900926	3.569973
H	21.947260	-2.207891	3.476191
H	23.350476	-2.198590	4.574222
H	23.594572	-2.470658	2.826569
C	22.765305	-0.148557	1.833573
H	22.890434	0.895583	1.509180
H	21.728336	-0.444190	1.613139
H	23.428193	-0.773855	1.206515
C	22.464618	0.395978	9.615805
H	21.550502	-0.191637	9.798976
H	22.223226	1.453643	9.793567
H	23.208010	0.095865	10.377731
C	24.377854	0.978922	8.126156
H	24.147106	2.058615	8.177283
H	24.913087	0.794706	7.178543
H	25.059003	0.734284	8.963903
C	23.423123	-1.371332	8.171336
H	22.506015	-1.987980	8.154585
H	24.004125	-1.648749	9.070333
H	24.031200	-1.650527	7.294768
C	20.886947	1.730202	2.876601
C	21.524052	2.871253	2.297777

C	21.027212	3.376506	1.082296
H	21.499625	4.261069	0.637126
C	19.928032	2.784674	0.437243
H	19.551851	3.199053	-0.506299
C	19.318432	1.652088	1.006708
H	18.468438	1.181023	0.495969
C	19.793121	1.096725	2.208790
C	22.689055	3.546511	3.016004
H	23.074864	2.820013	3.754804
C	22.192552	4.770184	3.813861
H	23.023649	5.253076	4.360175
H	21.436701	4.450479	4.555706
H	21.718788	5.518712	3.152984
C	23.847203	3.912419	2.070764
H	24.177486	3.038460	1.480043
H	24.713193	4.281865	2.650014
H	23.565287	4.711875	1.360497
C	19.144349	-0.140411	2.819824
H	19.854963	-0.539588	3.567531
C	17.870272	0.262111	3.578640
H	18.111028	1.060639	4.305166
H	17.438399	-0.580765	4.141818
H	17.098630	0.601349	2.863960
C	18.846215	-1.252786	1.799030
H	19.751549	-1.547126	1.238652
H	18.082480	-0.939613	1.062895
H	18.454378	-2.149129	2.314042
C	20.352630	1.691765	8.166856
C	19.425182	0.716623	8.682976
C	18.590473	1.085224	9.755452
H	17.883998	0.352293	10.163638
C	18.653436	2.370405	10.336130
H	18.001537	2.627719	11.180329
C	19.593902	3.299832	9.852211
H	19.674597	4.284621	10.331679
C	20.462940	2.979314	8.791275
C	19.377593	-0.685606	8.074401
H	20.425853	-0.965085	7.852161
C	18.637868	-0.688484	6.722983
H	19.077218	0.069753	6.047990
H	17.564922	-0.455268	6.844515
H	18.720191	-1.672475	6.226468
C	18.805518	-1.756091	9.016785
H	19.315436	-1.757167	9.997751
H	18.928115	-2.757841	8.567094
H	17.722879	-1.612352	9.191799
C	21.543924	3.960251	8.344121
H	22.175780	3.412283	7.619523

C	20.941222	5.162156	7.594423
H	20.385822	4.809235	6.710974
H	21.729493	5.854766	7.247575
H	20.244852	5.731295	8.239771
C	22.437748	4.415806	9.514789
H	22.873973	3.556173	10.054205
H	21.874390	5.021950	10.248823
H	23.269530	5.040693	9.140845
C	18.651490	4.542988	4.719168
C	18.307800	5.782521	5.326009
H	18.205466	5.831108	6.416079
C	18.096630	6.928674	4.544919
H	17.832740	7.871744	5.041647
C	18.219758	6.887757	3.142656
H	18.059426	7.791274	2.542645
C	18.567961	5.669289	2.529482
H	18.697893	5.603697	1.441272
C	18.778316	4.517574	3.302908
H	19.084088	3.578119	2.832606
N	15.646541	1.259789	5.869949
N	14.492795	1.242453	5.700188

D-N_2-bridge (filename K6*a*)

Fe	3.263936	0.193360	4.260589
N	4.552031	1.455611	4.483995
N	5.279760	2.338853	4.856915
Fe	6.734102	3.381139	5.206229
N	1.472097	0.477295	3.462561
