Supporting Information

for

Iron(II) Hydride Complex of a Ligand with two Adjacent *β*-Diketiminate Binding sites and its Reactivity

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1. Experimental Procedure

[(PYR)$_2$Fe$_4$(μ-O)(μ-H)$_2$] (3). Slow evaporation of the volatiles from a benzene-d_6 solution of **2** (presumably containing traces of water) led to the formation of dark brown crystals of **3**. IR (KBr): $\tilde{\nu}$ = 3056 (w), 2961 (s), 2925 (m), 2866 (m), 1640 (w), 1579 (m), 1521 (s), 1458 (s), 1430 (s), 1405 (s), 1374 (vs), 1356 (vs), 1321 (s), 1266 (s), 1223 (s), 1183 (s), 1152 (s), 1099 (m), 1055 (m), 1018 (s), 935 (m), 836 (m), 825 (m), 795 (m), 759 (s), 729 (w), 707 (w), 627 (m) cm^{-1}; elemental analysis calcd (%) for $C_{78}H_{104}N_{10}OFe_4$ (1421.14 gmol^{-1}): C 65.92, H 7.38, N 9.86;found (%): C 64.90, H 7.09, N 9.01.

[(PYR)Fe$_2$(μ-CH$_3$COO)$_2$] (5'). [(PYR)Fe$_2$(μ-Br$_2$] (**1**) (80.0 mg, 93 µmol) was stirred together with potassium acetate (18 mg, 186 µmol) in tetrahydrofuran for 16 h at room temperature. The reaction mixture was filtered and the solvent was removed under reduced pressure. Extraction of the residue with *n*-hexane and cooling to −30 °C afforded **5'** as red crystals (27 mg, 33 µmol, 36%). ^{1}H NMR (400 MHz, C_6D_6): δ = 71.68 (6H, CH_3COO), 26.27 (1H, C$H_{4\text{-Pyr}}$), 19.68 (4H, CH_{Ar}), 5.45 (12H, CH(CH_3)$_2$), −3.36 (12H, CH(CH_3)$_2$), −4.23(4H, CH(CH$_3$)$_2$), −25.93 (2H, CH_{Ar}), −44.56 (6H, CH_3), −45.03 (6H, CH_3) ppm; IR (KBr): $\tilde{\nu}$ = 3057 (w), 2960 (s), 2927 (m), 2867 (m), 1637 (m), 1599 (s), 1570 (s), 1555 (s), 1513 (s), 1437 (vs), 1406 (vs), 1392 (vs), 1381 (vs), 1356 (vs), 1322 (s), 1274 (s), 1225 (s), 1183 (m), 1161 (m), 1056 (w), 1021 (m), 935 (w), 787 (m), 760 (m), 734 (w), 706 (w), 654 (w), 624 (w)cm^{-1}; elemental analysis calcd (%) for $C_{43}H_{57}N_5O_4Fe_2$ (819.65 gmol^{-1}): C 63.01, H 7.01, N 8.54; found (%): C 63.00, H 7.27, N 8.10.

2. ^{1}H NMR Spectroscopic Data

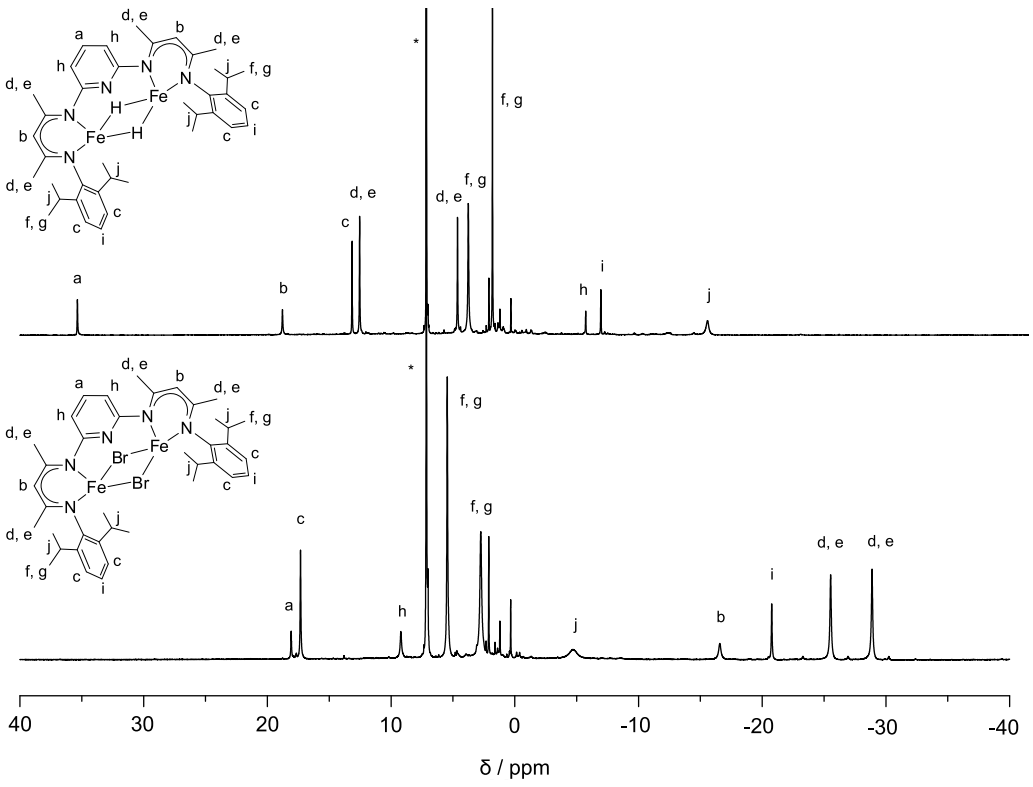


Fig. S1 ^{1}H NMR spectra of [(PYR)Fe$_2$(μ-Br)$_2$] (**1**) (bottom) and [(PYR)Fe$_2$(μ-H)$_2$] (**2**) (top), measured for C_6D_6 solutions (*). In case of the CH_3 groups belonging to the *i*Pr residues only two representatives are labelled.

