## Supporting Information

# N-Alkyl substituted triazenide-bridged homoleptic iron(II) dimers with an exceptionally short Fe–Fe bond

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## Experimental

**General Procedures.** All other manipulations were performed under the argon atmosphere using standard Schlenk and glovebox techniques. Solvents were distilled using MB SPS-800 and were used without further purification. New triazine ligands $HN_3{}^tBuR$ (R = Et, $^i$Pr, $^n$Bu) featuring different alkyl substituents at 1,3-N centers ligands were prepared as reported in our earlier report.[1] $Fe[N(SiMe_3)_2]_2$ was synthesized according to the published procedure.[2] The infrared spectra were obtained as Nujol mulls on a Bruker Vector 22 FT-IR spectrometer at room temperature and registered from 4000 to 400 $cm^{-1}$. Thermogravimetric analyses (TGA) were performed with a TGA/DSC 1 STARe System from Mettler Toledo. Around 8 mg of the sample were sealed in a 100 ml Al crucible in the glovebox and heated under argon atmosphere at a heating rate of 5 °C/min. Fitting of the curves was done using origin software. $^{57}$Fe Mössbauer spectra were recorded on powder samples contained in Delrin cups at 5 K on a strong-field Mössbauer spectrometer equipped with an Oxford Instruments Spectromag 4000 cryostat containing an 8 T split-pair superconducting magnet. The spectrometer was operated in a constant acceleration mode in transmission geometry. The isomer shifts were referenced against that of a room-temperature metallic iron foil. Analysis of the data was performed with the WMOSS Mössbauer Spectral Analysis Software (www.wmoss.org, 2012–2013, Web Research, Edina) and with a home-made program (SimuMoss software. C. Charavay, S. Segard, F. Edon, M. Clémancey, G. Blondin. CEA/iRTSV, CNRS, Univ. Grenoble Alpes).[3] EPR assays were all carried out at helium temperatures using a Bruker EMX spectrometer operating at X-band with double cavity. The instrument settings were as follows: 100 kHz modulation frequency, 6.5-22mW microwave power, 5 G modulation amplitude. The wide range $^1$H NMR spectra of Fe(II) complexes in the range -150 ppm to 500 ppm were recorded in $CDCl_3$ on AVANCE HD 400 spectrometer operating at 400.13 MHz. Samples for magnetic susceptibility measurements using the Evans method were prepared by dissolving a weighed

amount of the iron(II) complex **3** in a measured amount of a deuterated chloroform solvent. The solution was transferred into a 5 mm NMR tube containing a 1 mm capillary with the deuterated chloroform as a reference. The peak separation of the solvent resonance between that of pure solvent (in the capillary) and that shifted by the paramagnetic solution (outside of the capillary) was used for determining the susceptibility in solution.

**Computational details**

All calculations were done in the framework of Density Functional Theory (DFT) using ADF 2018[4,5] on complex **1**. Geometry optimizations were carried out with OLYP as a pure GGA or B3LYP as a hybrid functional, and dispersion terms were included through the Grimme3 correction. A T2ZP basis set was used throughout all calculations, with a small core for OLYP calculations and all electrons for B3LYP ones. Default integration and grid accuracy parameters were used. Open-shell singlet calculations were run either by imposing initial spin densities on the Fe atoms potential with MODIFYSTARTPOTENTIAL or by using the standard broken symmetry approach with spin flipping. The final spin densities were then controlled after each calculation. Indeed, single points on the X-ray structures with singlet calculations always converged to local null spin projections whatever the starting conditions. Geometry optimizations allowed to reach some other low-lying configurations depending on initial conditions. Mössbauer parameters were calculated following an already reported protocol[6] with B3LYP and the TZ2P basis set. The hyperfine coupling tensor components were calculated[7] from the B3LYP optimized geometry in triplet state. ADF 2018 was used with the scalar ZORA Hamiltonian[8] and ZORA-QZ4P all electron basis sets for Fe and N atoms, the rest being treated with TZ2P all electron ZORA basis sets. The spin-orbit ZORA Hamiltonian either did not converge or converged to non-consistent A values, which can be explained by the impossibility to impose a spin-only value within a two-component approach and by the existence of other low-lying spin states values. We also employed Orca 4.2[9,10] with the scalar ZORA approach

and the spin-orbit perturbation method, together with ZORA adapted def2-tzvp basis set, the uncontracted core-properties CP(PPP) basis set for Fe and IGLO-II for N atoms together with an increased grid accuracy of 6. The RIJCOSX approximation was employed to speed up the calculations of Coulomb and exchange integrals. The spin-orbit coupling was taken into account through the mean-field / effective nuclear charge approach with 1-electron terms.

**Synthesis of new iron(II) triazenide complexes**

**$[Fe_2(N_3{}^tBuEt)_4]$ (1).** To a pre-stirred solution of $Fe[N(SiMe_3)_2]_2$ (0.89g, 2.36 mmol) in *n*-hexane was added 0.67 g (4.72 mmol) of $HN_3{}^tBuEt$ at 0 °C and then the temperature was allowed to increase gradually to room temperature. The dark brown mixture obtained was stirred for 18 h, after which the volatile materials were removed under vacuum. Brown crystals of the complex were obtained by crystallization in anhydrous hexane at -20 °C. Yield, 0.79 g (54%). Anal.: Calcd for $C_{24}H_{56}N_{12}Fe_2$ (624.5): C 46.12, H 8.96, N 26.90; found C 46.21, H 9.06, N 26.82%. FT-IR (Nujol, $cm^{-1}$): 1678w, 1516m, 1461m, 1375m, 1305m, 1203w, 1078w, 1017w, 972w.

Using above method, complexes **2** and **3** were also synthesized from the reactants given below in the parentheses and purified by crystallization in anhydrous hexane at -20 °C.