N	3.618413	-1.600366	3.433472
C	-0.885035	-0.597064	3.509869
C	0.681235	-0.616292	3.335578
C	1.240559	-1.909795	3.191338
H	0.494316	-2.694225	3.105829
C	2.570425	-2.384107	3.081216
C	2.651564	-3.886447	2.614559
C	-1.586449	-1.739364	2.723394
H	-2.680613	-1.616477	2.813221
H	-1.352914	-2.743739	3.115984
H	-1.334960	-1.721164	1.647840
C	-1.609406	0.709036	3.103201
H	-2.693626	0.570092	3.269853
H	-1.462061	0.961890	2.041469
H	-1.296952	1.579995	3.692553
C	-1.124213	-0.848277	5.023571
H	-2.207995	-0.832357	5.245399
H	-0.633919	-0.083663	5.644248
H	-0.715496	-1.822687	5.340897
C	1.939038	-4.768787	3.680623

H	0.907611	-4.443407	3.892983
H	2.492523	-4.755613	4.636181
H	1.899364	-5.816706	3.329904
C	1.910443	-4.019678	1.255834
H	0.843176	-3.752434	1.329090
H	1.976370	-5.060911	0.888038
H	2.365958	-3.360047	0.496146
C	4.055644	-4.504317	2.422176
H	3.929363	-5.579316	2.195404
H	4.687831	-4.429811	3.320251
H	4.610578	-4.055628	1.585152
C	1.070052	1.807916	3.151070
C	0.762825	2.743649	4.182259
C	0.373212	4.047877	3.824481
H	0.129078	4.768509	4.616131
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H	-0.076423	5.441886	2.218992
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H	0.522488	3.828687	0.427450
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H	-0.825441	3.636644	6.427493
H	-0.565800	2.139282	7.366137
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C	1.498022	1.265633	0.666975
H	2.327406	0.683702	1.115353
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H	0.140397	-0.425970	1.029012
H	0.838073	-0.390561	-0.601663
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C	2.024837	2.005580	-0.577867
H	2.472960	1.285817	-1.286818
H	2.787686	2.763837	-0.328744
H	1.208212	2.515930	-1.121405
C	4.972425	-1.892099	3.153258
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H	6.118091	-4.304008	6.141001
C	4.577818	-1.210778	0.708999
H	3.525870	-1.301788	1.034766
C	4.895671	0.291770	0.576122
H	4.653245	0.838102	1.508227
H	4.317842	0.763832	-0.234436
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H	6.126804	7.282866	2.799176
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H	3.632912	3.300598	1.326367
H	3.023922	4.431229	2.552229
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H	5.633981	6.449174	0.708233
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C	9.863552	3.006601	3.083803
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H	9.831448	0.792665	3.158755
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C	10.924275	4.108033	2.902247
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C	5.904826	4.426804	7.736752
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C	5.167930	3.245822	9.750708
H	5.381015	2.552121	10.576546
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C	4.663635	5.152061	7.715263
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H	8.160163	3.207248	8.101565
C	7.464643	1.284383	8.709391
H	7.137676	1.043576	7.683611