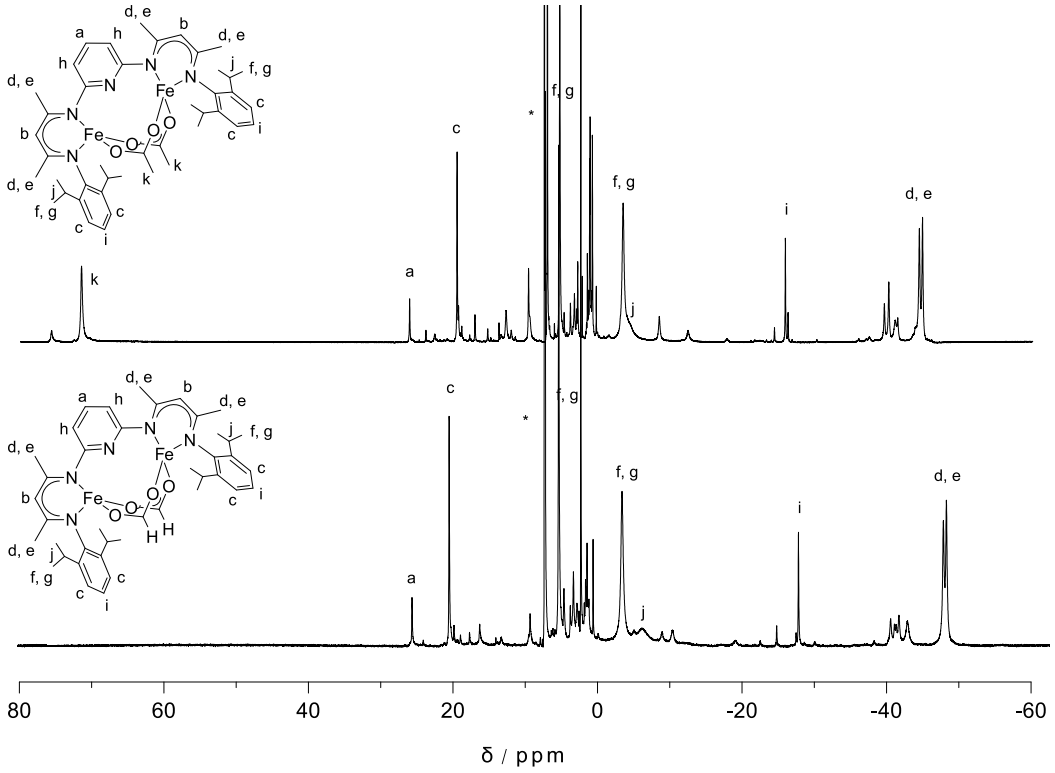


Fig. S2 ^{1}H NMR spectra of [(PYR)Fe$_2$(μ-HCOO)$_2$] (**5**) (bottom) and [(PYR)Fe$_2$(μ-CH$_3$COO)$_2$] (**5'**) (top), measured for C_6D_6 solutions (*). In case of the CH_3 groups belonging to the *i*Pr residues only two representatives are labelled.

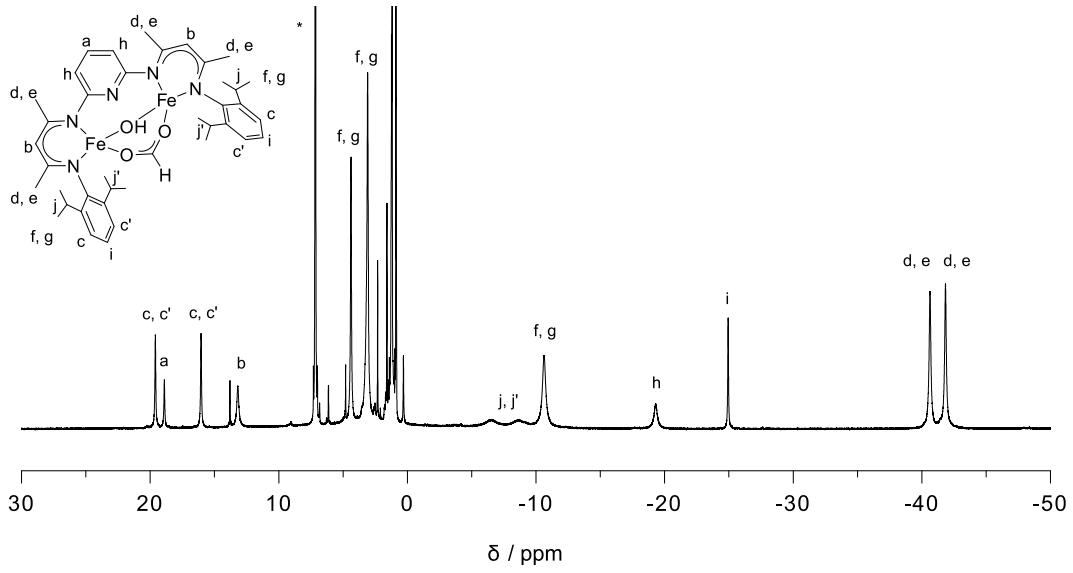


Fig. S3 ^{1}H NMR spectrum of [(PYR)Fe$_2$(μ-HCOO)(μ-OH)] (**6**) measured for C_6D_6 solutions (*). In case of the CH_3 groups belonging to the *i*Pr residues only two representatives are labelled.

3. Mößbauer Data

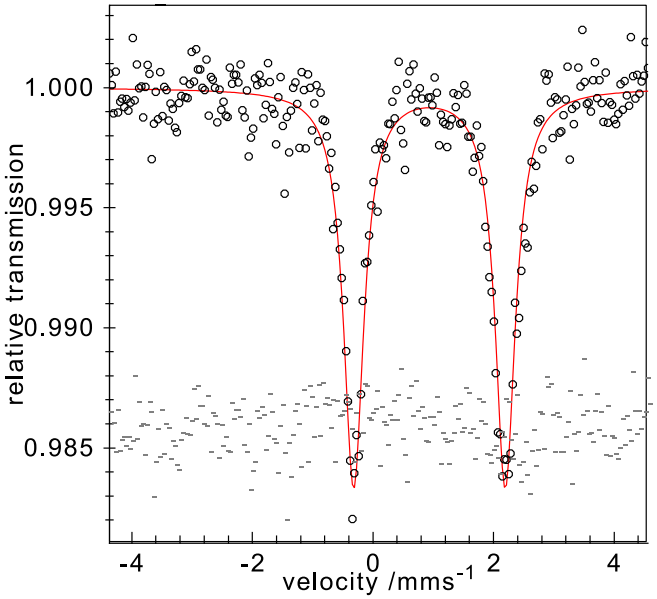


Fig. S4 Mößbauer spectrum of solid [(PYR)$Fe_2(\mu\text{-Br})_2$] (**1**) at 80 K. The simulation shows one doublet for **1** with an isomeric shift of δ = 0.94 mms^{-1} and a quadrupole splitting of ΔE_Q = 2.51 mms^{-1} (representing 100% of the total iron).