**$[Fe_2(N_3{}^tBu{}^iPr)_4]$ (2).** $Fe[N(SiMe_3)_2]_2$ (0.86 g, 2.47 mmol) and $HN_3{}^tBu{}^iPr$ (0.78 g, 4.95 mmol) in anhydrous hexane. Yield, 1.12 g (67%). Anal.: calcd for $C_{28}H_{58}N_{12}Fe_2$ (674.5): C 49.81, H 8.59, N 24.90; found C 49.93, H 8.68, N 24.82%. FT-IR (Nujol, $cm^{-1}$): 1451m, 1355m, 1241s, 1200m, 1108m, 1032m, 992s, 840s, 674m, 613w, 553w.

**$[Fe_2(N_3{}^tBu{}^nBu)_4]$ (3).** $Fe[N(SiMe_3)_2]_2$ (0.83 g, 2.21 mmol) and $HN_3{}^tBu{}^nBu$ (0.57 g, 5.17 mmol) in anhydrous hexane. Yield, 1.60 g (61%). Anal.: calcd for $C_{32}H_{60}N_{12}Fe_2$ (724.6): C 52.99, H 8.28, N 28.13; found C 53.09, H 8.19, N 28.03%. FT-IR (Nujol, $cm^{-1}$): 1673w, 1512m, 1456s, 1388s, 1300m, 1265m, 1209m, 1027w, 734w, 660w, 580w.

**X-ray crystallography:** Crystal structures of the **1** and **3** were measured using Mo radiation (λ = 0.71073 Å) on an Oxford Diffraction Gemini diffractometer equipped with an Atlas CCD detector. Intensities were collected at 150 K (for **1**) or 100 K (for **3**) by means of the CrysalisPro software.[11] Reflection indexing, unit-cell parameters refinement, Lorentz-polarization correction, peak integration and background determination were carried out with the CrysAlisPro software.[11] An analytical absorption correction was applied using the modeled faces of the crystal.[12] The resulting sets of hkl were used for structure solutions and refinements. The structures were solved with the ShelXT[13] structure solution program using the intrinsic phasing solution method and by using Olex2[14] as the graphical interface. The model was refined with version 2018/3 of ShelXL[15] using least-squares minimization.

CCDC 1555083 and 1555084 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Date Centre via www.ccdc.cam.ac.uk/data_request/cif.

## References

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Table S1. Crystallographic and refinement data for new Fe(II) triazenide complexes.

| Compound | **1** | **3** |
|---|---|---|
| Empirical formula | $C_{24}H_{56}Fe_2N_{12}$ | $C_{32}H_{72}Fe_2N_{12}$ |
| Formula weight | 624.5 | 736.7 |
| Crystal system | Orthorhombic | Monoclinic |
| Space group | *Pccn* | *C*2/*c* |
| a (Å) | 12.1992(15) | 19.115(2) |
| B (Å) | 12.3984(18) | 11.7866(8) |
| C (Å) | 21.399(3) | 21.137(2) |
| α (°) | 90 | 90 |
| β (°) | 90 | 120.907(16) |
| γ (°) | 90 | 90 |
| V (Å³) | 3236.6(7) | 4086.0(9) |
| Z | 4 | 4 |
| μ ($mm^{-1}$) | 0.94 | 0.75 |
| Temperature (K) | 150 | 100 |
| Measured reflections | 16252 | 42383 |
| Independent reflections ($R_{int}$) | 4014 | 5396 (0.068) |
| Data/restrains/parameters | 4014/0/181 | 5396/0/216 |
| Goodness of fit | 1.04 | 1.11 |
| R[$F^2>2\sigma$ ($F^2$)] | 0.064 | 0.055 |
| *w*R ($F^2$) | 0.190 | 0.162 |
| Residual electron density (e.$Å^{-3}$) | −1.20 to 1.54 | −0.85 to 0.79 |
| CCDC no. | 1555083 | 1555084 |

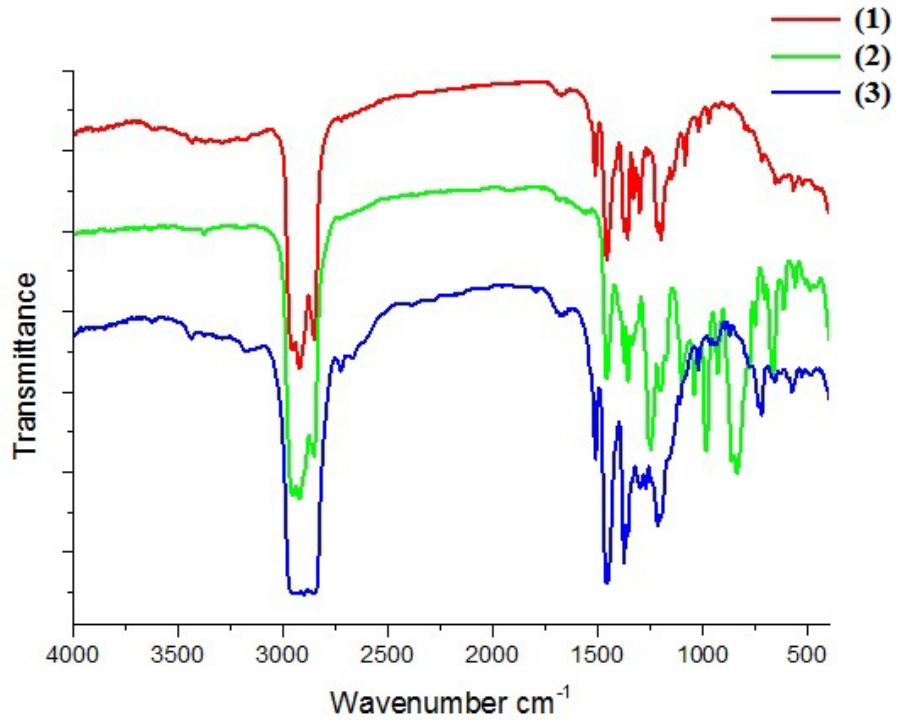


Figure S1: FT-IR spectra of the new Fe(II) complexes **1-3**.

