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SUPPORTING INFORMATION

Triptycene-based diiron(II) mesocate: spin-crossover in solution

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1. Materials and Methods

All commercially available starting materials and solvents were purchased from Sigma-Aldrich or VWR, and used without further purification. 2,3,6,7-tetraaminotriptycene chlorohydrate was obtained using a known procedure[S1]. Further details on synthesis of the L compound have been reported by our group in a recent publication.[S2] ^{1}H- and ^{13}C-NMR and 2D-NMR spectra were recorded on a Bruker AVANCEIII 400 MHz (operating at 9.37 T, 400 MHz), equipped with a 5 mm BBO probe head with Z-gradient (Bruker BioSpin). The ^{1}H VT-NMR ranging from 193 K to 293 K, in CD_3OD were recorded on a Bruker AVANCE 400 MHz (operating at 9.37 T) spectrometer. Deuterated solvents used for NMR analysis (DMSO, CD_3CN, CD_3OD) were purchased and used as received. Chemical shifts are reported in ppm with the residual solvent as internal reference, while 2D spectra were graphically referenced.

High-resolution mass spectra were recorded on a Sciex X500B QTOF System (Framingham, USA) operated in the ESI mode.

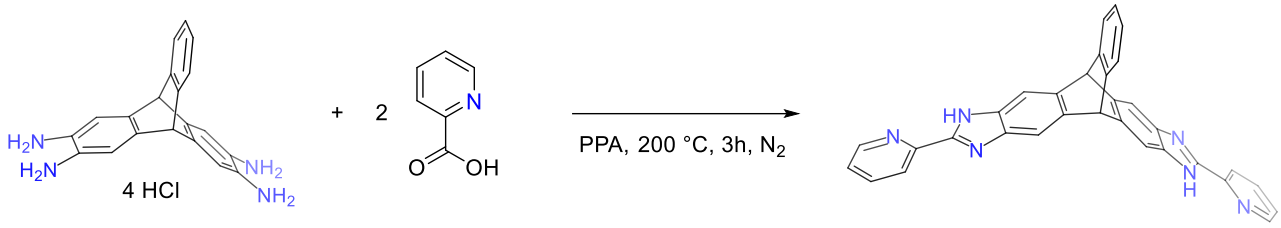
UV-Vis spectra were recorded on an Agilent (Santa Clara, CA, USA) 8453 spectrophotometer equipped with a 1024 photodiode array detector (190-1100 nm wavelength range) and a quartz optical cell of 1 cm path length. Low temperature optical spectra were obtained with a magnetically stirred optical quartz cell inserted into a USP-203-A cryostat (UNISOKU, Oaka, Japan) connected with the Agilent spectrophotometer.

For the Fourier Transform-Infrared analysis (FT-IR), a Nicolet FT-IR iS10 spectrometer (Nicolet, Madison, WI, USA) equipped with attenuated total reflectance (ATR) sampling accessory (Smart iTR with diamond plate) was used. Sixteen scans in the 4000–500 cm^{-1} range were co-added. Well-ground powder samples were used, and spectra were obtained after pressing the sample onto an ATR diamond crystal at room temperature (20 °C).

The solvent used in the electrochemical experiments (MeCN) was distilled over CaH_2 and stored under nitrogen over molecular sieves. Supporting electrolyte ($[Bu_4N]PF_6$, 50 mM) was used without further purification. Electrochemical measurements (cyclic voltammetry) were performed in a conventional three-electrode cell, using a PAR273 potentiostat/galvanostat. The working electrode was a platinum microsphere, and the counter electrode was a platinum foil. A silver wire immersed in a solution of AgCl in MeCN and $[Bu_4N]PF_6$ 50 mM was used as a pseudo reference electrode and was calibrated using ferrocene as an internal standard. Thus, the potential of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ reported in this work has been referred to the Fc^+/Fc couple.[S3]

2. Synthetic Procedures

2.1 Ligand **L**



Ortho-pyridinecarboxylic acid (62 mg, 0.5 mmol, 2.5 eqv.) is added, under N_2 atmosphere, to a suspension of the 2,3,6,7-tetramminotriptycene chlorohydrate, (100 mg, 0.2 mmol, 1 eqv.) in polyphosphoric acid (3 mL). The reaction mixture is stirred at 100 °C for 1 h, and then the temperature is increased to 200 °C. After three hours, the reaction mixture is cooled down to room temperature and water (30 mL) is added. The formed suspension is stirred for 3 hours and then the pH is adjusted to 7-8 by addition of solid sodium bicarbonate. The suspension is finally filtered and washed with H_2O and cold MeOH to obtain the product as a brown solid. Yield = 55 mg, 56%. ^{1}H-NMR (400 MHz, DMSO-d$_6$) δ 12.97 (s, 2H, N*H*), 8.68 (d, 2H, C*H*$_a$), 8.24 (d, 2H, C*H*$_d$), 7.94 (t, 2H, C*H*$_c$), 7.74 (s, 2H, C*H*$_{e,f}$), 7.62 (d, 2H, C*H*$_{e,f}$), 7.48 (m, 4H, C*H*$_b$ + C*H*$_{i,l}$), 7.01 (m, 2H, C*H*$_{j,k}$), 5.77 (t, 2H, C*H*$_{g,h}$). ^{13}C-NMR (100 MHz, DMSO-d$_6$) δ 150.60, 149.26, 148.52, 145.79, 141.26, 140.97, 139.72, 137.46, 132.32, 132.30, 125.01, 124.36, 123.43, 121.06, 114.17, 107.51, 52.78. HRMS (ESI, methanol) m/z: 489.1821 $[M+H^+]^+$; calc. m/z = 489.1822 $[M+H^+]^+$; error= 0.2 ppm.

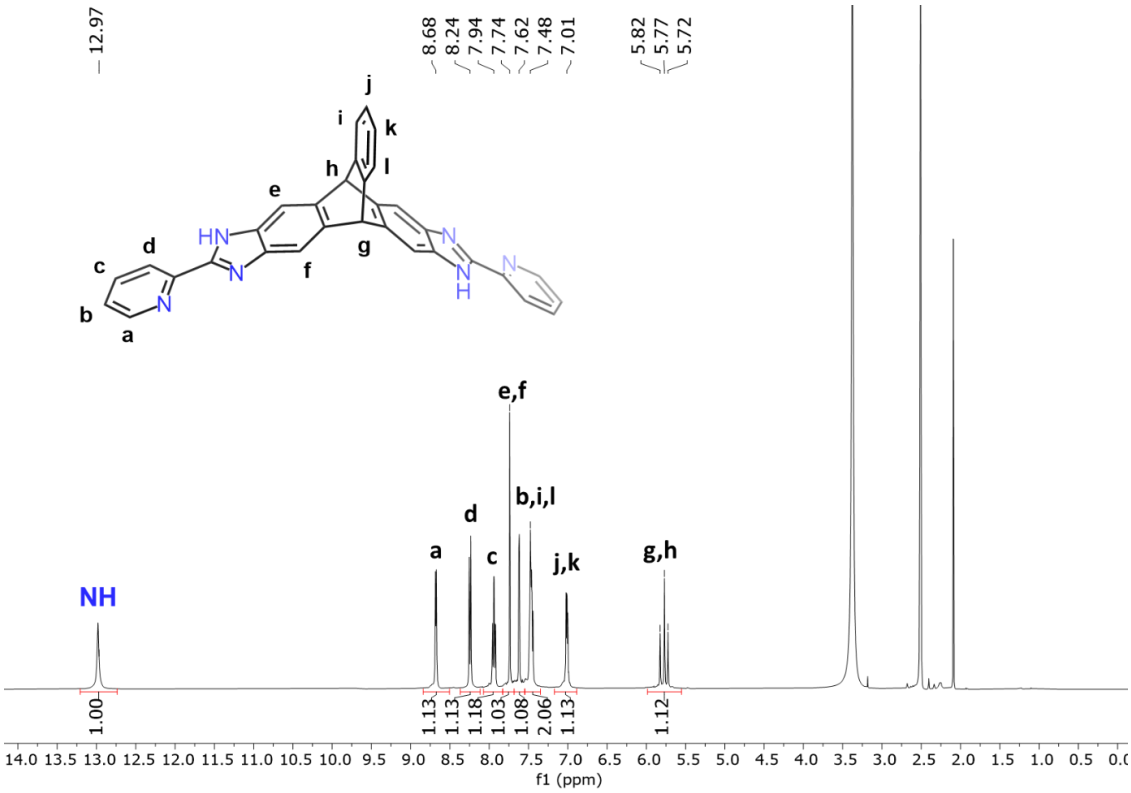


Figure S1a ^{1}H-NMR spectrum of **L** in DMSO-d_6 at 298 K.

The tautomeric equilibrium between *syn* and *anti* forms is slow on the NMR timescale (DMSO-d_6, 303 K), and the tautomers can be distinguished by the different set of peaks observed for the bridgehead protons.[S2] Specifically, *syn* and *anti* forms are highlighted using green and red circles, respectively, as illustrated in Figure S1b. In the *syn* tautomer the two N-H protons face the same side of the triptycene unit; this makes the bridgehead protons inequivalent, giving two distinct singlets at 5.72 and 5.82 ppm. On the contrary, in the *anti* form, the N-H protons face the opposite sides of the ligand. In this situation, the bridgehead protons are symmetrically equivalent and produce a unique singlet at 5.77 ppm. As it results from the ratio of the protons' integrals, the free ligand is equally distributed between the *syn* and *anti* forms.