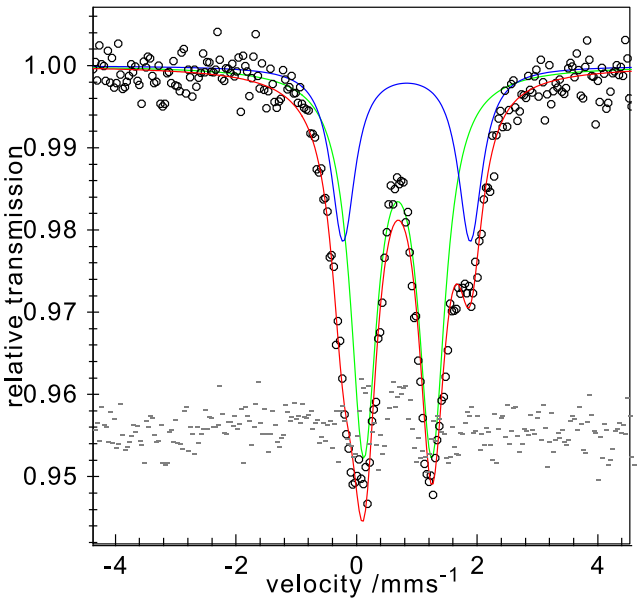


Fig. S5 Mößbauer spectrum of solid [(PYR)$Fe_2(\mu\text{-H})_2$] (**2**) at 80 K. The simulation shows one doublet for **2** with an isomeric shift of δ = 0.68 mms^{-1} and a quadrupole splitting of ΔE_Q = 1.13 mms^{-1} (representing 70% of the total iron) and a second doublet for another species with an isomeric shift of δ = 0.83 mms^{-1} and a quadrupole splitting of ΔE_Q = 2.11 mms^{-1} (30% of the total iron).

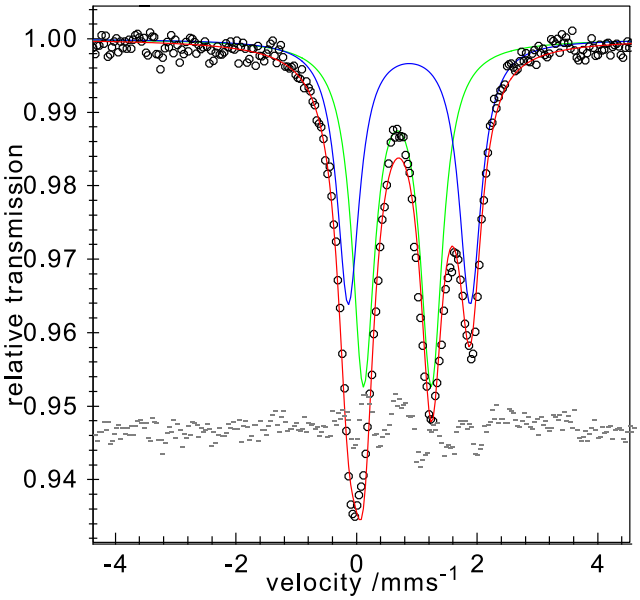


Fig. S6 Mößbauer spectrum of solid [(PYR)$Fe_2(\mu\text{-H})_2$] (**2**) at 80 K. The simulation shows one doublet for **2** with an isomeric shift of δ = 0.68 mms^{-1} and a quadrupole splitting of ΔE_Q = 1.13 mms^{-1} (representing 56% of the total iron) and one second doublet for another species (44% of the total iron) with an isomeric shift of δ = 0.87 mms^{-1} and a quadrupole splitting of ΔE_Q = 2.02 mms^{-1}.

4. Crystallographic Data

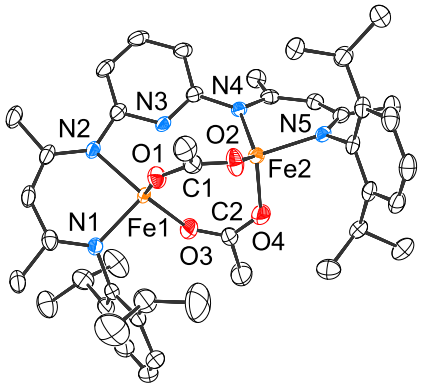


Fig. S7 Molecular structure of [(PYR)$Fe_2(\mu\text{-}CH_3COO)_2$] (**5'**); ellipsoids are set at 50% probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths /Å and angles /°: Fe1-N1 2.056(2), Fe1-N2 2.030(2), Fe1-O1 2.0674(19), Fe1-O3 1.980(2), Fe2-N4 2.002(2), Fe2-N5 2.028(2), Fe2-O2 1.9577(19), Fe2-O4 2.031(2), C1-O1 1.250(3), C1-O2 1.257(3), C2-O3 1.247(3), C2-O4 1.246(3), Fe1···Fe2 3.4741(7), N1-Fe1-N2 88.86(8), O1-Fe1-N1 103.22(8), O1-Fe1-N2 97.37(8), O1-Fe1-O3 120.88(8), N1-Fe1-O3 97.78(8), N2-Fe1-O3 137.97(9), Fe1-O1-C1 137.24(19), Fe1-O3-C2 143.1(2), O1-C1-O2 125.0(3), O3-C2-O4 124.9(3), Fe2-O2-C1 130.69(17), Fe2-O4-C2 127.22(19), N4-Fe2-N5 93.93(8), O2-Fe2-N4 128.80(9), O2-Fe2-N5 105.23(8), O2-Fe2-O4 114.99(10), O4-Fe2-N4 105.66(9), O4-Fe2-N5 103.13(8).