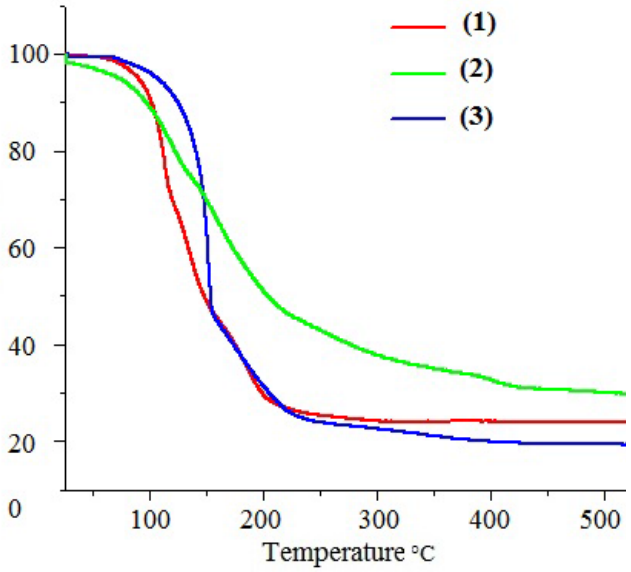


Figure S2. TGA curves of **1-3**.

Even though not very volatile, the TGA curves of these dimeric complexes $[Fe_2(N_3\text{-}^t\text{BuR})_4]$ [R = Et (**1**), $^i$Pr (**2**), $^n$Bu (**3**)] do indicate gradual loss of the triazene ligands in 2 to 3-decomposition steps with the end residues at 450 °C corresponding mostly to the metallic iron

(e.g., 18% exp vs. 17.9% calcd. for **1** and 15% exp vs. 15.1% calcd. for **3**). This is further supported by the Fe 2p XPS spectrum of **1** decomposed *in-situ* at 500 °C for 2 h, producing about 55% metallic Fe(0) component (Figure S3). The presence of some iron oxide particles during decomposition indicates the high air-sensitivity of this complex.

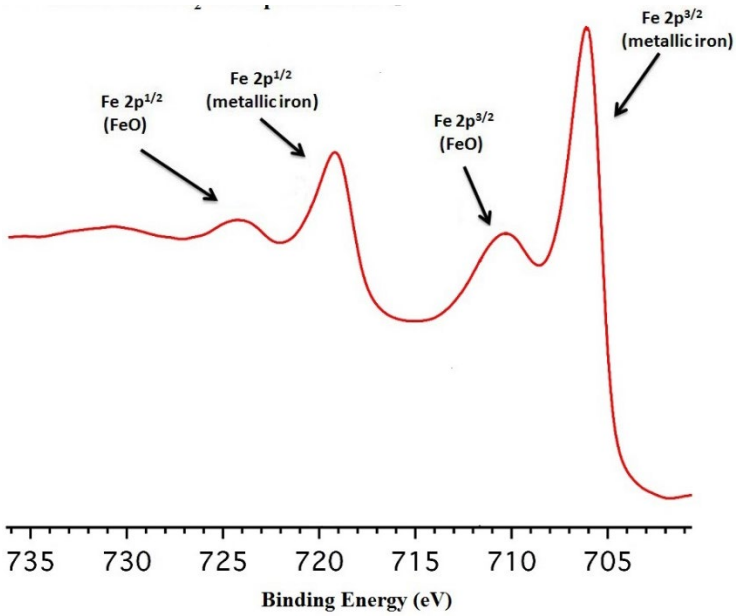


Figure S3. Fe 2p XPS spectrum of the complex **1** decomposed *in situ* at 500°C.

Cyclic voltammetry was performed on **1-3** to understand the electrochemical properties of these complexes. Experiments were conducted under a constant flow of argon gas using a standard three-electrode setup with a glassy carbon working disc electrode and a platinum wire auxiliary electrode and colomel saturated electrode reference electrode. The dimeric complexes **1**-**3** showed an irreversible oxidation process (Fig. S4a). The voltammograms exhibited highest oxidation potential for the complex with the bulkiest ligand (1.86 V for **3** as compared to 1.78 and 1.73 V for **1** and **2**, respectively). No clear-cut effect of the ligand on the evolution of the oxidation potential was found and the complexes with $N_3{}^t Bu^n Bu$ ligand has the highest oxidation potential.

To understand the electrochemical behavior of the dimers, electrolysis was performed on the representative example $[Fe_2(N_3{}^t BuEt)_4]$ (**1**) to calculate the number of electrons involved in the oxidation process. It is an electro-analytical process that determines the quantity of electricity (Q in coulomb) experimentally by completely oxidizing or reducing a known quantity of a chemical compound. The working electrode was kept at a constant potential and the current that flows through the circuit was measured. As the electroactive molecules were consumed, the

current also decreased, approaching zero when the conversion was complete. Cyclic voltammetry of **1** was performed before electrolysis experiment in anhydrous dichloromethane in order to assess the potential needed to oxidize these complexes in an electrolysis experiment. Cyclic voltammetry was then performed after electrolysis to verify if all the quantity was consumed (Fig. S4b). The sample mass, molecular mass, number of electrons in the electrode reaction, and number of electrons passed during the experiment are all related by Faraday's laws (eq. 1).

$$Q = mFne^{-} \qquad (1)$$

Where Q = electrical charge, measured experimentally by calculating the area under the curve I (A) vs time (min); m = number of mole of the compound; F = Faraday's constant (96500); and $ne^-$ = number of electrons involved in the electrochemical process.

The potential of the working electrode needed to completely oxidize the quantity of a chemical compound in an electrolysis experiment is determined by cyclic voltammetry and it corresponds to the oxidation peak of the compound.

Number of electrons involved in the oxidation of **1** (assuming that the electrochemical process is a one electron process):

$Q_{theoratical}$ = 0.02 x 96500 x 1/ 652.7 = 2.956 coulomb

$Q_{experimental}$ = 3.5 coulomb

$Q_{experimental}/Q_{theoratical}$ = 3.5 / 2.956 = 1.18 electron

Therefore, the oxidation of the dimers is a one-electron process that corresponds to the oxidation from $Fe^{II}$ to $Fe^{III}$.