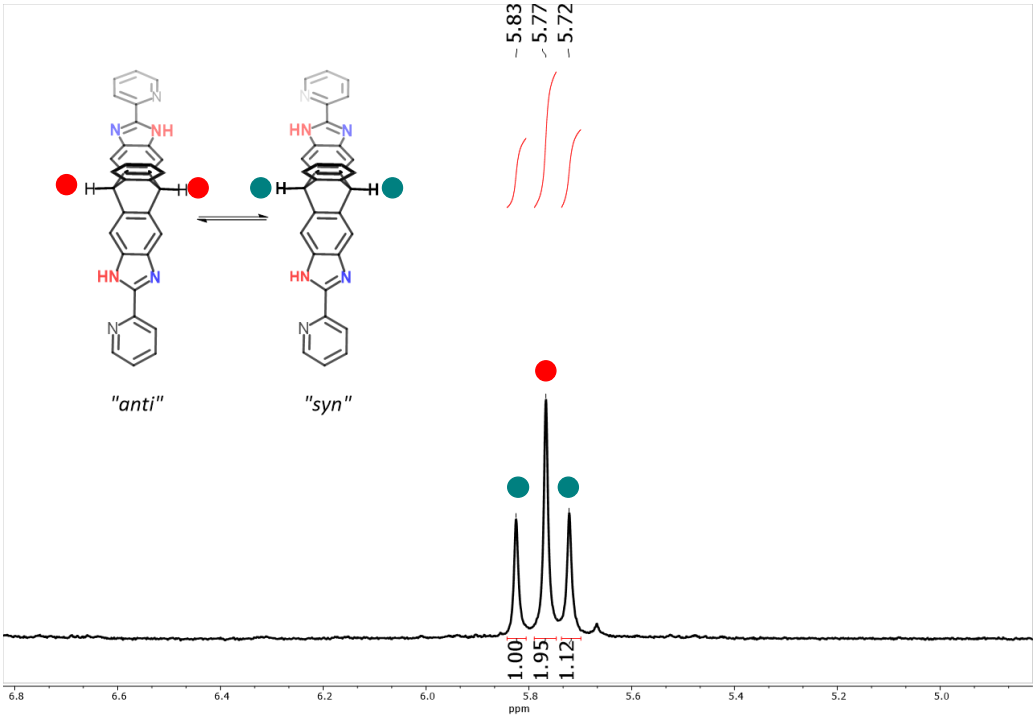


Figure S1b Detail of ^{1}H-NMR spectra of ligand **L** in DMSO-d_6 at 298K. The three signals of the bridgehead protons can be distinguished between those from the "*syn*" tautomer (two singlet) and those from the "*anti*" tautomer (central singlet).

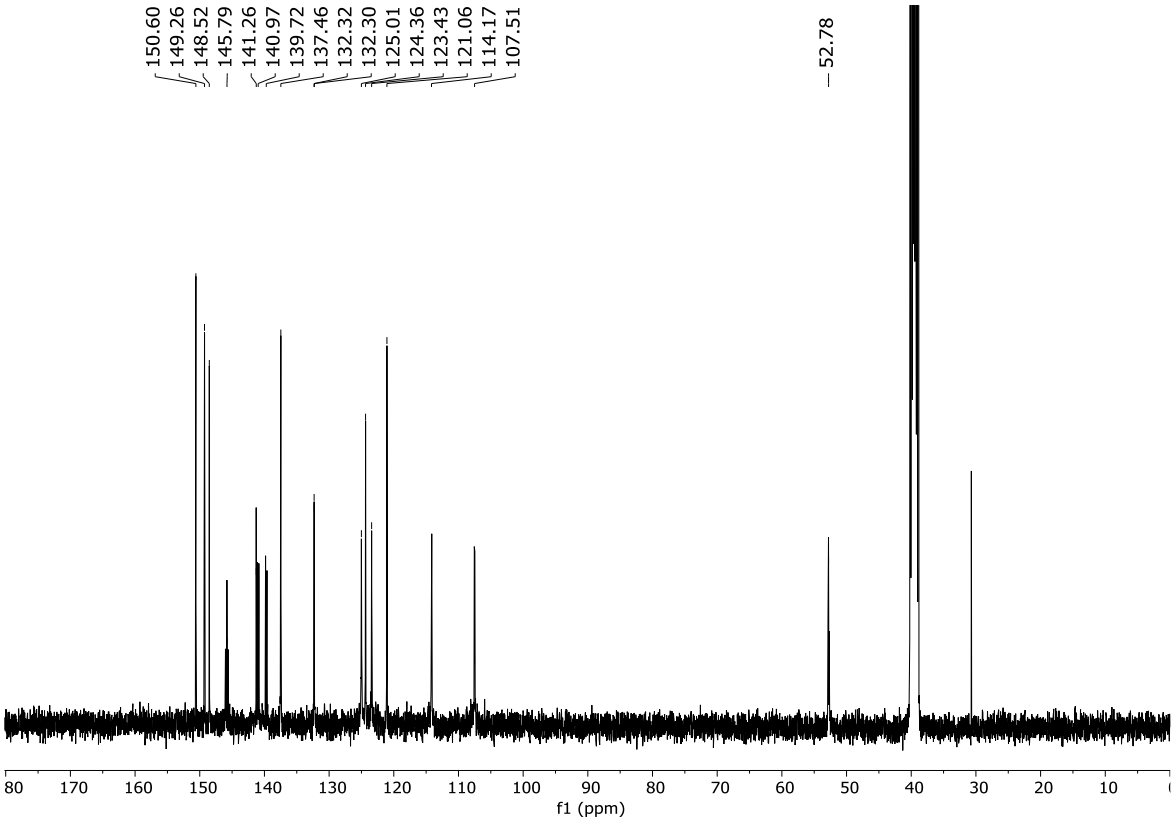


Figure S2 ^{13}C-NMR spectrum of **L** in DMSO-d_6 at 298 K. The signal at 30 ppm is due to the CH_3 of residual acetone used to clean the NMR tube.

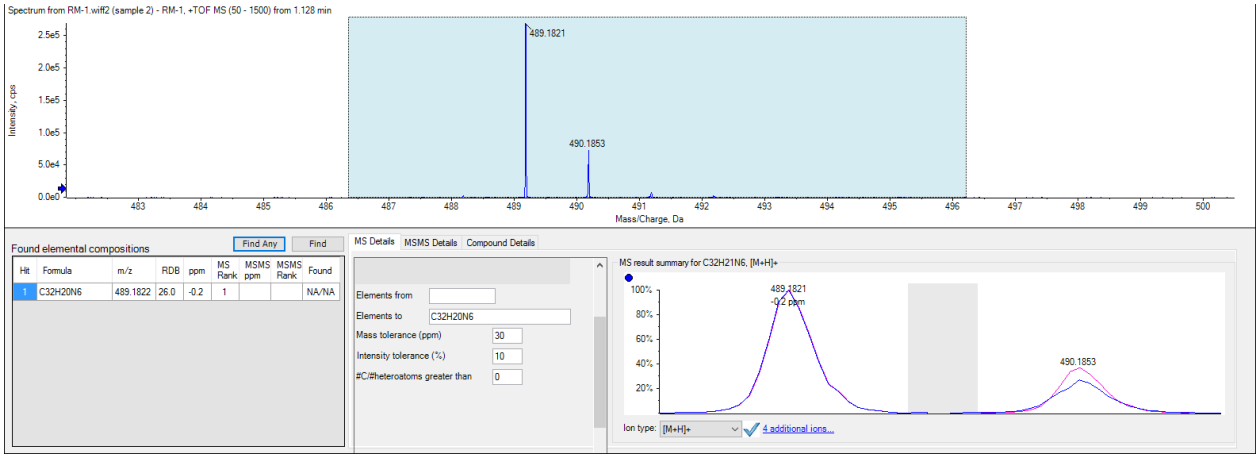
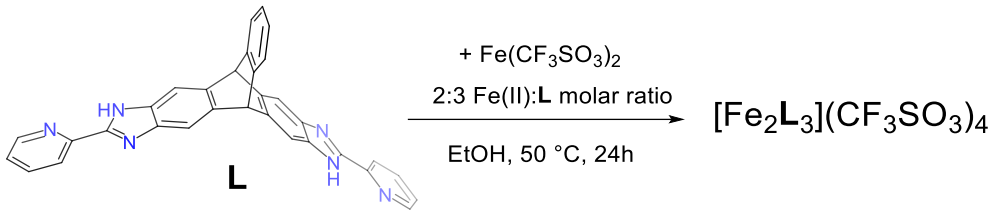


Figure S3 HRMS-ESI of **L** in MeOH. Up: zoom scan of the peak at 489.1821 m/z obtained from the experimental HRMS-ESI spectrum. Bottom: calculated spectrum of the adduct [**L**+H]$^+$ superimposed to the experimental one.

2.2 $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$



A solution of $Fe(CF_3SO_3)_2$ (10.6 mg, 0.03 mmol, 2 eqv.) in ethanol (2 mL) is added to a suspension of ligand **L** (22.5 mg, 0.046 mmol, 3 eqv.) in ethanol (3 mL). The reaction mixture is heated at 50 °C for 24 hours. The red-brownish solution is then cooled down to room temperature, filtered on a 0.45 µm syringe filter and added to diethyl ether (30 mL) to obtain a red precipitate that is decanted, washed 2 times with diethyl ether (10 mL per wash) and dried under vacuum to obtain a vivid red solid. (22 mg, 67%). ^{1}H-NMR (400 MHz, 298 K, CD_3CN) δ 70.19 (s broad, 6H), 50.24 (s, 6H), 40.95 (s, 6H), 26.95 (s, 6H), 7.43 (d, 3H), 7.19 (dd, 3H), 6.78 (dd, 3H), 5.19 (s, 3H), 4.94 (d, 3H), 4.64 (s, 3H), -5.46 (s, 6H), -14.56 (s, 6H). $C_{100}H_{60}N_{18}O_{12}F_{12}S_4Fe_2$ + $7H_2O$ (MW: 2299.74): calc. C 52.22%, H 3.24%, N 10.96%; exp. C 52.18%, H 3.69%, N 10.59%. HRMS (ESI, methanol) m/z: 787.6911 $[M–2H^+]^{2+}$, 525.4629 $[M–H^+]^{3+}$, 394.3492 $[M]^{4+}$; calc. m/z = 394.3490 $[M]^{4+}$; error= 1.2 ppm.