H	6.802835	0.795871	9.453113
H	8.468163	0.835977	8.811121
C	8.214777	3.129857	10.259437
H	8.251904	4.214491	10.457735
H	9.252753	2.750338	10.250424
H	7.689532	2.652286	11.108084
C	4.450518	6.267319	6.688429
H	5.446800	6.716442	6.512874
C	3.530598	7.394882	7.185916
H	3.854195	7.788623	8.166907
H	2.480770	7.059557	7.283491
H	3.534818	8.230551	6.462947
C	3.975270	5.739878	5.318557
H	4.548245	4.849172	5.013579
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H	2.909174	5.456787	5.336648
O	7.903309	1.720716	5.476564
C	1.965280	-0.997676	6.778186
C	1.858520	-2.365652	6.404650
C	1.111532	-0.536066	7.821614
H	2.497243	-2.724775	5.595646
H	1.165737	0.521650	8.112236
C	0.946226	-3.221035	7.035621
C	0.193811	-1.397303	8.443526
H	0.888627	-4.270511	6.716525
H	-0.460098	-1.006544	9.234510
C	0.100312	-2.747465	8.057773
C	9.118108	1.661424	6.017261
C	9.845586	2.828617	6.393512
C	9.745810	0.400770	6.227443
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H	9.193606	-0.504664	5.943933
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C	11.029664	0.314248	6.785374
H	11.661071	3.651923	7.225356
H	11.486370	-0.673324	6.935586
C	11.735982	1.476760	7.152385
K	4.465528	1.309445	7.467410
K	7.048557	0.609501	3.218801
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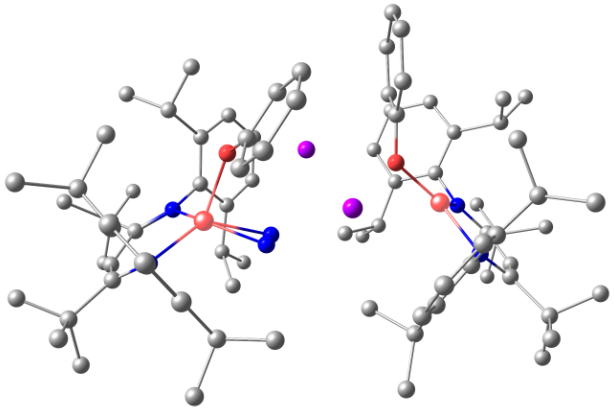
N_2 bound side-on to Fe1 inside bowl



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O       13.918233000      3.487172000      5.381393000
N       11.811177000      0.857500000      6.746756000
N       12.451492000      0.984701000      3.853476000
C        9.685436000     -0.582309000      7.194813000
C       10.804411000      0.077303000      6.300556000
C       10.678591000     -0.243172000      4.931632000
H        9.837389000     -0.897091000      4.716827000
C       11.339455000      0.229122000      3.770329000
C       10.548815000     -0.140311000      2.448552000
C        8.284540000     -0.273179000      6.594910000
H        8.131678000      0.815571000      6.494019000
H        7.498421000     -0.667279000      7.264976000
H        8.124494000     -0.728631000      5.603614000
C        9.934233000     -2.116491000      7.161354000
H       10.927917000     -2.363212000      7.575147000
H        9.893637000     -2.522428000      6.136099000
H        9.170694000     -2.639935000      7.766779000
C        9.603565000     -0.158486000      8.680343000
H        9.317891000      0.897155000      8.804095000
H       10.537793000     -0.311745000      9.234765000
H        8.825249000     -0.774210000      9.168460000
C       11.181904000      0.245478000      1.088806000
H       12.096083000     -0.323258000      0.860722000
H       11.427524000      1.312146000      1.005600000
H       10.448877000      0.013713000      0.294124000
C        9.176543000      0.591705000      2.539579000
H        9.312362000      1.678969000      2.667586000