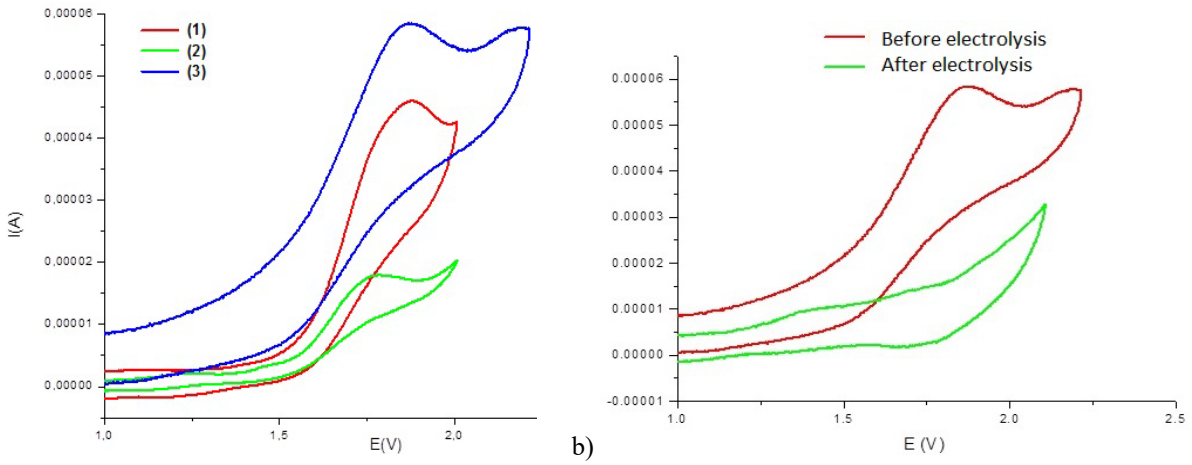


Figure S4. a) Voltammogram of **1-3**, and b) Cyclic voltammogram of **1** in anhydrous $CH_2Cl_2$, 0.1 M ($^n$Bu$_4$N)$PF_6$, 100 mV.

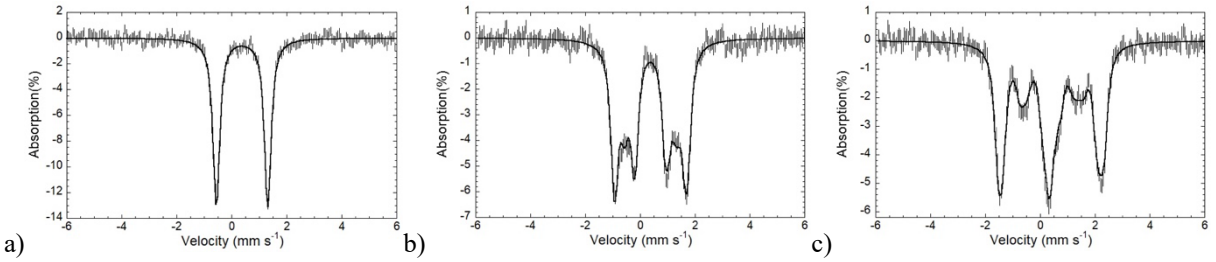


Figure S5**.** Mössbauer spectra of **1** recorded at 5K under magnetic fields applied parallel to the γ ray of 0.06 T (a), 3 T (b) and 7 T (c) and simulations under the assumption of an S = 0 spin. Hashed vertical bars: experimental data, solid line: spectra calculated with the following parameters $\delta = 0.37\ (1)$ mm $s^{-1}$ and $\Delta E_Q = 1.87\ (3)$ mm $s^{-1}$.

The electron paramagnetic resonance (EPR) measurements on the representative complex **1** at helium temperature (parallel and perpendicular modes) showed partial oxidation of this Fe(II)-Fe(II) complex, even though the samples were prepared in an inert atmosphere. Two forms of paramagnetic species were observed. The first corresponds to the oxidation of a Fe(II) ion to Fe(III) (low spin, S=1/2, Figure S6b), while the second species exhibits a high integer spin, consistent with the Fe(III)-Fe(III) dimer (Figure S6a).

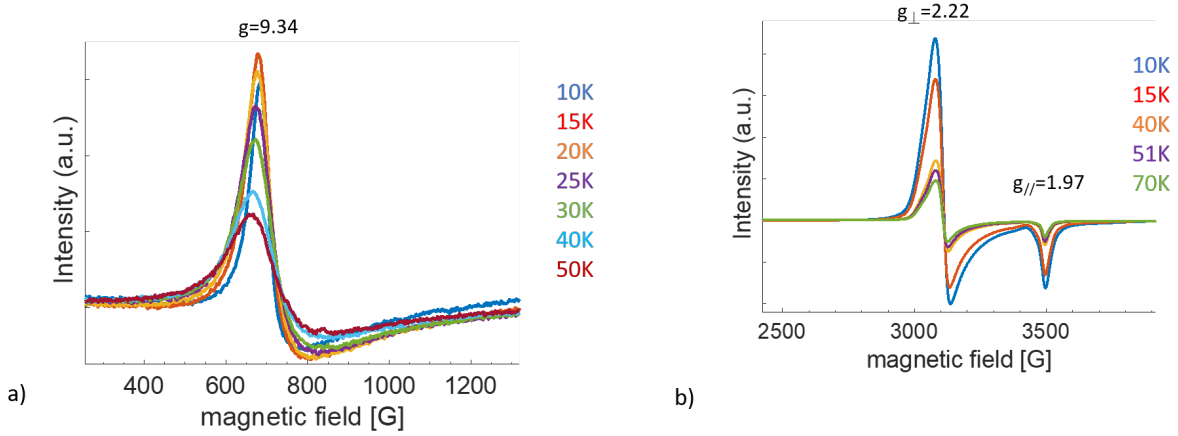


Figure S6: EPR spectra for complex **1** in parallel (a) and perpendicular (b) modes at different temperatures.