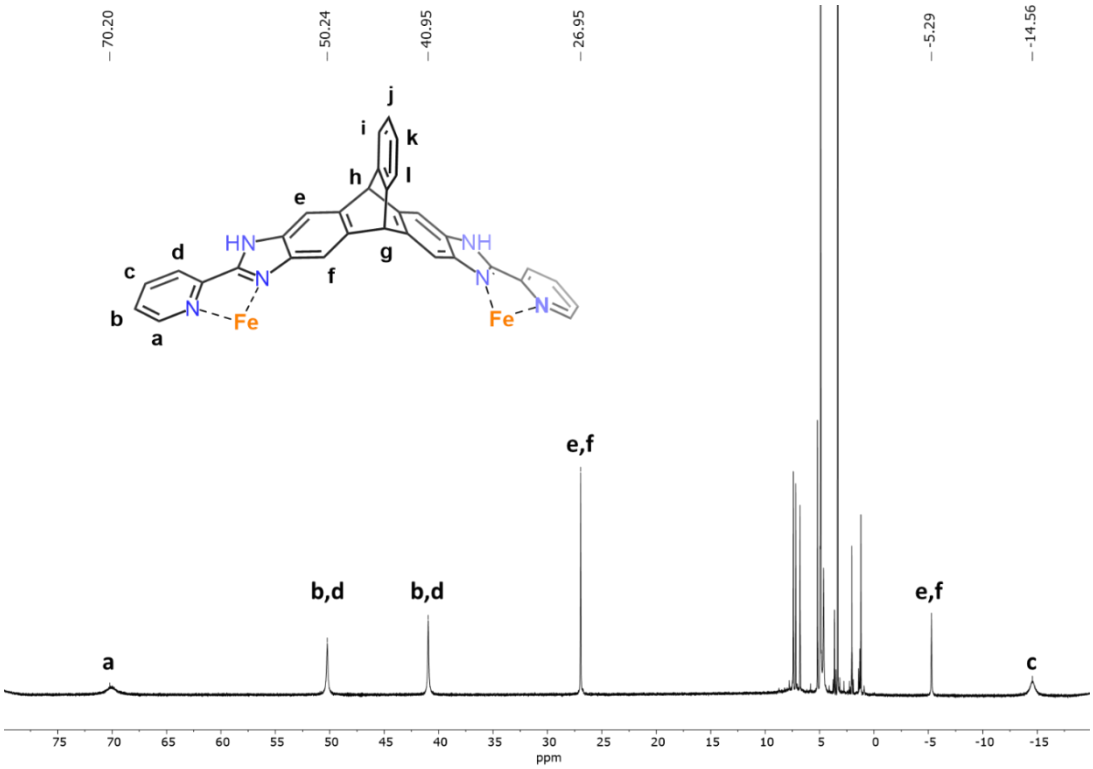


Figure S4 Paramagnetic ^{1}H-NMR spectrum of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K. Correct assignment of protons *b*, *d*, *e* and *f* was not possible on the basis of this experiment.

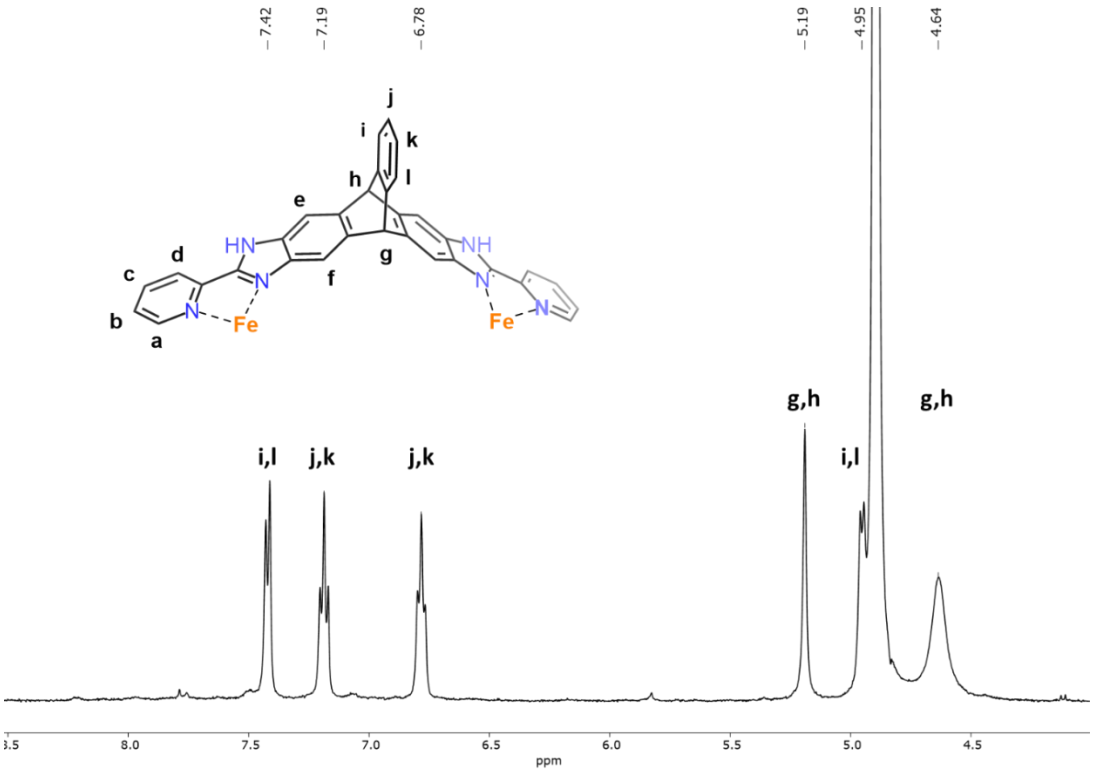


Figure S5 Diamagnetic region of ^{1}H-NMR spectrum of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K. Correct assignment of protons *g*, *h*, *i*, *j*, *k*, and *l* was not possible on the basis of this experiment.