H        8.573249000      0.237143000      3.391392000
H        8.593940000      0.424704000      1.614435000
C       10.281317000     -1.670762000      2.381858000
H       11.223394000     -2.247577000      2.380687000
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C	8.661670000	3.573153000	7.422124000
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H	15.368609000	1.118414000	9.045337000
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H	14.991541000	0.283317000	10.576736000
C	12.972572000	-1.328514000	9.679730000
H	12.015152000	-1.656250000	9.244605000
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C	14.016730000	-1.187875000	2.591808000
H	12.949982000	-1.426789000	2.422958000
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*
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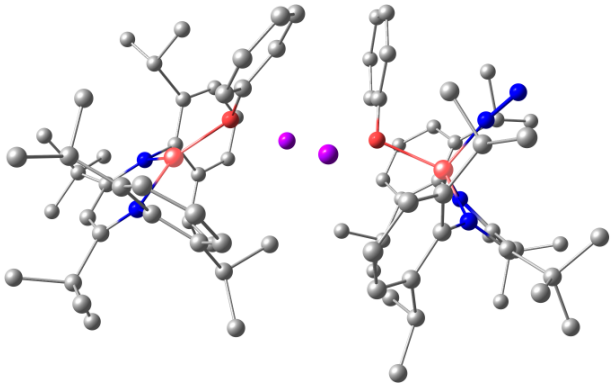
N_2 bound end-on to Fe2 outside of bowl



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C	20.027714000	1.652630000	0.343550000
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C	22.550053000	3.237850000	2.761617000
H	22.726341000	2.953625000	3.813513000
C	22.082409000	4.707256000	2.737068000
H	22.818294000	5.355091000	3.245209000
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H	18.853317000	-2.844875000	3.227734000
C	19.850887000	1.513965000	8.445887000
C	19.113572000	0.331077000	8.808104000
C	18.094501000	0.436508000	9.773457000
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H	17.012925000	1.707107000	11.174944000
C	18.563174000	2.791358000	10.099473000
H	18.382582000	3.730263000	10.640329000
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C	19.491348000	-1.019498000	8.198062000
H	20.597165000	-1.059963000	8.185110000
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C	19.685915000	5.072155000	8.171018000
H	19.300268000	4.677104000	7.215291000
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H	18.840887000	5.449180000	8.779838000

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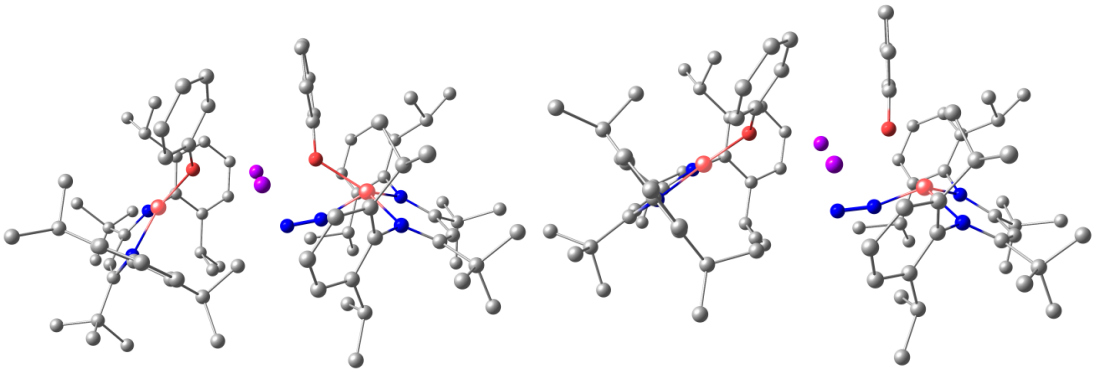
H       21.808875000      5.319767000      9.966205000
C       18.581030000      3.988490000      4.222358000
C       18.649375000      5.356576000      4.603558000
H       18.697018000      5.606721000      5.666418000
C       18.655830000      6.378657000      3.645214000
H       18.710513000      7.422925000      3.979504000
C       18.596505000      6.084456000      2.268949000
H       18.604528000      6.889826000      1.525304000
C       18.563292000      4.738543000      1.869549000
H       18.570478000      4.470037000      0.805674000
C       18.563678000      3.710240000      2.826741000
H       18.619534000      2.663217000      2.503255000
N       22.099175000      4.732133000      5.952998000
N       21.369056000      3.869943000      5.748399000
*
```

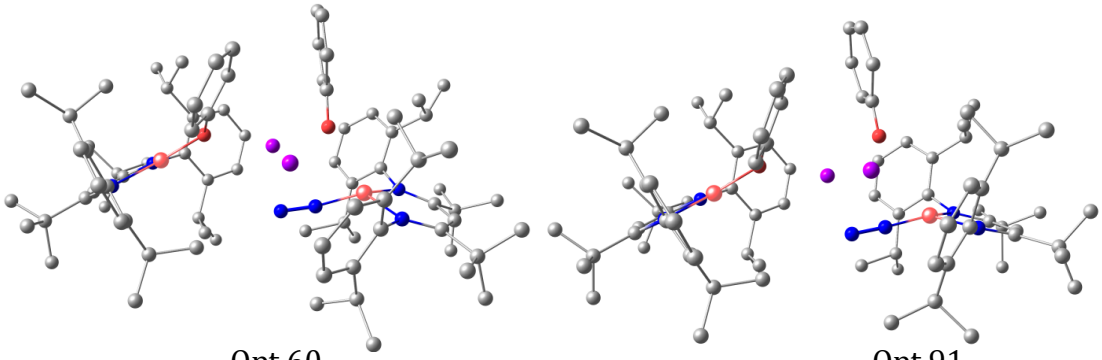
Table S-3. Electronic energies of optimized alternative binding modes of N_2 to **D** in kcal/mol.