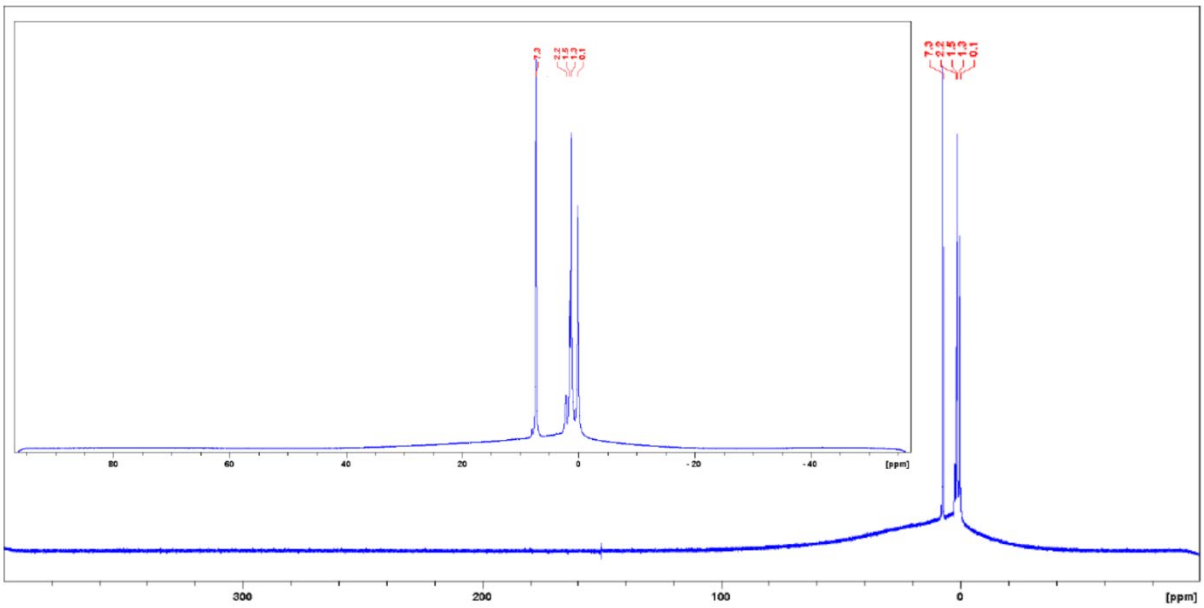


Figure S7: Wide range $^{1}$H NMR spectrum of the Fe-complex **1** in $CDCl_3$.

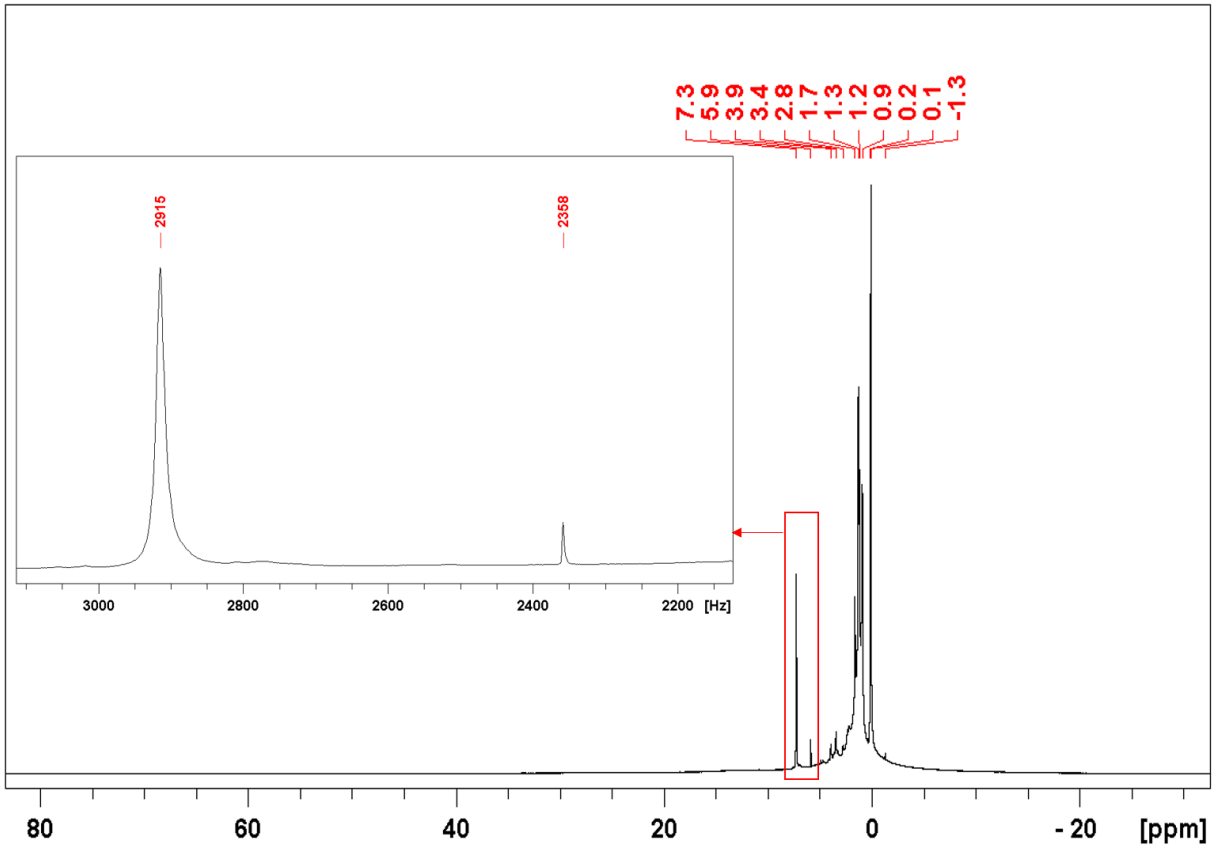


Figure S8: Wide range $^{1}$H NMR spectrum of the Fe-complex **3** in $CDCl_3$ containing a capillary of the pure solvent within the NMR tube. The inset shows the frequency difference in Hz between the pure solvent resonance and the shifted resonance in the presence of paramagnetic species.