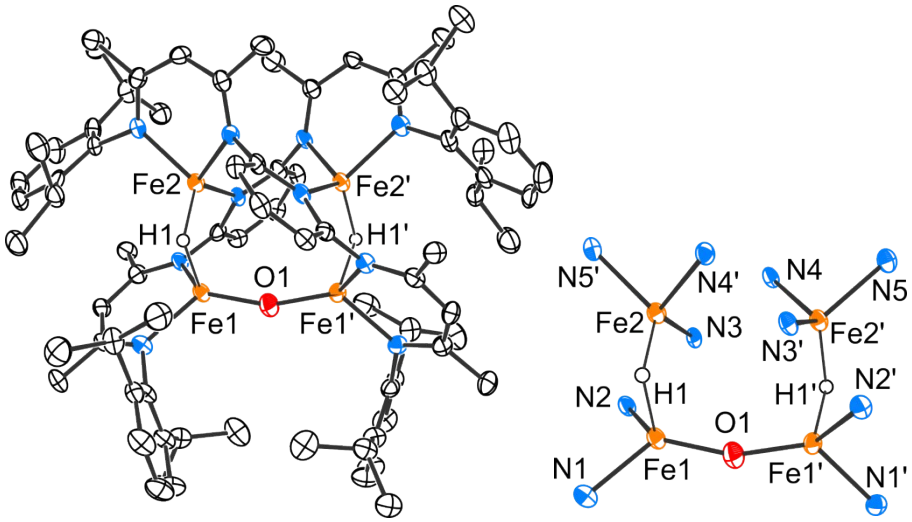
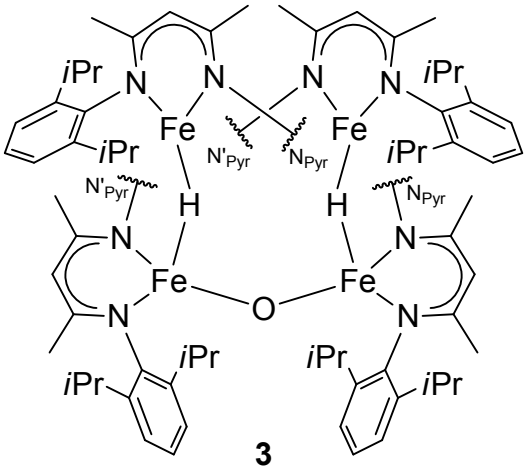


Fig. S8 Molecular structure of $[(PYR)_2Fe_4(\mu\text{-}O)(\mu\text{-}H)_2]$ (**3**) (left) and the truncated core (right); ellipsoids are set at 50% probability. Hydrogen atoms beside the bridging hydride ligands have been omitted for clarity. Selected bond lengths /Å and angles /°: Fe1–N1 2.003(4), Fe1–N2 2.051(3), Fe1–H1 1.75(5), Fe1–O1 1.7756(12), Fe2–N3 2.124(4), Fe2–N4' 2.027(3), Fe2–N5' 2.060(4), Fe2–H1 1.66(5), Fe1···Fe2 2.7922(10), Fe1···Fe1' 3.4988(13), Fe2···Fe2' 3.6658(13), Fe1-H1-Fe2 110(2), Fe1-O1-Fe1' 160.3(3), N1-Fe1-N2 92.88(15), H1-Fe1-N2 100.8(14), H1-Fe1-O1 101.8(15), N1-Fe1-O1 127.3(2), H1-Fe2-N5' 122.9(16), N4'-Fe2-N5' 90.43(15), N3-Fe2-N4' 118.26(15), H1-Fe2-N3 110.9(16).



3

Compound **3** crystallizes in a monoclinic space group (C_2/c) with four molecules in the asymmetric unit cell. One half of each molecule is generated by symmetry operation (C_2). All iron centers in **3** are surrounded by their ligands in a tetrahedral geometry. Fe2 is coordinated by three nitrogen atoms, two of the *β*-diketiminate binding pocket (N4' and N5') and one of the pyridine ring (N3). Additionally, Fe2 is bridged by one hydride ligand to Fe1. Fe1 is further coordinated by the two nitrogen atoms of one *β*-diketiminate binding pocket (N1 and N2) and by one bridging oxo ligand. The hydride ligands could be located from the electron density difference map. The Fe-H distances (1.75(5) Å and 1.66(5) Å) are slightly longer compared to the Fe-H distances in *β*-diketiminate iron(II) hydride complexes (**I**; 1.40 − 1.56 Å),[1] but still in the range of Fe-H bond lengths found for other dinuclear iron hydride compounds (1.51 − 1.94 Å).[2] The Fe-H-Fe angle amounts to 110(2)°. The Fe1···Fe2 distance is 2.7922(19) Å, which is much shorter compared to the corresponding value of the precursor compound 1 (3.0332(7) Å). Regarding the Fe1-O1 distance of 1.7756(12) Å and the almost linear Fe1-O1-Fe1' angle of 160.3(3)° the possibility of a hydroxo bridge can be excluded: For instance, Fe-O distances of 1.95 − 2.08 Å are reported for μ-hydroxo diiron complexes.[3] Furthermore the observed values for **3** fit very well to the metric data reported by Holland and coworkers for the only known structurally characterized $Fe^{II}(\mu\text{-}O)Fe^{II}$ moiety (Fe-O 1.7503(4) Å; Fe-O-Fe 167.55(14)°).[4]

5. XAS

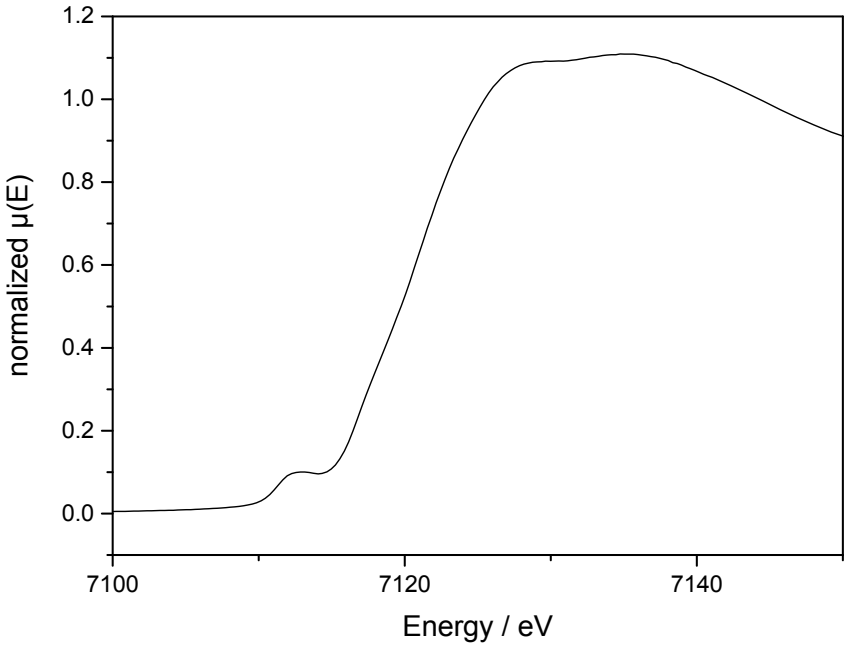


Fig. S9 XANES spectrum of complex **2**.