N_2 Complex	**E_{elec} (kcal/mol)**
D + N_2	-4666869.83
D (constrained Fe-Fe) + N_2	-4666869.61
D-N_2 (N_2-end-on-Fe1-inside)	-4666891.24
N_2-side-on-Fe1-inside	-4666877.56
N_2-end-on-Fe2-outside	-4666888.09
D-N_2-bridge	-4666914.36

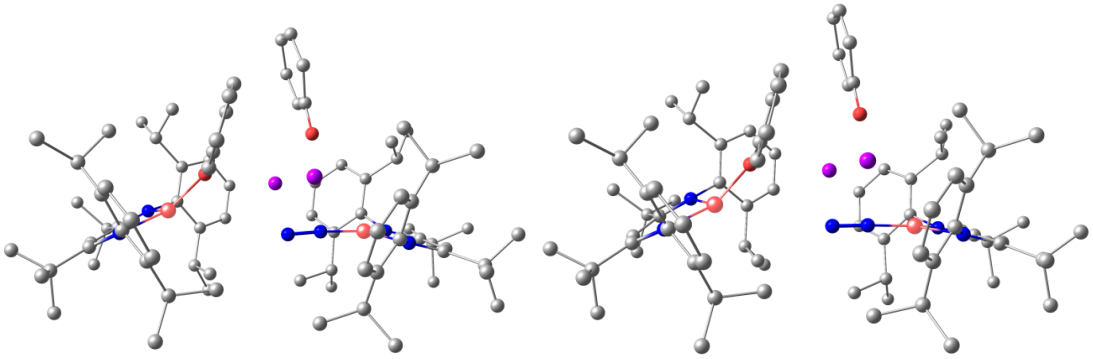
Figure S-3. Optimization of N_2 bound end-on on Fe2 with phenoxide dissociating
When N_2 was bound end-on to Fe2 in the bowl of complex **D**, the optimization iterations revealed the Fe2-phenoxide ligand dissociating. Below are selected structures along the geometry optimization followed by a table with bond lengths of interest. As the optimization progresses, the N-N bond length and the Fe2-OPh bond length increase while the Fe2-N2 and Fe1-N1 distances decrease. Fe2 starts as tetrahedral but as the Fe2-N2 interaction decreases, the geometry changes toward trigonal pyramidal. The axial OPh dissociates to form a trigonal plane at Fe2. As the OPh moves away from the core of the complex, Fe1 goes from a trigonal planar geometry to trigonal pyramidal to open a coordination site for the N_2 ligand, reducing the Fe1-N1 distance. Through the majority of the iterations the Fe1-N1 distance fluctuates but does not begin to contract until OPh is far from Fe2. We attribute these fluctuations from the loose structure described in the paper. No local minimum was found in this calculation. The spontaneous dissociation of OPh, followed by the contraction of the FeNNFe core, is consistent with **D-N_2-bridge** being a local minimum on the way to KOPh dissociation and formation of **N**.



Opt 1 Opt 30



Opt 60 Opt 91



Opt 120 Opt 137

	N1-N1, Å	N2-Fe2, Å	N1-Fe1, Å	Fe2-OPh, Å
Opt 1	1.16	1.78	4.62	2.03
Opt 30	1.19	1.74	4.63	2.21
Opt 60	1.19	1.73	4.58	2.58
Opt 91	1.19	1.71	4.90	3.25
Opt 120	1.21	1.68	4.29	3.97
Opt 137	1.21	1.69	4.00	4.23

Table S4. Point energies of the BP86 geometries at the B3LYP/def2-SVP(Fe:def2-TZVP) level were calculated, and they are consistent with the conclusions drawn from the BP86 calculations described above. Doing frequency calculations to derive enthalpies and entropies was not feasible using the B3LYP functional.