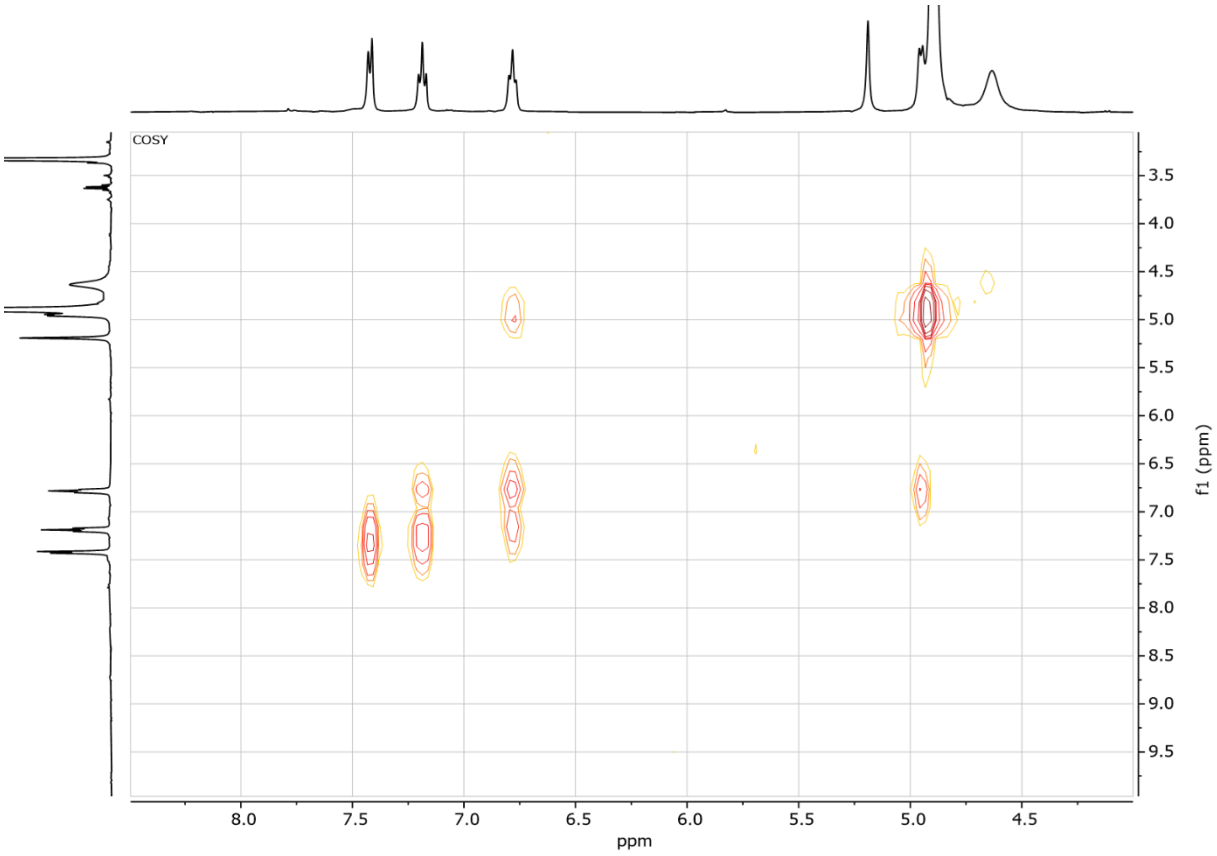
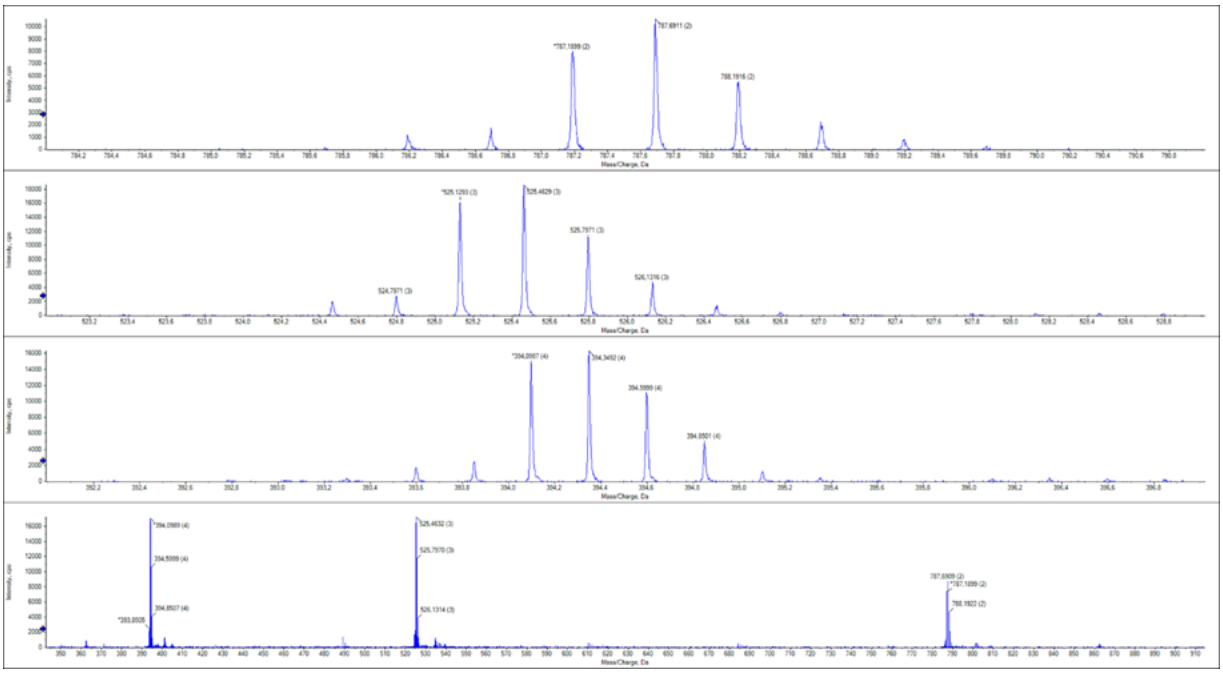
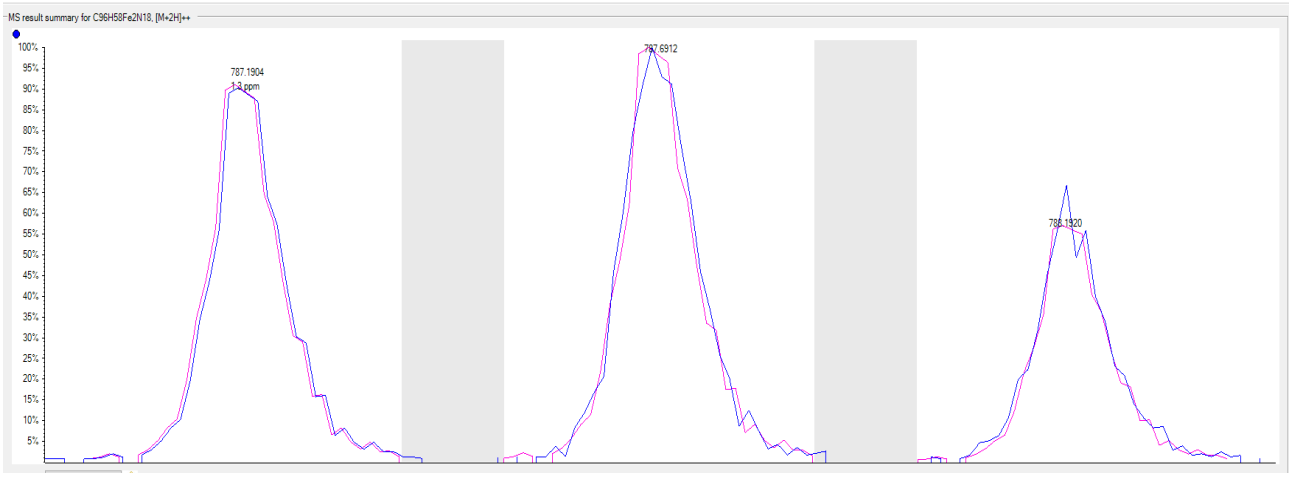


Figure S6 ^{1}H-^{1}H-COSY of the diamagnetic region of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K.





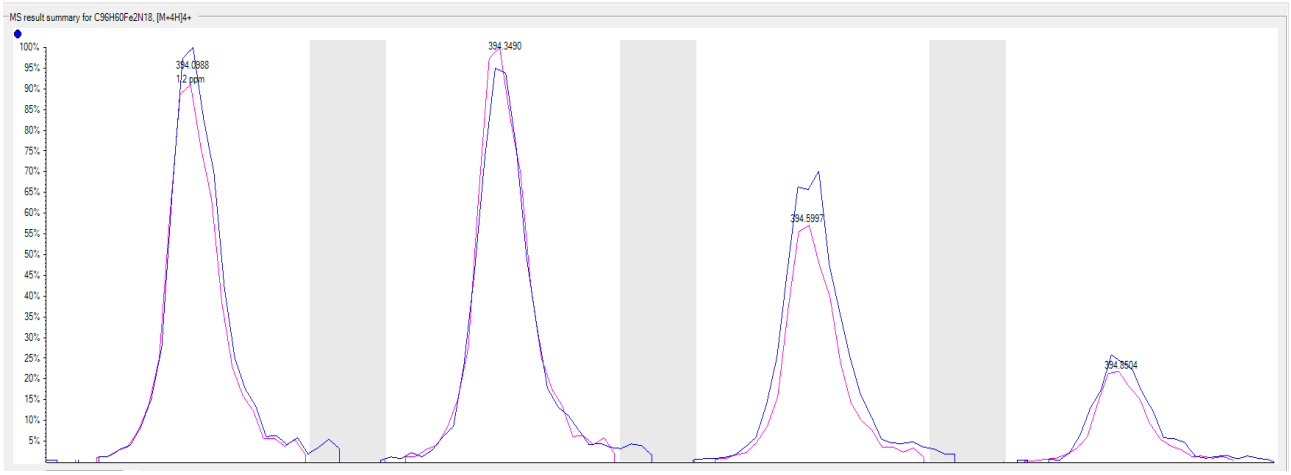
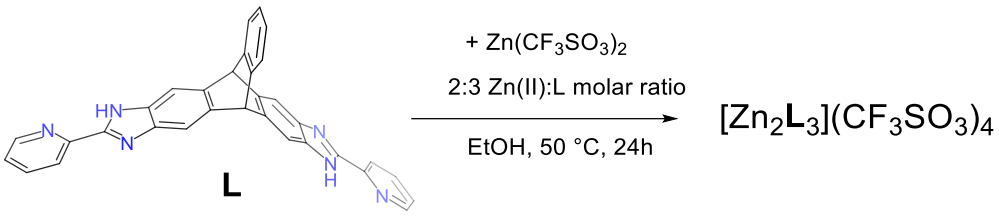


Figure S7 HRMS-ESI full spectrum of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in MeOH. Up: Full spectrum and zoom scans of the peaks at 787.6911 $[M–2H^+]^{2+}$, 525.4629 (100) $[M–H^+]^{3+}$, 394.3492 $[M]^{4+}$ m/z. Bottom: calculated spectrum of the $[M–2H^+]^{2+}$ and $[M]^{4+}$ peaks superimposed to the experimental one.