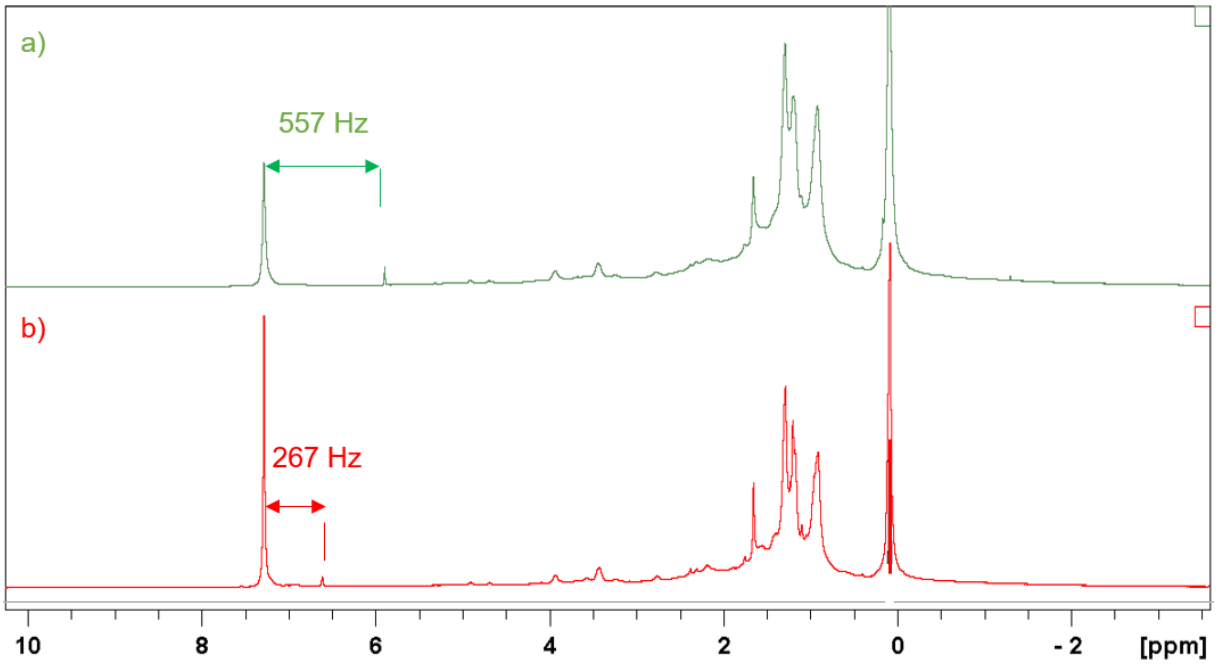


Figure S9: $^{1}$H NMR spectra of the Fe-complex **3** taken in two different concentration in $CDCl_3$: a) $1 \times 10^{-4}$ mol/ml, and b) $0.5 \times 10^{-4}$ mol/ml. The different concentration of **3** causes change in the frequency difference between the pure solvent resonance (taken in a capillary inside the NMR tube) and the shifted resonance in the presence of the paramagnetic **3**.

Magnetic susceptibility ($\chi_m$ = 0.00332 $cm^3$/mol) and effective magnetic moment ($\mu_{eff}$ = 2.81 μB) of the complex **3** was calculated by Evans method using following equations 2 and 3, respectively:

$$\chi m = \frac{3\,\Delta f}{4\pi F c} \qquad (2)$$

$$\mu_{eff} = \sqrt{8}\,(\chi_m T) \qquad (3)$$

Where

Δf (frequency difference between the pure and the shifted resonance of the solvent) = 557 Hz

F (magnetic field of NMR instrument) = $400 \times 10^6$ (Hz)

c (concentration) = $1 \times 10^{-4}$ mol/ml

T (Temperature) = 298 K

A lower concentration of **3** ($0.5 \times 10^{-4}$ mol/ml) caused less shifting of the solvent resonance and, therefore, lower frequency difference with the pure solvent resonance (267 Hz, Fig. S9). Using above equations 2 and 3, the magnetic susceptibility ($\chi_m$ = 0.00318 $cm^3$/mol) and effective magnetic moment ($\mu_{eff}$ = 2.76 μB) were calculated.

Table S2. Spin state ordering from single points on the X-ray structure of complex **1** with OLYP, B3LYP and TPSSH for various spin states and configurations: spin densities on each Fe atom (ρFe) and total bonding energies E in eV.

| Functional | Spin | ρFe | E |
|---|---|---|---|
| OLYP | 0 | 0.0 | -494.18 |
| | 1 | 1.01 | -494.52 |
| B3LYP | 0 | 0.0 | -591.29 |
| | 1 | 1.02 | -590.63 |
| TPSSH | 0 | 0.0 | -571.14 |
| | 1 | 1.01 | -571.77 |

Table S3. Molecular data from geometry optimizations of complex **1** with OLYP and B3LYP for various spin states and configurations: bond lengths in Å, spin density (ρFe) on Fe atoms, Mössbauer parameters in mm $s^{-1}$ and total bonding energies E in eV.

| Functional | Spin | d(Fe-Fe) | $d(Fe-N)_{av}$ | ρFe | δ | $\Delta E_Q$ | E |
|---|---|---|---|---|---|---|---|
| OLYP | 0 | 2.25 | 1.98 | +/-1.02 | | | -514.36 |
| | 0 | 2.36 | 2.02 | +/-1.84 | | | -514.09 |
| | 0 | 2.20 | 1.98 | 0.0 | 2.44 | 0.64 | -514.34 |
| | 1 | 2.16 | 1.99 | 1.02 | 1.51 | 0.60 | -514.66 |
| B3LYP | 0 | 2.25 | 1.95 | 0.0 | 2.13 | 0.42 | -610.68 |
| | 1 | 2.14 | 1.98 | 1.02 | 1.51 | 0.40 | -611.17 |