Sample 2 vs DFT					Fe-N			Fe-Fe			Fe••C			Fe••C			Fe••N			Fe•••C		
fit	R-factor	red. Chi-sq.	ΔE_0	R range	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²	n	r	σ²
1	0.194	802.78	3.227	1 - 2.5	2	2.03	1.0															
2	0.036	218.83	1.960	1 - 2.5	2	2.02	0.8	1	2.54	7.6												
3	0.004	27.13	1.748	1 - 2.5	3	2.03	3.3	1	2.54	8.1												
4	0.033	45.46	1.720	1 - 5.0	3	2.03	3.3	1	2.54	8.2												
5	0.031	47.51	2.195	1 - 5.0	3	2.03	3.3	1	2.55	8.3	4	3.08	47.7									
6	0.018	31.42	2.009	1 - 5.0	3	2.03	3.3	1	2.54	8.2	4	4.60	3.4	9	3.92	72.7						
7	0.018	35.01	1.340	1 - 5.0	3	2.02	3.3	1	2.54	8.2	4	3.34	13.6	9	3.73	27.9	2	4.57	0.9			
8	**0.017**	**37.52**	**2.167**	**1 - 5.0**	**3**	**2.03**	**3.3**	**1**	**2.55**	**8.2**	**4**	**3.07**	**79.8**	**9**	**3.92**	**48.0**	**2**	**4.58**	**1.0**	**9**	**5.19**	**24.8**
DFT					3	2.19		1	2.61		4	2.95		9	3.88		2	4.53		9	4.86	

Table S1 Summary of EXAFS fitting for **2**. Bold line represents the best fit for the system (fit 8). r is in units of Å; σ² is in units of 10^{-3} Å; ΔE_0 is in units of eV; R represents the goodness of the fit (GOF) and is defined $R = \frac{\sum_i^N [\chi_{dat}(R_i) - \chi_{th}(R_i)]^2}{\sum_i^N [\chi_{dat}(R_i)]^2}$ (value from ifeffit package); reduced chi-square is a second GOF-factor defined by $\chi_\vartheta^2 = \chi^2/(N - N_{vars})$ and $\epsilon^2 = \frac{1}{N}\sum_i^N [\chi_{dat}(R_i) - \chi_{th}(R_i)]^2 / (\chi_{dat}(R_i))^2$. Fourier transform range: 2 - 12 Å^{-1}. The fit was optimzied in R space with a k-weight of 3. The fitting range is 1.0-2.5 and 1.0-5.0 for fits 1-3 and 4-8, respectively.

6. Density Functional Calculations

Geometry optimizations were performed in redundant internal coordinates without symmetry restrictions for different spin states of [PYR)$Fe_2(\mu\text{-H})_2$] (**2**) using the Gaussian09 program package.[5] The molecular structure of [(PYR)$Fe_2(\mu\text{-Br})_2$] (**1**) as determined by X-ray diffraction analysis, with the bromide ligand substituted by hydrido ligands, was used as starting geometry. The B3LYP functional[6] was employed together with def2 basis sets, taken from the EMSL Basis Set Exchange Database[7]: the def2-TZVPD basis set[8] was used for Fe, N, and the two bridging hyride ligands H1 and H2. For all remaining C and H atoms, the def2-SVP basis set[9] was employed. Very tight convergence criteria were chosen for the SCF procedure and a pruned (99,590) "ultrafine" integration grid was used for numerical integrations. Visualisation of molecular structures was accomplished with the program Gauss View (Gaussian, Inc.).

An open-shell singlet state, where four unpaired electrons per iron center couple antiferromagnetically, was found to represent the ground state. The corresponding nonet state with a ferromagnetic coupling of the 2x4 unpaired electrons is 19.9 kJ/mol higher in energy. In contrast to the structure of **1** there is no C_2 axis in the structure of **2**. To simulate the effect of the solvent Toluene, for all spin states a reoptimisation has been done employing the Polarizable Continuum Model (PCM) as implemented in Gaussian, resulting in minor structural changes (table S2, S3).

spin state	Mulliken atomic spin density	rel. energy (kJ/mol)	rel. energy (kJ/mol) in Toluene
singlet (closed shell)	0	228.5	230.6
triplet	Fe1:-0.01, Fe2: 2.08	141.5	144.7
quintet	Fe1: 0.18, Fe2: 3.71	58.7	58.6
septet	Fe1: 3.76, Fe2: 2.17	36.6	36.8
nonet	Fe1: 3.82, Fe2: 3.82	19.9	19.0
singlet (open-shell)	Fe1: 3.70, Fe2:-3.70	0	0

Table S2. Relative electronic energies of different spin states of **2** (each at optimised geometry) and Mulliken atomic spin densities at the Fe atoms.

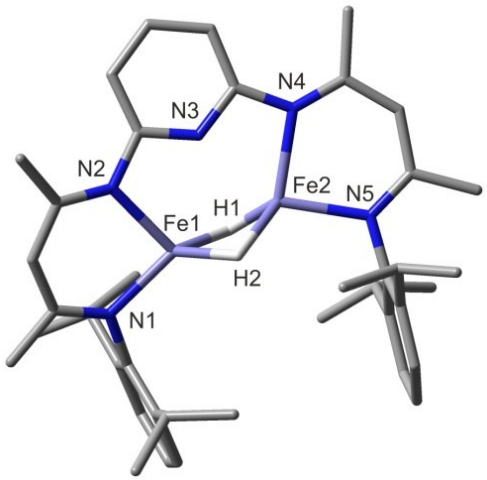


Fig. S10. Calculated molecular structure of [PYR)$Fe_2(\mu\text{-H})_2$] (**2**), B3LYP/Def2-SVP/Def2-TZVPD (open-shell singlet). Hydrogen atoms apart from H1, H2 have been omitted for clarity.

bond lengths /Å and angles /°	isolated molecule	molecule in Toluene (PCM)
Fe1-N1	2.045	2.053
Fe1-N2	2.090	2.098
Fe1-N3	2.431	2.420
Fe1-H1	1.786	1.796
Fe1-H2	1.813	1.821
Fe1···Fe2	2.607	2.626
Fe2-N5	2.029	2.033
Fe2-N4	2.072	2.076
Fe2-N3	2.606	2.642
Fe2-H1	1.791	1.794
Fe2–H2	1.766	1.772
N1-Fe1-N2	90.3	89.9
H1-Fe1-N1	120.3	120.2
H1-Fe1-N2	133.5	133.8
N1-Fe1-H2	120.7	121.2
N2-Fe1-H2	116.7	116.9
H1-Fe1-H2	79.0	78.9
Fe1-H1-Fe2	93.6	94.0
N4-Fe2-N5	91.5	91.4
H1-Fe2-N5	124.4	125.5
H1-Fe2-N4	112.9	112.3
N5-Fe2-H2	125.5	126.8
N4-Fe2-H2	125.6	123.5
H1-Fe2-H2	80.1	80.2
Fe1-H2-Fe2	93.5	93.9

Table S3. Selected bond lengths /Å and angles /° of the open-shell singlet ground state of **2**.