Compound	E (Hartrees)	E (kcal/mol)	E_{rel}(kcal/mol)
D	-7323.385476	-4595497.6	0
D-constrained	-7323.387415	-4595498.8	-1.2
D-N_2	-7432.88602	-4664210.3	
D-N_2 – (**D** + N_2)			-11.4
D-N_2-bridge	-7432.909462	-4664225.0	
D-N_2-bridge – (**D** + N_2)			-26.1
M	-4128.819021	-2590875.2	
M-N_2	-4238.320333	-2659588.4	
M-N_2 – (**M** + N_2)			-11.8
N_2	-109.4824303	-68701.3	

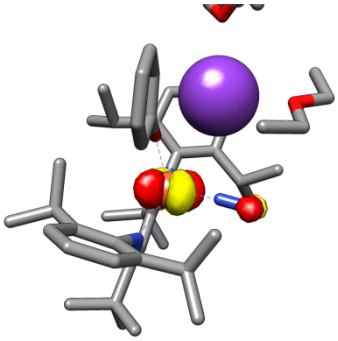
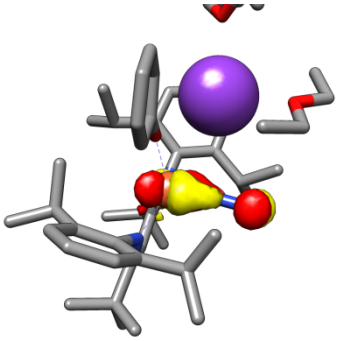
Key orbitals of N_2 complexes. Point calculations at the B3LYP/def2-SVP(Fe:def2-TZVP) level were used to plot key orbitals. Orbital plots were created using the orca_plot module, and visualized using CHIMERA.[9] Quasirestricted orbitals are shown, unless otherwise indicated. Because of the relatively small basis set used for the ligands, these details should be considered tentative.

Table S5. Mulliken charges and spin populations on key atoms in **M-N_2.**

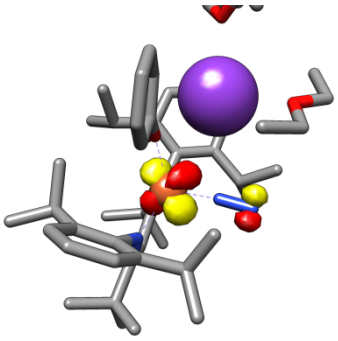
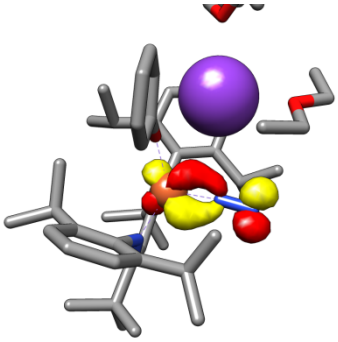
atom	charge	spin
Fe	+0.62	+3.24
K	+0.49	0
O	-0.53	+0.04
N (internal)	-0.10	-0.01
N (terminal)	-0.23	-0.36

Figure S-4. Frontier orbitals of **M-N_2** with substantial *d* character. For orbitals 231 and 232, the overlap between the alpha and beta electrons was relatively low (0.92-0.93), suggesting contribution from a resonance structure with a radical on N_2 antiferromagnetically coupled to high-spin iron(II).[10] This picture is supported by the spin and charge on the N_2 indicated in Table S3.

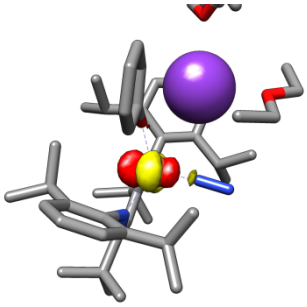