Table S4. Components of the hyperfine coupling tensor A (MHz), computed with various functionals and basis sets for complex **1**.

| | Functional | Basis | $A_1$ | $A_2$ | $A_3$ |
|---|---|---|---|---|---|
| ADF | OLYP | TZ2P/QZ4P(Fe, N) | -22.7 | -20.4 | -7.8 |
| | OPBE | TZ2P/QZ4P(Fe, N) | -23.6 | -21.8 | -2.2 |
| | PBE | TZ2P/QZ4P(Fe, N) | -18.8 | -16.3 | 2.6 |
| | B3LYP | TZ2P/QZ4P(Fe, N) | -21.8 | -20.0 | -1.5 |
| Orca | OLYP | Def2-tzvp/CP(PPP) | -27.1 | -20.3 | -7.2 |
| | OPBE | Fe/IGLO-II N | -31.6 | -20.5 | -9.4 |

Cartesian coordinates

a) B3LYP geometry S=1 state.

| | | | |
|---|---|---|---|
| Fe | -0.821673000 | 0.682798000 | 13.362892000 |
| Fe | 0.821673000 | -0.682798000 | 13.362892000 |
| N | -1.512272000 | -0.250783000 | 14.966140000 |
| N | -1.164935000 | -1.466568000 | 15.230223000 |
| N | -0.175952000 | -1.915145000 | 14.540915000 |
| N | -1.850165000 | -0.517983000 | 12.177666000 |
| N | -1.225733000 | -1.405550000 | 11.487137000 |
| N | 0.031159000 | -1.528576000 | 11.757135000 |
| C | 0.070080000 | -3.372189000 | 14.719518000 |
| C | -0.987512000 | -4.146366000 | 13.917009000 |
| C | 1.467319000 | -3.670462000 | 14.166774000 |
| C | 0.014635000 | -3.774170000 | 16.199593000 |
| C | -2.478716000 | 0.269520000 | 15.934745000 |
| C | -1.877917000 | 0.439972000 | 17.327897000 |
| C | 0.721608000 | -2.382300000 | 10.788368000 |
| C | 0.762892000 | -1.770778000 | 9.389741000 |
| C | -3.325577000 | -0.530608000 | 11.977840000 |
| C | -3.877453000 | 0.769716000 | 12.570407000 |
| C | -3.689408000 | -0.604175000 | 10.488608000 |
| C | -3.907747000 | -1.737003000 | 12.730564000 |
| H | -0.806243000 | -5.221967000 | 13.974450000 |
| H | -1.980834000 | -3.937034000 | 14.314364000 |
| H | -0.970002000 | -3.839513000 | 12.871791000 |
| H | 1.695581000 | -4.732022000 | 14.269697000 |
| H | 2.228721000 | -3.107047000 | 14.706984000 |
| H | 1.534463000 | -3.420220000 | 13.109015000 |
| H | 0.218679000 | -4.842074000 | 16.297065000 |
| H | 0.763551000 | -3.228191000 | 16.774192000 |
| H | -0.964090000 | -3.565449000 | 16.626273000 |
| H | -2.812476000 | 1.235771000 | 15.557635000 |
| H | -3.356121000 | -0.385711000 | 15.976678000 |
| H | -2.594285000 | 0.915313000 | 18.002144000 |
| H | -0.977928000 | 1.051658000 | 17.277806000 |
| H | -1.603859000 | -0.531100000 | 17.739555000 |
| H | 1.737083000 | -2.520528000 | 11.158677000 |
| H | 0.249750000 | -3.370573000 | 10.755696000 |
| H | 1.375343000 | -2.379241000 | 8.720456000 |
| H | 1.175534000 | -0.763816000 | 9.430413000 |
| H | -0.243940000 | -1.707137000 | 8.978133000 |
| H | -4.957266000 | 0.821698000 | 12.426033000 |
| H | -3.682009000 | 0.829001000 | 13.639409000 |
| H | -3.431109000 | 1.638740000 | 12.085658000 |
| H | -4.774969000 | -0.625847000 | 10.375656000 |
| H | -3.306810000 | 0.266381000 | 9.955100000 |
| H | -3.273607000 | -1.498411000 | 10.029462000 |