Cartesian coordinates (Å) for the optimised theoretical structure of [PYR)$Fe_2(\mu\text{-}H)_2$] (**2**):

Open-shell singlet state (in toluene), E = -4318,48368571 hartree

	x	y	z
Fe	-1.379984	0.814902	0.062246
Fe	1.232944	0.781801	-0.201102
N	3.107202	0.017757	-0.391316
N	1.908187	2.690149	-0.659662
N	-0.265425	2.956400	-0.112185
N	-2.388159	2.611205	0.461476
N	-3.139095	-0.218013	0.289876
C	4.133405	0.658172	-0.931499
C	4.076733	1.996697	-1.405353
C	5.467991	-0.047168	-1.065143
C	3.064474	2.961478	-1.276420
C	3.258714	-1.312518	0.121475
C	3.352415	4.312333	-1.902280
C	3.618331	-1.494484	1.482772
C	2.976808	-2.426927	-0.710120
C	0.896031	3.586877	-0.329872
C	3.694403	-2.801572	1.984517
C	3.901353	-0.316335	2.414459
C	3.069130	-3.712429	-0.155978
C	2.568862	-2.272948	-2.174533
C	-1.392560	3.566709	0.297182
C	0.977279	4.980260	-0.114461
C	3.425329	-3.906181	1.177406
C	2.805902	-0.173299	3.487563
C	5.294847	-0.401460	3.062673
C	3.558183	-2.964750	-3.130613
C	1.135447	-2.778562	-2.417360
C	-1.383728	4.963391	0.501709
C	-0.179762	5.640809	0.295858
C	-3.666903	2.769539	0.821021
C	-4.307095	0.292825	0.645188
C	-3.016941	-1.612507	-0.019694
C	-4.534715	1.671338	0.914882
C	-4.264518	4.123449	1.138306
C	-5.515488	-0.615444	0.765023
C	-3.227582	-2.051431	-1.353768
C	-2.616887	-2.526407	0.989748
C	-3.033545	-3.408410	-1.648869
C	-3.642859	-1.095867	-2.472735
C	-2.439644	-3.873004	0.638555
C	-2.377776	-2.095640	2.436427
C	-2.644524	-4.317797	-0.666237
C	-2.520145	-0.919824	-3.512095
C	-4.953201	-1.528063	-3.155884
C	-3.359261	-2.773559	3.411011
C	-0.923157	-2.343934	2.873690
H	4.976657	2.336819	-1.916773
H	6.203624	0.580684	-1.582865

H	5.366796	-0.995909	-1.611571
H	5.870287	-0.303631	-0.072994
H	4.126766	4.212430	-2.674207
H	3.726226	5.033459	-1.157443
H	2.454221	4.745960	-2.364161
H	3.968079	-2.958029	3.031119
H	3.880987	0.600373	1.807950
H	2.854907	-4.581222	-0.783707
H	2.579654	-1.199199	-2.411314
H	1.908392	5.527507	-0.220171
H	3.490189	-4.916934	1.588504
H	2.778367	-1.052519	4.152148
H	1.809847	-0.067039	3.030925
H	2.990490	0.714832	4.114396
H	5.495639	0.501726	3.661810
H	6.091840	-0.488772	2.307317
H	5.380138	-1.268737	3.737478
H	3.569736	-4.056989	-2.982422
H	4.588086	-2.600505	-2.990599
H	3.274892	-2.777014	-4.179232
H	0.412947	-2.265439	-1.765858
H	1.051233	-3.861037	-2.227620
H	0.834484	-2.598483	-3.462432
H	-2.257924	5.513552	0.828532
H	-0.141980	6.718819	0.474291
H	-5.554328	1.910589	1.213615
H	-5.327510	4.027707	1.392087
H	-4.181326	4.808751	0.280553
H	-3.753944	4.595866	1.991871
H	-6.390824	-0.071761	1.141321
H	-5.312432	-1.462521	1.435602
H	-5.773573	-1.050805	-0.212376
H	-3.189826	-3.761059	-2.671629
H	-3.821674	-0.110151	-2.019784
H	-2.132906	-4.588955	1.405379
H	-2.554704	-1.011825	2.493013
H	-2.499488	-5.371595	-0.917831
H	-2.299335	-1.868519	-4.028569
H	-1.590161	-0.570101	-3.038773
H	-2.813523	-0.182828	-4.277990
H	-5.266055	-0.775390	-3.897950
H	-5.773666	-1.647481	-2.430799
H	-4.839089	-2.486409	-3.688164
H	-3.214186	-3.866093	3.436291
H	-4.408630	-2.584889	3.135611
H	-3.207860	-2.395757	4.435506
H	-0.213673	-1.832542	2.206946
H	-0.676711	-3.418196	2.873177
H	-0.759167	-1.965940	3.896288
H	0.072552	0.440337	1.093880
H	-0.190551	0.307949	-1.184772