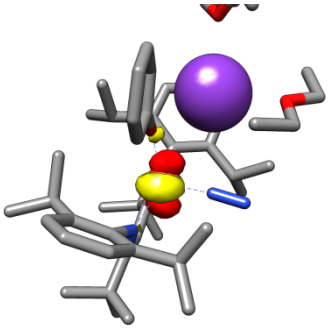
231 (alpha) (beta)

232 (alpha) (beta)

233 234

235

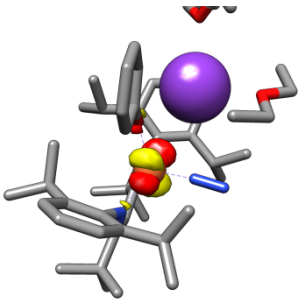
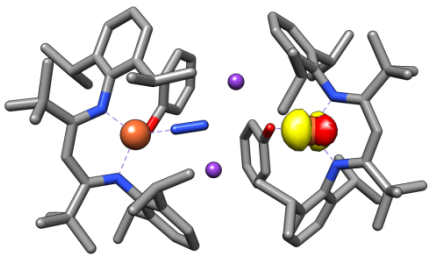


Table S-4. Mulliken charges and spin populations on key atoms in **D-N_2.**

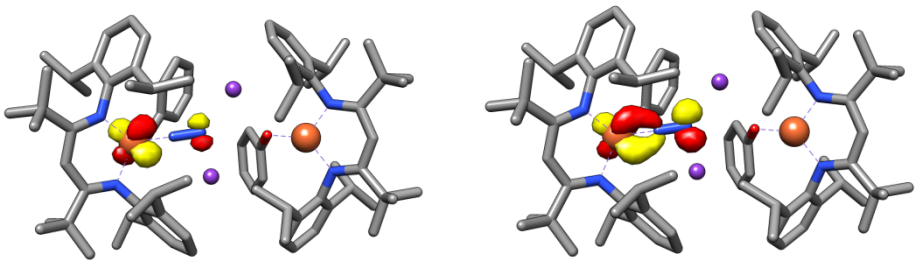
atom	charge	spin
Fe	+0.51	+3.08
Fe (bound to N_2)	+0.64	+3.30
K (same for both)	+0.52	0
O	-0.57	+0.02
O (on Fe bound to N_2)	-0.47	+0.05
N (internal)	-0.07	-0.07
N (terminal)	-0.28	-0.41

Figure S-5. Frontier orbitals of **D-N_2** with substantial *d* character. For orbitals 372-374, the overlap between the alpha and beta electrons was relatively low (~0.90). The occupation of the N_2 π* orbital in orbitals 372 and 374 suggests a contribution from a resonance structure with a radical on N_2 antiferromagnetically coupled to high-spin iron(II).[10] This picture is supported by the spin and charge on N_2 in Table S4.

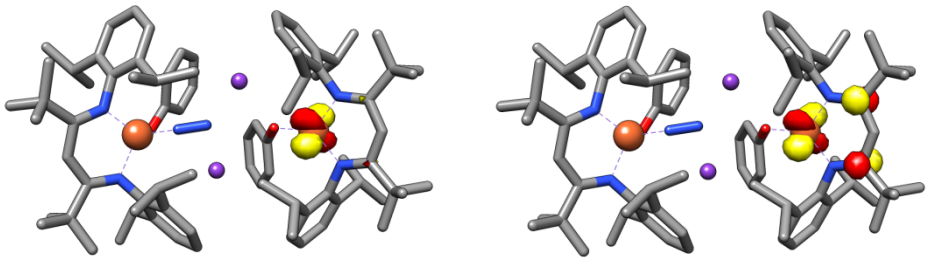
371



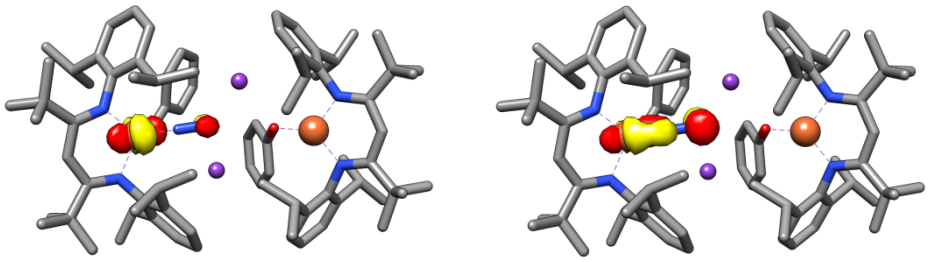
372 (alpha) (beta)



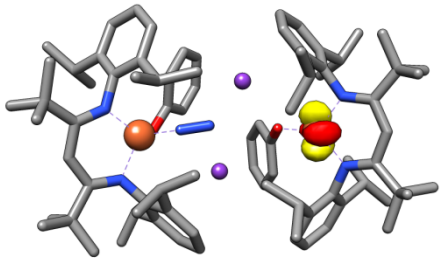
373 (alpha) (beta)



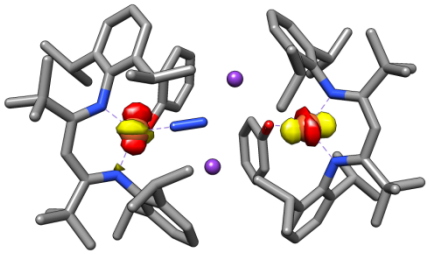
374 (alpha) (beta)



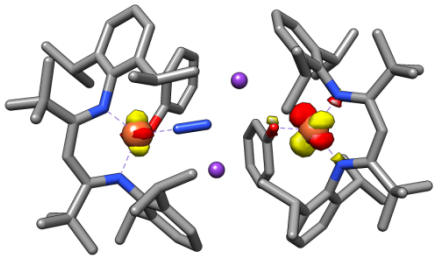
375



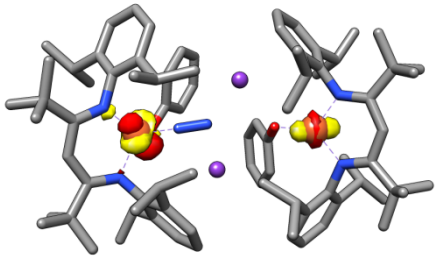
376



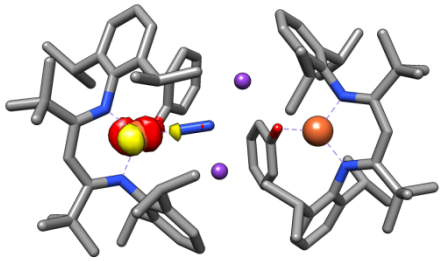
377



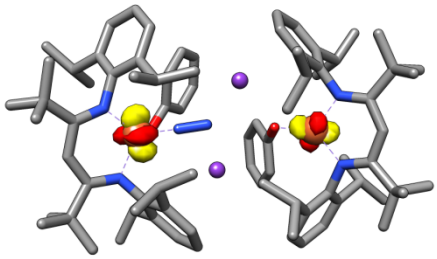
378



379



380



References

[1] Schubert, E. M. *J. Chem. Educ.* **1992**, *69*, 62.

[2] Chiang, K. P.; Barrett, P. M.; Ding, F.; Smith, J. M.; Kingsley, S.; Brennessel, W. W.; Clark, M. M.; Lachicotte, R. J.; Holland, P. L. *Inorg. Chem.* **2009**, *48*, 5106.