2.3 $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$



A solution of $Zn(CF_3SO_3)_2$ (7.4 mg, 0.02 mmol, 2 eqv.) in ethanol (2 mL) is added to a suspension of ligand **L** (15.0 mg, 0.031 mmol, 3 eqv.) in ethanol (3 mL). The reaction mixture is heated for 24 hours at 50 °C. The yellow-brownish solution is then cooled down to room temperature, filtered on a 0.45 µm syringe filter and added to diethyl ether (30 mL) to obtain a yellow precipitate that is decanted, washed 2 times with diethyl ether (10 mL per wash) and dried under vacuum to obtain a faint yellow solid. (17 mg, 76%). ^{1}H-NMR (400 MHz, 298 K, CD_3OD) δ 8.32 (d, 6H, C*H*$_{Py}$), 8.19 (t, 6H, C*H*$_{Py}$), 7.97 (s, 6H, C*H*$_{Tript}$), 7.74 (d, 6H, C*H*$_{Py}$), 7.55 (t, 6H, C*H*$_{Py}$), 7.41(d, 3H, C*H*$_{Tript}$), 6.95 (t, 3H, C*H*$_{Tript}$), 6.87 (t, 3H, C*H*$_{Tript}$), 6.82 (d, 3H, C*H*$_{Tript}$), 6.79 (s, 6H, C*H*$_{Tript}$), 5.92 (s, 3H, C*H* $_{Bridgehead}$), 4.04 (s, 3H, $_{Bridgehead}$); ^{13}C-NMR (100 MHz, 298 K, CD_3OD) δ 148.91, 147.93, 143.71, 143.57, 143.44, 143.38, 142.49, 141.04, 137.00, 133.70, 127.14, 125.62, 125.35, 123.50, 122.76, 122.13, 118.84, 111.22, 108.61, 54.31, 53.37; HR-MS (ESI, methanol) m/z: 399.0956 $[M]^{4+}$, 531.7915 $[M–1H^+]^{3+}$, 582.1123 $[M+CF_3SO_3^-]^{3+}$, 872.6633 $[M-1H^+ + CF_3SO_3^-]^{2+}$, 947.6446 $[M+2CF_3SO_3^-]^{2+}$; calc. m/z = 582.7804 $[M+CF_3SO_3^-]^{3+}$; error= 0.7 ppm.

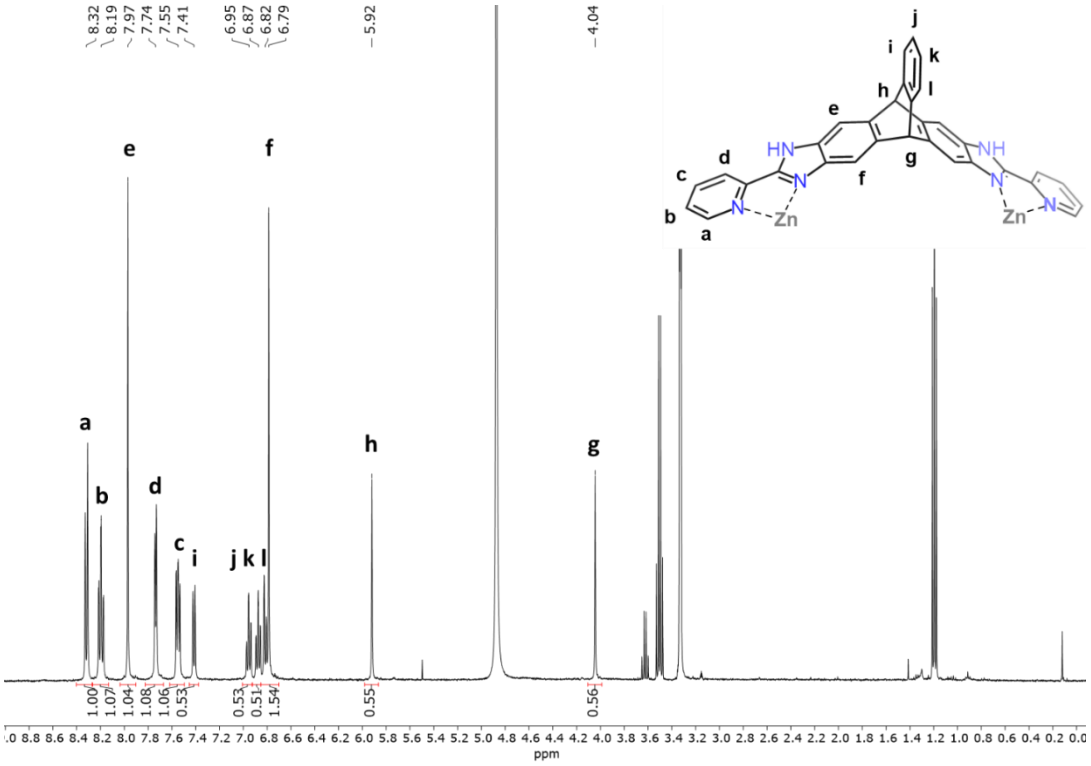


Figure S8 ^{1}H-NMR spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K. NH proton is not visible due to exchange whit deuterium of the solvent.

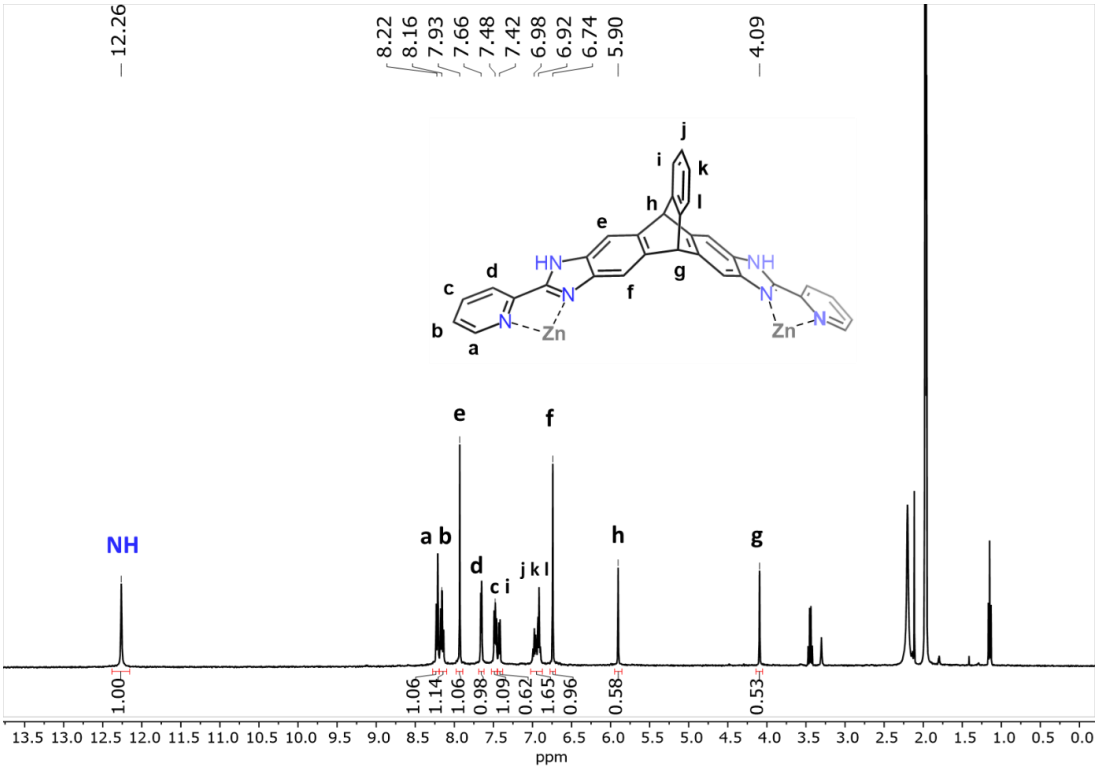


Figure S9 ^{1}H-NMR spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3CN at 298 K.

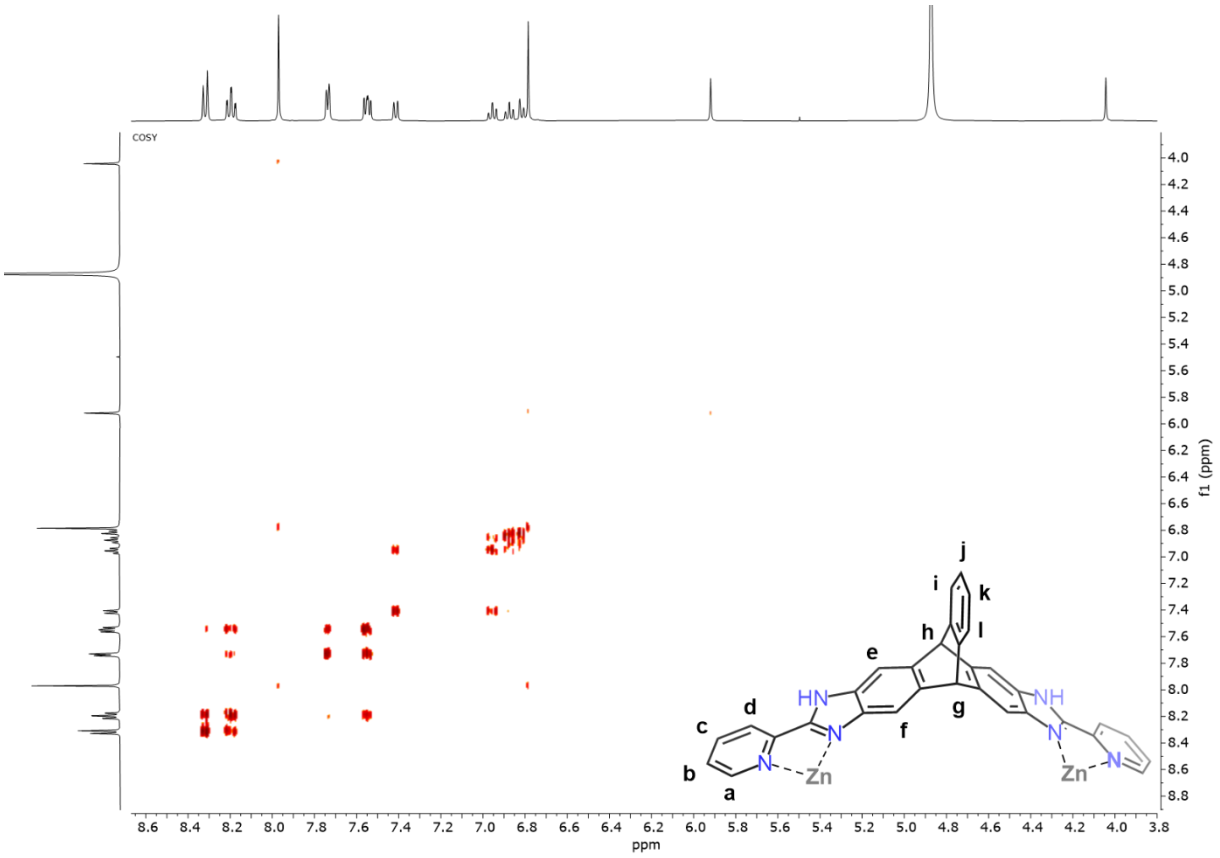


Figure S10 ^{1}H-^{1}H-COSY spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K.