Open-shell singlet state (isolated molecule), E = -4318,47725164 hartree

	x	y	z
Fe	-1.353242	0.820412	0.084592
Fe	1.239235	0.796701	-0.191172
N	3.090159	-0.008158	-0.394767
N	1.950812	2.685760	-0.660044
N	-0.210260	2.959659	-0.085906
N	-2.329130	2.618951	0.510798
N	-3.109543	-0.199843	0.321060
C	4.131851	0.608792	-0.930514
C	4.107719	1.950885	-1.397404
C	5.447661	-0.130467	-1.067313
C	3.114900	2.935237	-1.271144
C	3.202800	-1.344716	0.111246
C	3.433292	4.281601	-1.891730
C	3.559041	-1.543094	1.470936
C	2.885613	-2.445124	-0.725600
C	0.943383	3.591002	-0.341295
C	3.592085	-2.853729	1.966999
C	3.881973	-0.377579	2.405557
C	2.935860	-3.734823	-0.176510
C	2.485404	-2.270928	-2.189855
C	-1.338253	3.573140	0.313208
C	1.014123	4.991926	-0.177092
C	3.285543	-3.945104	1.155696
C	2.781041	-0.185968	3.465373
C	5.263367	-0.521467	3.068842
C	3.448731	-2.998298	-3.146047
C	1.033179	-2.717333	-2.435683
C	-1.340789	4.977282	0.461442
C	-0.145677	5.656624	0.218116
C	-3.588983	2.776878	0.932847
C	-4.261215	0.312608	0.722192
C	-3.010369	-1.585493	-0.034158
C	-4.463150	1.685407	1.036962
C	-4.156762	4.125683	1.320749
C	-5.475865	-0.586097	0.849430
C	-3.271963	-1.981357	-1.372326
C	-2.585034	-2.531813	0.933513
C	-3.105608	-3.330894	-1.713026
C	-3.705840	-0.985384	-2.448061
C	-2.437825	-3.869268	0.537292
C	-2.286087	-2.145159	2.381442
C	-2.694906	-4.272925	-0.771167
C	-2.594876	-0.764616	-3.491680
C	-5.023113	-1.394420	-3.131508
C	-3.249956	-2.825646	3.371629
C	-0.823606	-2.437910	2.760437
H	5.017388	2.273116	-1.902984
H	6.201767	0.482609	-1.576337
H	5.321792	-1.070374	-1.624079
H	5.839235	-0.409034	-0.076839

H	4.232405	4.174796	-2.636946
H	3.784907	5.003631	-1.136875
H	2.553517	4.718205	-2.385665
H	3.861504	-3.023538	3.012541
H	3.907927	0.538914	1.798776
H	2.693142	-4.593431	-0.807756
H	2.539065	-1.197795	-2.423870
H	1.937524	5.544577	-0.314041
H	3.317141	-4.959012	1.562787
H	2.704297	-1.064761	4.126660
H	1.796881	-0.032570	2.996575
H	2.998531	0.691144	4.097175
H	5.497978	0.374276	3.666872
H	6.063762	-0.647752	2.322526
H	5.304086	-1.388493	3.748042
H	3.415817	-4.090794	-3.003284
H	4.492489	-2.677644	-3.001149
H	3.176894	-2.794900	-4.194782
H	0.331243	-2.170263	-1.789673
H	0.902161	-3.794212	-2.241164
H	0.743560	-2.529442	-3.482605
H	-2.219757	5.532663	0.765511
H	-0.117218	6.741520	0.351577
H	-5.466326	1.926103	1.385917
H	-5.187874	4.022045	1.680970
H	-4.167402	4.817497	0.463845
H	-3.562645	4.595077	2.119933
H	-6.330977	-0.047337	1.276290
H	-5.260494	-1.461726	1.478095
H	-5.772261	-0.979306	-0.135129
H	-3.300613	-3.651357	-2.739595
H	-3.882379	-0.018273	-1.955706
H	-2.112452	-4.610601	1.271511
H	-2.434401	-1.059293	2.472124
H	-2.572863	-5.320572	-1.058001
H	-2.374243	-1.693055	-4.043829
H	-1.661551	-0.427341	-3.015776
H	-2.899574	-0.001928	-4.227433
H	-5.349330	-0.612450	-3.836596
H	-5.833223	-1.549068	-2.401278
H	-4.913468	-2.328320	-3.706379
H	-3.133527	-3.921851	3.360764
H	-4.303283	-2.602846	3.140198
H	-3.052545	-2.482138	4.400372
H	-0.125900	-1.928644	2.080130
H	-0.602771	-3.517184	2.727988
H	-0.614064	-2.086845	3.784222
H	0.094121	0.419172	1.099421
H	-0.184202	0.324591	-1.170741

Nonet state (in Toluol), E = -4318,47645872 hartree

	x	y	z
Fe	-1.378574	0.817195	0.044330
Fe	1.240383	0.786337	-0.169071
N	3.107095	0.007121	-0.395790
N	1.930963	2.686454	-0.654148
N	-0.240376	2.956298	-0.103168
N	-2.366379	2.620753	0.471057
N	-3.138453	-0.202813	0.296696
C	4.133019	0.636523	-0.948435
C	4.084773	1.975133	-1.422271
C	5.457990	-0.083156	-1.099273
C	3.081224	2.947571	-1.285288
C	3.249849	-1.325835	0.113083
C	3.371421	4.294340	-1.918249
C	3.623188	-1.514407	1.469892
C	2.947114	-2.435453	-0.717961
C	0.920690	3.586226	-0.330790
C	3.695510	-2.823641	1.966659
C	3.928625	-0.342420	2.402351
C	3.037106	-3.723177	-0.168695
C	2.520658	-2.274936	-2.176456
C	-1.366820	3.570620	0.304041
C	1.001806	4.980861	-0.129670
C	3.408985	-3.923637	1.159419
C	2.866376	-0.212288	3.509843
C	5.341479	-0.428331	3.007592
C	3.500066	-2.959553	-3.147988
C	1.086208	-2.784232	-2.404934
C	-1.355318	4.968603	0.499329
C	-0.153053	5.644731	0.282155
C	-3.639717	2.785389	0.845605
C	-4.298402	0.313920	0.669636
C	-3.027332	-1.597793	-0.016760
C	-4.513785	1.692541	0.945680
C	-4.225693	4.141003	1.176921
C	-5.509936	-0.587681	0.803951
C	-3.258637	-2.033214	-1.348571
C	-2.620414	-2.515441	0.986688
C	-3.079750	-3.391511	-1.647155
C	-3.681789	-1.074234	-2.461624
C	-2.459130	-3.863074	0.631839
C	-2.359290	-2.089121	2.430968
C	-2.685417	-4.304847	-0.670418
C	-2.578616	-0.919324	-3.524917
C	-5.012741	-1.488254	-3.115828
C	-3.341315	-2.752320	3.415262
C	-0.904717	-2.361159	2.853747
H	4.982394	2.306666	-1.943123
H	6.194932	0.538753	-1.622214
H	5.339869	-1.027913	-1.649044
H	5.867861	-0.349064	-0.112892