[3] Chiang, K. P.; Scarborough, C. C.; Horitani, M.; Lees, N. S.; Ding, K.; Dugan, T. R.; Brennessel, W. W.; Bill, E.; Hoffman, B. M.; Holland, P. L. *Angew. Chem., Int. Ed.* **2012**, *51*, 3658. Rodriguez, M. M.; Stubbert, B. D.; Scarborough, C. C.; Brennessel, W. W.; Bill, E.; Holland, P. L. *Angew. Chem., Int. Ed.* **2012**, *51*, 8247. Yu, Y.; Smith, J. M.; Flaschenriem, C. J.; Holland, P. L. *Inorg. Chem.* **2006**, *45*, 5742.

[4] Neese, F. *ORCA,* current manual and description available at http://cec.mpg.de/forum/.

[5] Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098. Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822.

[6] (a) Neese, F.; Wennmohs, F.; Hansen, A.; Becker, U. *Chem. Phys.* **2009**, *356*, 98-109; (b) Kossmann, S.; Neese, F. *Chem. Phys. Lett.* **2009**, *481*, 240-43.

[7] (a) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1993**, *99*, 4597. (b) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1994**, *101*, 9783. (c) van Lenthe, E.; van Leeuwen, R.; Baerends, E. J.; Snijders, J. G. *Int. J. Quantum Chem.* **1996**, *57*, 281.

[8] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

[9] Pettersen, E. F.; Goddard, T. D.; Huang, C. C.; Couch, G. S.; Greenblatt, D. M.; Meng, E. C.; Ferrin, T. E. *J. Comput. Chem.* **2004** , *25*, 1605.

[10] Dugan, T. R.; Bill, E.; MacLeod, K. C.; Christian, G. J.; Cowley, R. E.; Brennessel, W. W.; Ye, S.; Neese, F.; Holland, P. L. *J. Am. Chem. Soc.* **2012**, *134*, 20352.