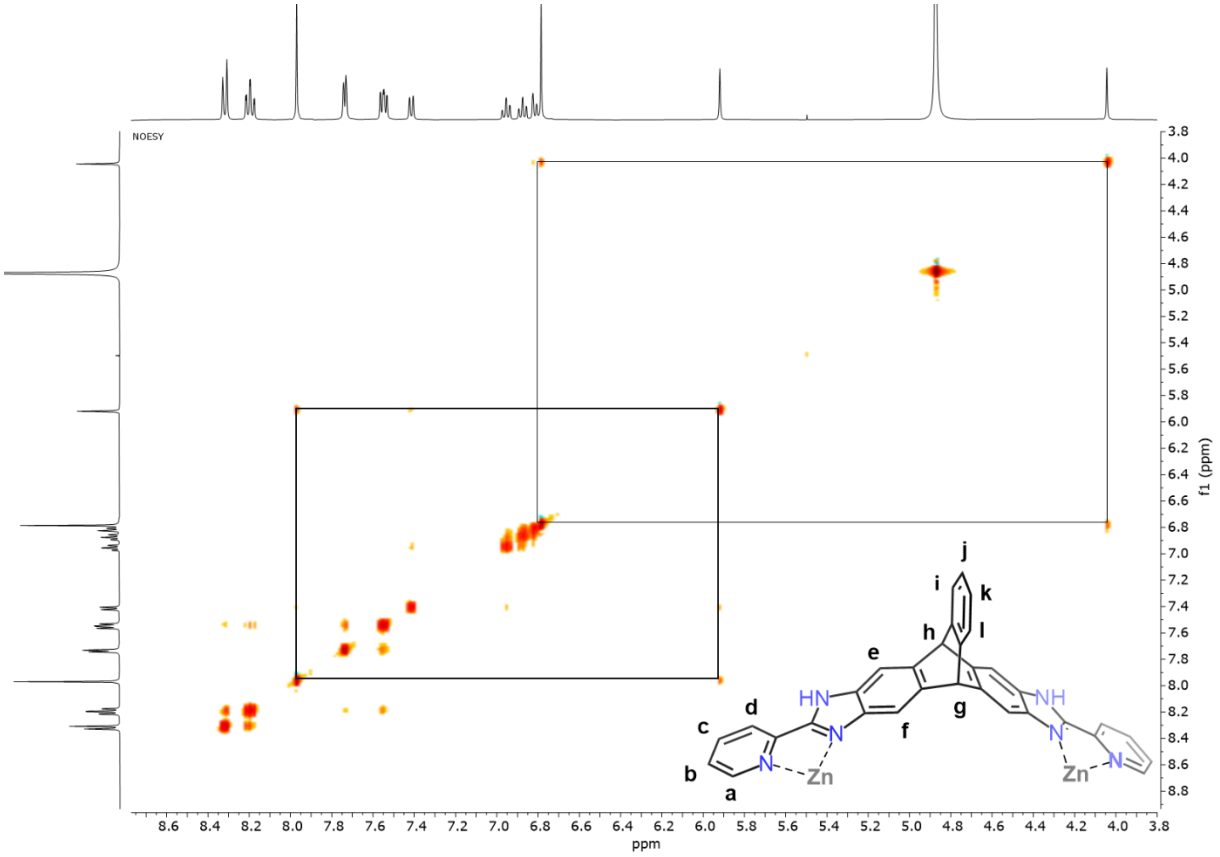


Figure S11 NOESY spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K.

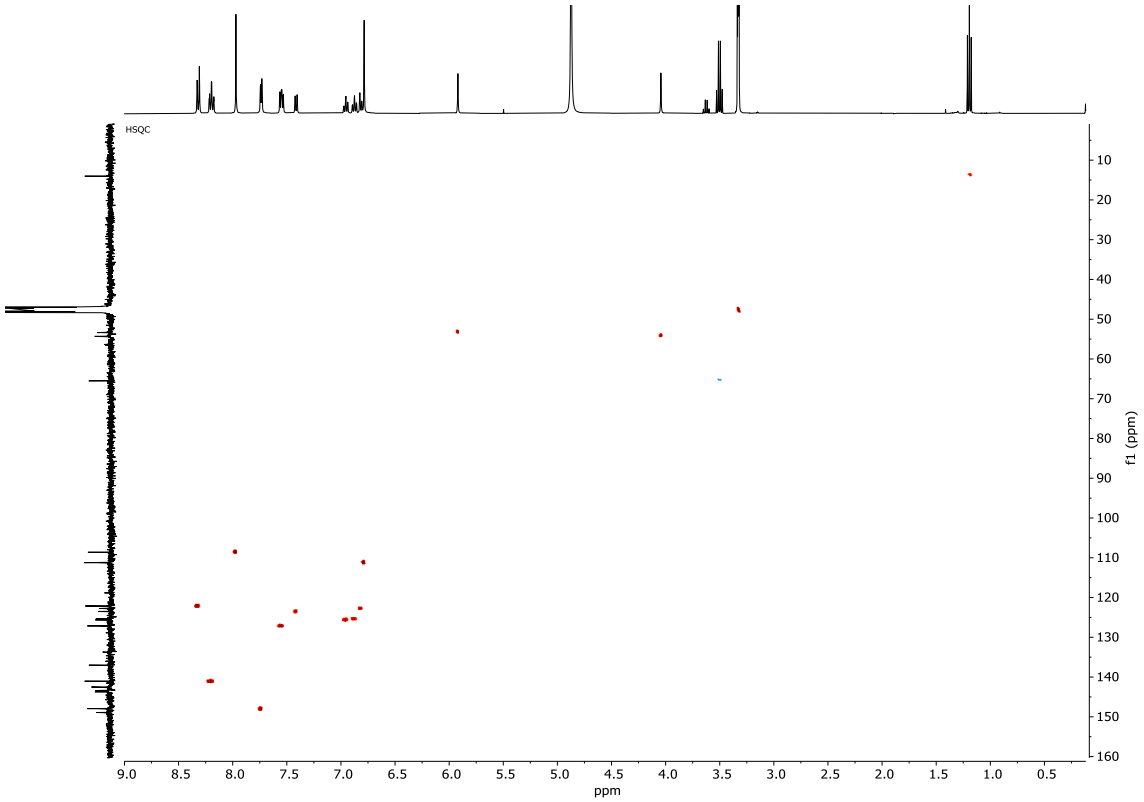


Figure S12 ^{1}H-^{13}C-HSQC spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K.

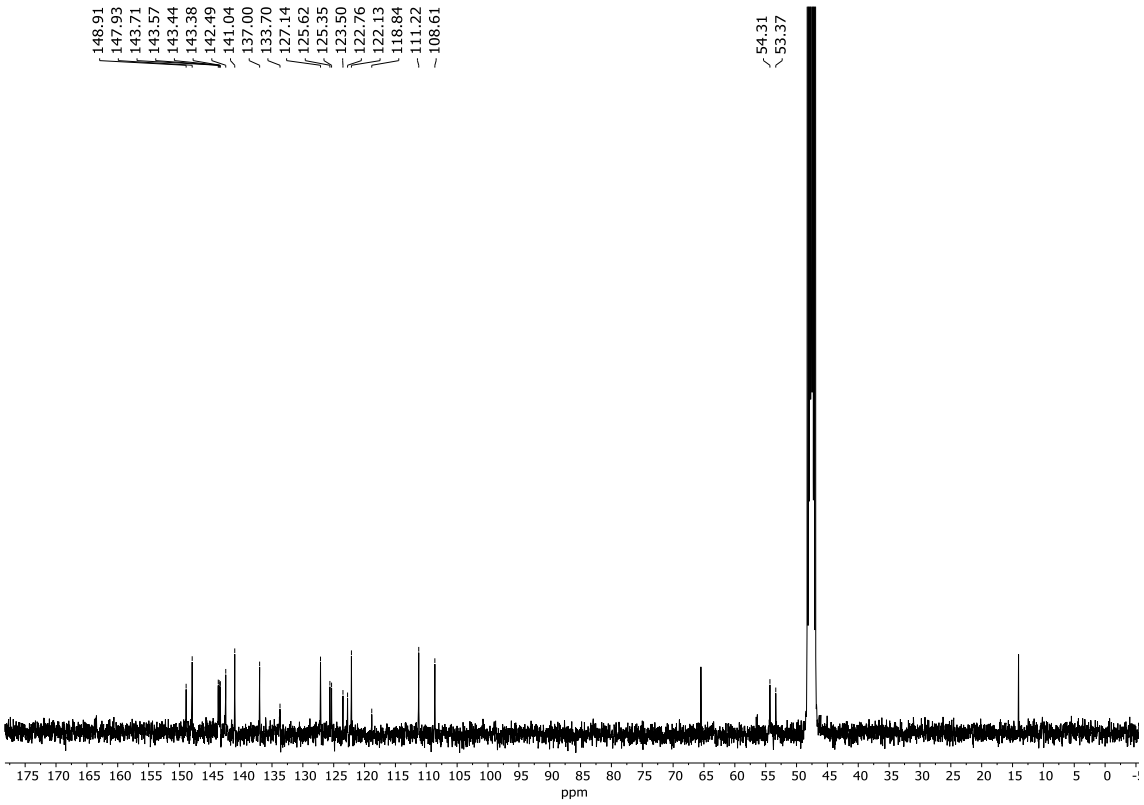


Figure S13 ^{13}C-NMR spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD at 298 K. Signals at 15 and 66 ppm are due to the CH_2-CH_3 of residual diethyl ether.