H	4.144163	4.189253	-2.690976
H	3.747513	5.017988	-1.177052
H	2.473194	4.727535	-2.380606
H	3.980620	-2.985285	3.009421
H	3.886679	0.579124	1.804240
H	2.808131	-4.588414	-0.796094
H	2.524581	-1.199985	-2.407773
H	1.932037	5.527452	-0.245884
H	3.471732	-4.936137	1.566534
H	2.863904	-1.095472	4.169714
H	1.856278	-0.107440	3.084974
H	3.066537	0.672695	4.136320
H	5.556508	0.468811	3.610865
H	6.116167	-0.503539	2.228198
H	5.449862	-1.303261	3.669119
H	3.516878	-4.052322	-3.004037
H	4.530645	-2.592814	-3.020355
H	3.202502	-2.768622	-4.192054
H	0.370088	-2.276938	-1.742111
H	1.007954	-3.868346	-2.222035
H	0.772403	-2.597850	-3.445040
H	-2.228157	5.521787	0.824256
H	-0.114759	6.724142	0.451307
H	-5.527986	1.937382	1.257778
H	-5.283884	4.048594	1.450950
H	-4.156860	4.827475	0.318837
H	-3.696800	4.609658	2.021267
H	-6.377038	-0.039598	1.192626
H	-5.302646	-1.436811	1.470486
H	-5.783101	-1.020048	-0.170567
H	-3.252410	-3.741930	-2.668012
H	-3.835398	-0.084363	-2.008385
H	-2.148025	-4.582280	1.393791
H	-2.517725	-1.002597	2.490026
H	-2.552604	-5.359602	-0.924738
H	-2.384968	-1.872445	-4.044166
H	-1.633693	-0.583716	-3.071504
H	-2.876233	-0.179026	-4.285986
H	-5.328593	-0.733949	-3.854956
H	-5.820316	-1.591442	-2.374011
H	-4.924403	-2.450712	-3.645602
H	-3.213475	-3.847083	3.437516
H	-4.390532	-2.546547	3.151957
H	-3.172567	-2.378356	4.438432
H	-0.194389	-1.858332	2.181608
H	-0.674956	-3.439099	2.849687
H	-0.725546	-1.987084	3.875182
H	0.068863	0.445483	1.149898
H	-0.177478	0.308553	-1.231340

Nonet state (isolated molecule), E = -4318,46967991 hartree

	x	y	z
Fe	-1.336318	0.821112	0.084044
Fe	1.256464	0.804171	-0.157002
N	3.090530	-0.039064	-0.390772
N	2.011934	2.676582	-0.644865
N	-0.140900	2.959760	-0.058218
N	-2.266282	2.635178	0.541877
N	-3.104518	-0.166637	0.338092
C	4.145512	0.555863	-0.923412
C	4.153427	1.901370	-1.381434
C	5.443155	-0.213472	-1.067245
C	3.181167	2.905219	-1.253947
C	3.169865	-1.383173	0.101963
C	3.529482	4.247071	-1.867005
C	3.525772	-1.604734	1.458269
C	2.821957	-2.466213	-0.745664
C	1.008277	3.590193	-0.343360
C	3.532212	-2.921609	1.938705
C	3.879645	-0.459055	2.406208
C	2.846960	-3.762945	-0.211708
C	2.418114	-2.267234	-2.205857
C	-1.270994	3.580043	0.324882
C	1.070191	4.995712	-0.228159
C	3.199024	-3.996408	1.116015
C	2.804125	-0.275014	3.493135
C	5.273154	-0.630067	3.037439
C	3.375744	-2.984795	-3.175368
C	0.963673	-2.703922	-2.455680
C	-1.280097	4.988379	0.425274
C	-0.091587	5.666534	0.151513
C	-3.507112	2.805590	1.013138
C	-4.236171	0.360506	0.774245
C	-3.038354	-1.546352	-0.047449
C	-4.399707	1.729644	1.123497
C	-4.033288	4.153327	1.459829
C	-5.466180	-0.515277	0.909369
C	-3.330258	-1.908800	-1.388792
C	-2.615965	-2.520335	0.893870
C	-3.200369	-3.254726	-1.758497
C	-3.759462	-0.882978	-2.437977
C	-2.505935	-3.852456	0.468813
C	-2.282056	-2.169594	2.343308
C	-2.795283	-4.224095	-0.842414
C	-2.670869	-0.683451	-3.509136
C	-5.107761	-1.239267	-3.090037
C	-3.246787	-2.843583	3.337211
C	-0.821915	-2.508737	2.691320
H	5.071799	2.206215	-1.881767
H	6.210450	0.384664	-1.574283
H	5.293739	-1.146625	-1.629274
H	5.829839	-0.507151	-0.079356

H	4.353985	4.134405	-2.582849
H	3.856125	4.969595	-1.101575
H	2.669923	4.685876	-2.393896
H	3.801986	-3.109429	2.981080
H	3.902689	0.467876	1.815245
H	2.581982	-4.608526	-0.851488
H	2.475169	-1.190842	-2.423338
H	1.986993	5.550805	-0.393914
H	3.210776	-5.015519	1.511005
H	2.733956	-1.163299	4.142388
H	1.811807	-0.104210	3.048322
H	3.044636	0.589552	4.133830
H	5.529312	0.250556	3.648941
H	6.057110	-0.748826	2.272722
H	5.318181	-1.511799	3.697188
H	3.339386	-4.078964	-3.046577
H	4.421232	-2.669952	-3.030639
H	3.100691	-2.766491	-4.220254
H	0.265817	-2.163900	-1.799625
H	0.828496	-3.783592	-2.280365
H	0.673166	-2.496348	-3.498569
H	-2.163335	5.548996	0.706240
H	-0.070122	6.755762	0.244134
H	-5.385505	1.982628	1.511042
H	-5.030281	4.049232	1.905748
H	-4.116652	4.852647	0.612857
H	-3.370568	4.613905	2.208157
H	-6.300766	0.032400	1.364521
H	-5.256431	-1.407865	1.515575
H	-5.790478	-0.881766	-0.076639
H	-3.419703	-3.550112	-2.787666
H	-3.890444	0.082081	-1.927572
H	-2.184015	-4.615204	1.182288
H	-2.398514	-1.082075	2.457230
H	-2.701987	-5.268301	-1.151725
H	-2.497059	-1.609931	-4.080968
H	-1.714417	-0.383603	-3.054578
H	-2.970736	0.099917	-4.224883
H	-5.426200	-0.438274	-3.777095
H	-5.903083	-1.375896	-2.340237
H	-5.044526	-2.169316	-3.678011
H	-3.160250	-3.942078	3.302901
H	-4.297707	-2.588285	3.129671
H	-3.021963	-2.525985	4.368623
H	-0.122184	-2.003856	2.009962
H	-0.630677	-3.592674	2.634869
H	-0.586554	-2.183072	3.717804
H	0.106552	0.405260	1.161699
H	-0.168618	0.336376	-1.211958

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