| | | | |
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| H | -4.998464000 | -1.740306000 | 12.672596000 |
| H | -3.608352000 | -1.708016000 | 13.778232000 |
| H | -3.531596000 | -2.663210000 | 12.296002000 |
| N | 1.512272000 | 0.250783000 | 14.966140000 |
| N | 1.164935000 | 1.466568000 | 15.230223000 |
| N | 0.175952000 | 1.915145000 | 14.540915000 |
| N | 1.850165000 | 0.517983000 | 12.177666000 |
| N | 1.225733000 | 1.405550000 | 11.487137000 |
| N | -0.031159000 | 1.528576000 | 11.757135000 |
| C | -0.070080000 | 3.372189000 | 14.719518000 |
| C | 0.987512000 | 4.146366000 | 13.917009000 |
| C | -1.467319000 | 3.670462000 | 14.166774000 |
| C | -0.014635000 | 3.774170000 | 16.199593000 |
| C | 2.478716000 | -0.269520000 | 15.934745000 |
| C | 1.877917000 | -0.439972000 | 17.327897000 |
| C | -0.721608000 | 2.382300000 | 10.788368000 |
| C | -0.762892000 | 1.770778000 | 9.389741000 |
| C | 3.325577000 | 0.530608000 | 11.977840000 |
| C | 3.877453000 | -0.769716000 | 12.570407000 |
| C | 3.689408000 | 0.604175000 | 10.488608000 |
| C | 3.907747000 | 1.737003000 | 12.730564000 |
| H | 0.806243000 | 5.221967000 | 13.974450000 |
| H | 1.980834000 | 3.937034000 | 14.314364000 |
| H | 0.970002000 | 3.839513000 | 12.871791000 |
| H | -1.695581000 | 4.732022000 | 14.269697000 |
| H | -2.228721000 | 3.107047000 | 14.706984000 |
| H | -1.534463000 | 3.420220000 | 13.109015000 |
| H | -0.218679000 | 4.842074000 | 16.297065000 |
| H | -0.763551000 | 3.228191000 | 16.774192000 |
| H | 0.964090000 | 3.565449000 | 16.626273000 |
| H | 2.812476000 | -1.235771000 | 15.557635000 |
| H | 3.356121000 | 0.385711000 | 15.976678000 |
| H | 2.594285000 | -0.915313000 | 18.002144000 |
| H | 0.977928000 | -1.051658000 | 17.277806000 |
| H | 1.603859000 | 0.531100000 | 17.739555000 |
| H | -1.737083000 | 2.520528000 | 11.158677000 |
| H | -0.249750000 | 3.370573000 | 10.755696000 |
| H | -1.375343000 | 2.379241000 | 8.720456000 |
| H | -1.175534000 | 0.763816000 | 9.430413000 |
| H | 0.243940000 | 1.707137000 | 8.978133000 |
| H | 4.957266000 | -0.821698000 | 12.426033000 |
| H | 3.682009000 | -0.829001000 | 13.639409000 |
| H | 3.431109000 | -1.638740000 | 12.085658000 |
| H | 4.774969000 | 0.625847000 | 10.375656000 |
| H | 3.306810000 | -0.266381000 | 9.955100000 |
| H | 3.273607000 | 1.498411000 | 10.029462000 |
| H | 4.998464000 | 1.740306000 | 12.672596000 |
| H | 3.608352000 | 1.708016000 | 13.778232000 |
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b) B3LYP geometry S=0 state.

| | | | |
|---|---|---|---|
| Fe | -0.868042000 | 0.719294000 | 13.360616000 |
| Fe | 0.868042000 | -0.719294000 | 13.360616000 |
| N | -1.541192000 | -0.243803000 | 14.908522000 |
| N | -1.162945000 | -1.449170000 | 15.189029000 |
| N | -0.142670000 | -1.895888000 | 14.540068000 |
| N | -1.841161000 | -0.483330000 | 12.174334000 |
| N | -1.212505000 | -1.399831000 | 11.521001000 |
| N | 0.040213000 | -1.553588000 | 11.804447000 |
| C | 0.122834000 | -3.341505000 | 14.845771000 |
| C | -0.958840000 | -4.201484000 | 14.167855000 |
| C | 1.501598000 | -3.709169000 | 14.286216000 |
| C | 0.115902000 | -3.604729000 | 16.360292000 |
| C | -2.624668000 | 0.189097000 | 15.804891000 |
| C | -2.227896000 | 0.229684000 | 17.280449000 |
| C | 0.664815000 | -2.538303000 | 10.906712000 |
| C | 0.612267000 | -2.157318000 | 9.427062000 |
| C | -3.309195000 | -0.479953000 | 11.861027000 |
| C | -3.918074000 | 0.812978000 | 12.414048000 |
| C | -3.562119000 | -0.538149000 | 10.345686000 |
| C | -3.966766000 | -1.694899000 | 12.540312000 |
| H | -0.763018000 | -5.262668000 | 14.337569000 |
| H | -1.940310000 | -3.961056000 | 14.576312000 |
| H | -0.983457000 | -4.021191000 | 13.093381000 |
| H | 1.705809000 | -4.764338000 | 14.475504000 |
| H | 2.291648000 | -3.129417000 | 14.765152000 |
| H | 1.554673000 | -3.551131000 | 13.210854000 |
| H | 0.333548000 | -4.657801000 | 16.549294000 |
| H | 0.876334000 | -3.005333000 | 16.862475000 |
| H | -0.852138000 | -3.366372000 | 16.795423000 |
| H | -2.925086000 | 1.185035000 | 15.480652000 |
| H | -3.491948000 | -0.468055000 | 15.678130000 |
| H | -3.053147000 | 0.621663000 | 17.879365000 |
| H | -1.355984000 | 0.865903000 | 17.431690000 |
| H | -1.986762000 | -0.770205000 | 17.637902000 |
| H | 1.704032000 | -2.636230000 | 11.219505000 |
| H | 0.191955000 | -3.516601000 | 11.047689000 |
| H | 1.147751000 | -2.900278000 | 8.831479000 |
| H | 1.070521000 | -1.182706000 | 9.258992000 |
| H | -0.418518000 | -2.114461000 | 9.078916000 |
| H | -4.992531000 | 0.824705000 | 12.222967000 |
| H | -3.774050000 | 0.897822000 | 13.489460000 |
| H | -3.488302000 | 1.691701000 | 11.932149000 |
| H | -4.636672000 | -0.512114000 | 10.153630000 |
| H | -3.106311000 | 0.315045000 | 9.841901000 |
| H | -3.154400000 | -1.449433000 | 9.914500000 |
| H | -5.045277000 | -1.690717000 | 12.366497000 |
| H | -3.789044000 | -1.683194000 | 13.615350000 |
| H | -3.554748000 | -2.619487000 | 12.136744000 |
| N | 1.541192000 | 0.243803000 | 14.908522000 |

| | | | |
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| N | 1.162945000 | 1.449170000 | 15.189029000 |
| N | 0.142670000 | 1.895888000 | 14.540068000 |
| N | 1.841161000 | 0.483330000 | 12.174334000 |
| N | 1.212505000 | 1.399831000 | 11.521001000 |
| N | -0.040213000 | 1.553588000 | 11.804447000 |
| C | -0.122834000 | 3.341505000 | 14.845771000 |
| C | 0.958840000 | 4.201484000 | 14.167855000 |
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| H | 0.763018000 | 5.262668000 | 14.337569000 |
| H | 1.940310000 | 3.961056000 | 14.576312000 |
| H | 0.983457000 | 4.021191000 | 13.093381000 |
| H | -1.705809000 | 4.764338000 | 14.475504000 |
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