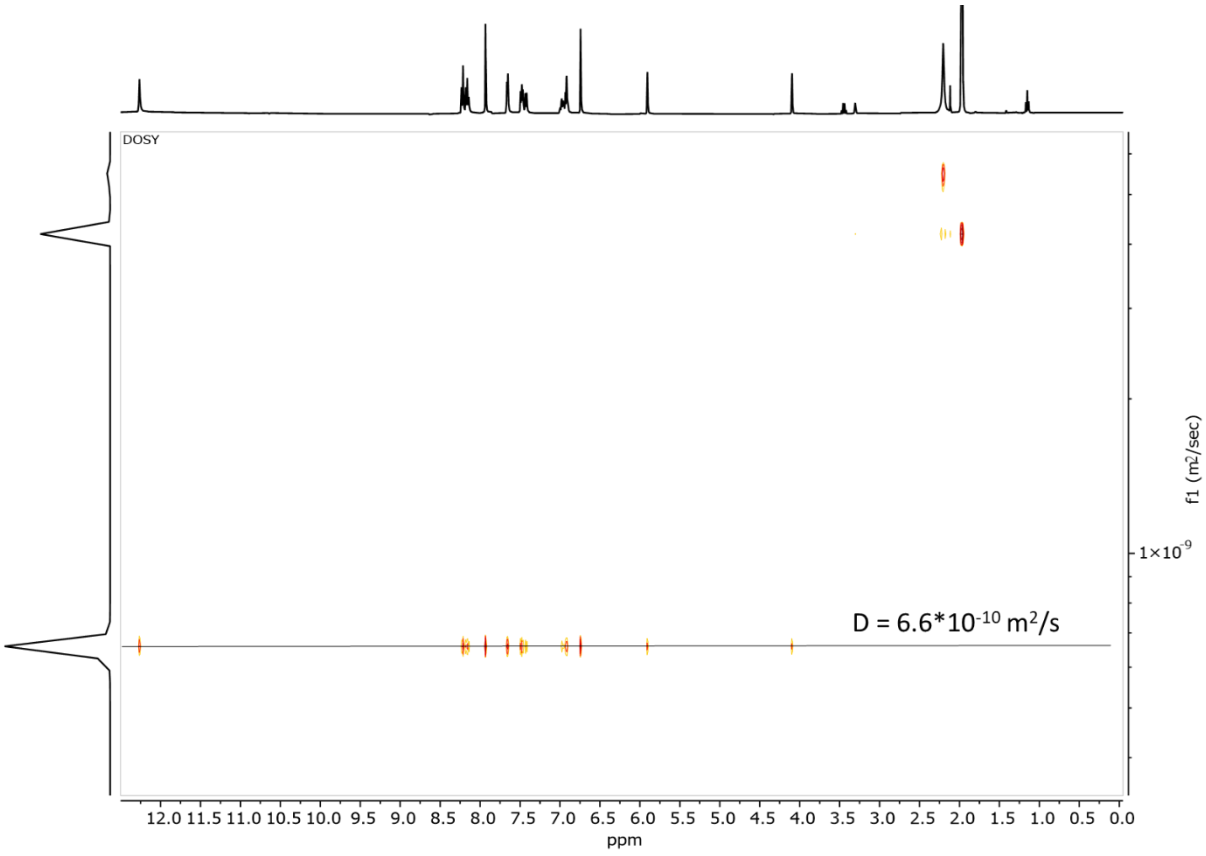


Figure S14 DOSY spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3CN at 292 K. Hydrodynamic radius, calculated with the Stoke-Einstein equation,[S4] was found to be 8.3 Å.

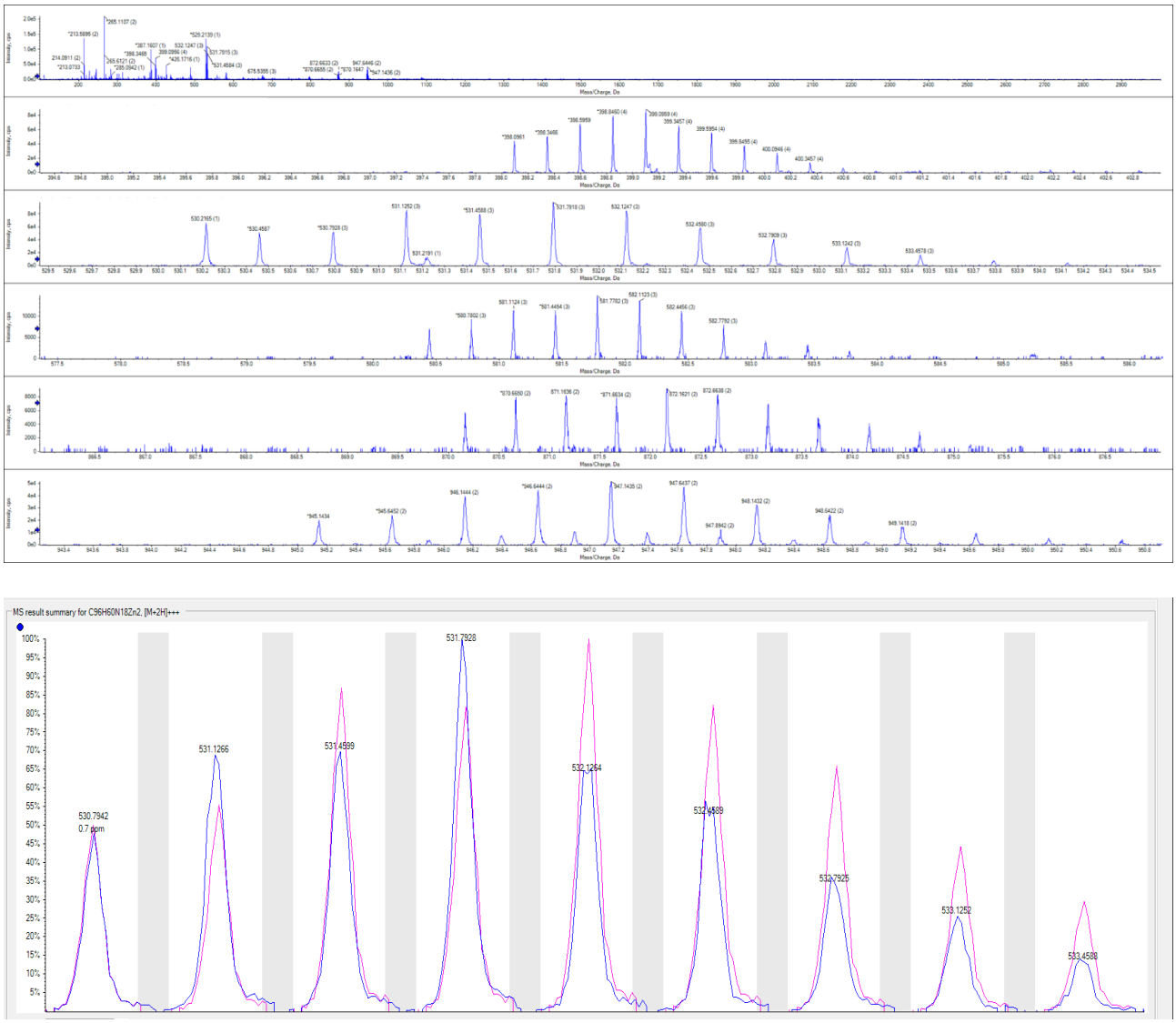


Figure S15 HRMS-ESI full spectrum of $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in MeOH. Up: Full spectrum and zoom scans of the peaks at 399.0956 $[M]^{4+}$, 531.7915 $[M–H^+]^{3+}$, 582.1123 $[M+CF_3SO_3^-]^{3+}$, 872.6633 $[M–H^+ +CF_3SO_3^-]^{2+}$, 947.6446 $[M+2CF_3SO_3^-]^{2+}$ m/z. Bottom: calculated spectrum of the $[M+CF_3SO_3^-]^{3+}$ peak superimposed to the experimental one.

3. FT-IR Spectra

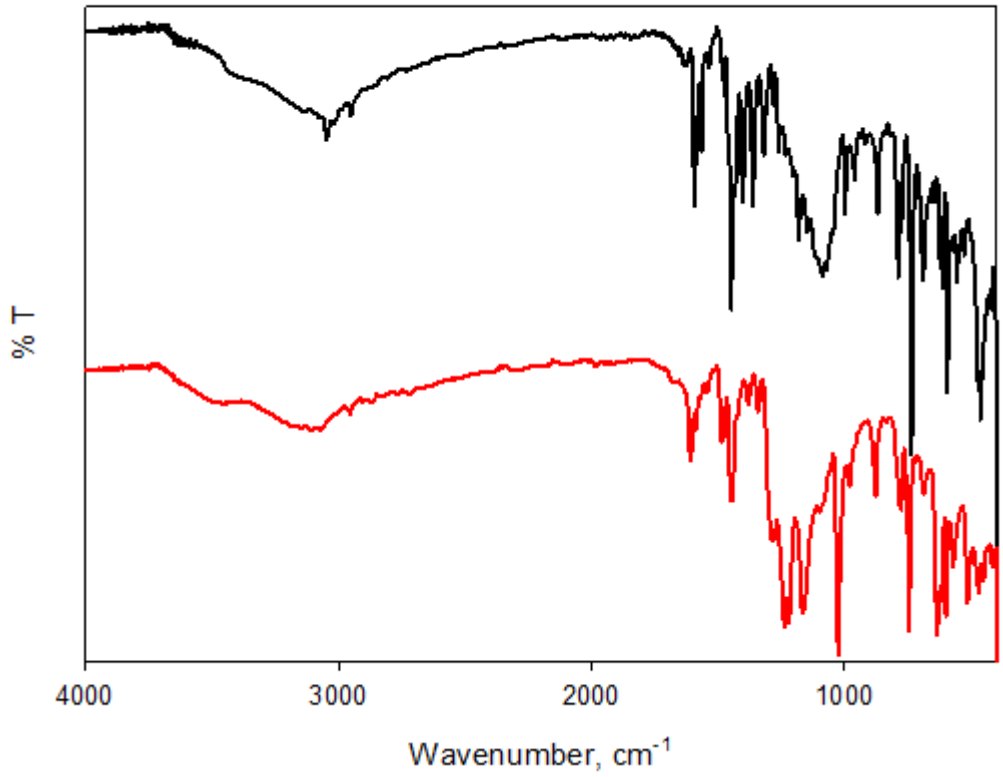


Figure S16 FT-IR (ATR) of ligand **L** (black line) and mesocate $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ (red line).

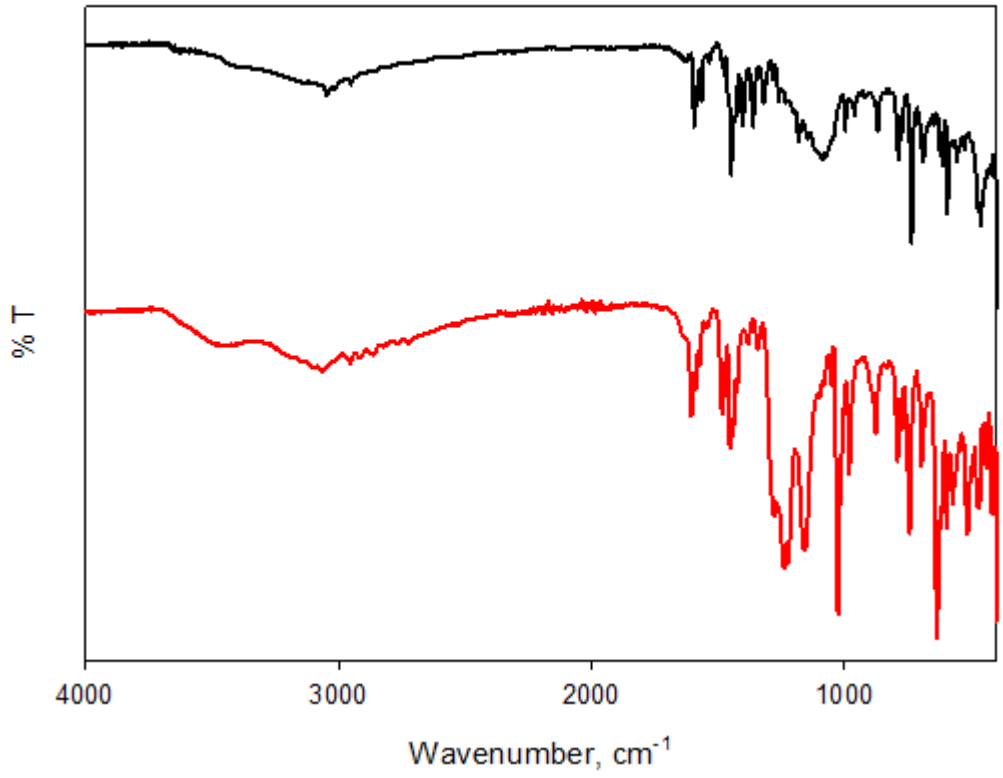


Figure S17 FT-IR (ATR) of ligand **L** (black line) and mesocate $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ (red line).

4. Cyclic Voltammetry

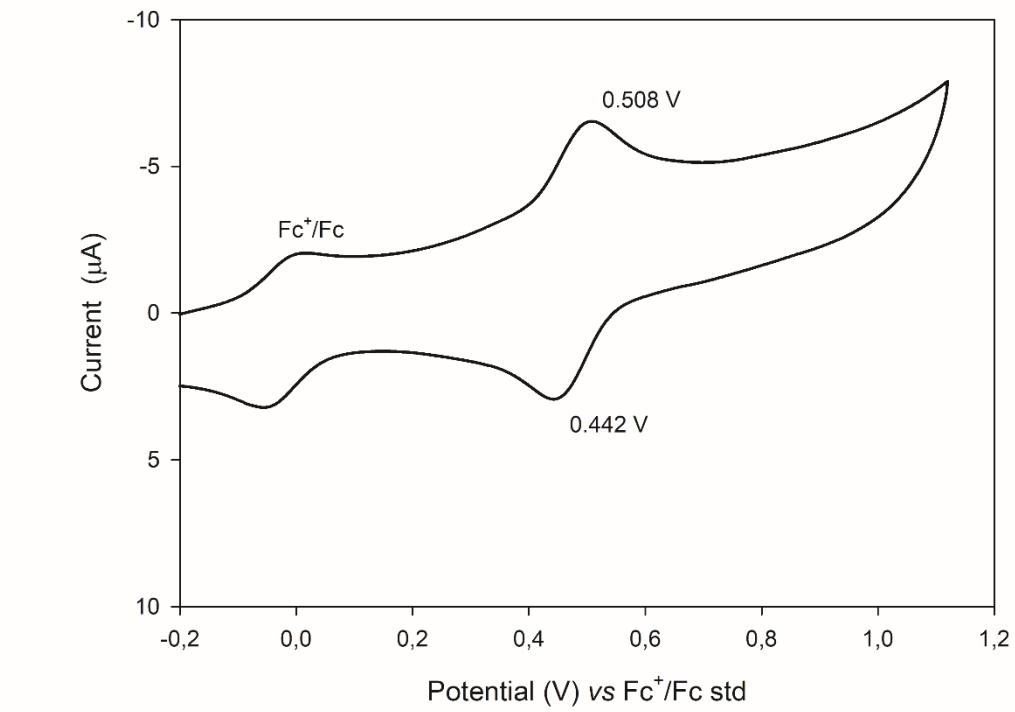


Figure S18 CV of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ 0.05 mM in CH_3CN with $TBAPF_6$ 50 mM vs (Fc^+/Fc). Scan rate 100 mV/s, $E_{1/2}$ = 0.475 mV, ΔE = 0.66 mV.

5. SCXRD study

The crystal structure of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ was determined by X-ray diffraction on single crystals. Crystal data and experimental details for data collection and structure refinement are reported in Table S1. Intensity data and cell parameters were recorded at 150(2) K on a Bruker D8 Venture PhotonII diffractometer (CuKα radiation λ = 1.54178 Å). The raw frame data were processed using SAINT and SADABS to yield the reflection data files.[S5] The structures were solved by Direct Methods using the SHELXT program[S6] and refined on F_o^2 by full-matrix least-squares procedures, using SHELXL-2018[S7] in the WinGX suite v.2021.2.[S8] All non-hydrogen atoms were refined with anisotropic atomic displacements, except for the carbon and fluorine atoms of a disordered triflate anion. The hydrogen atoms were included in the refinement at idealized geometry and refined "riding" on the corresponding parent atoms. In view of the presence of disordered electron density which could not be properly modelled, the structure was subjected to the program SQUEEZE.[S9] The program calculated a void volume of 1924 $Å^3$ and 469 electrons per unit cell, which corresponds to eleven diethyl ether molecules per unit cell. The solvent contribution to the diffraction pattern was removed and modified F_o^2 written to a new HKL file. The number of electrons corresponding to the solvent molecules were included in the formula, formula weight, calculated density, μ and F(000). The weighting scheme used in the last cycle of refinement was $w = 1/ [\sigma^2 F_o^2 + (0.1143P)^2 + 3.9857P]$, where $P = (F_o^2 + 2F_c^2)/3$. The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. 2332708 and can be obtained free of charge on application to the CCDC, 12 Union Road, Cambridge, CB2 IEZ, UK (e-mail deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

Compound	$[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$
empirical formula	$(C_{96}H_{60}Fe_2N_{18})\cdot 4(CF_3SO_3)\cdot 6.5(C_4H_{10}O)\cdot 4(H_2O)$
M	3135.09
crys syst	Monoclinic
space group	*P*21/*m*
a/Å	16.4651(5)
b/Å	23.3184(7)
c/Å	17.2067(5)
β/°	97.467(1)
V/Å^3	6550.3(3)
Z	2
ρ /g cm^{-3}	1.590
μ /mm^{-1}	3.264
F(000)	3300
total reflections	183920
unique reflections (R_{int})	14438 (0.0521)
observed reflections *[F_o>4σ(F_o)]*	13322
GOF on F^{2a}	1.005
R indices *[F_o>4σ(F_o)]*[b] *R_1*, *wR_2*	0.0538, 0.1651
largest diff. peak and hole (eÅ^{-3})	1.646,-0.847

[a]Goodness-of-fit S = $[\Sigma w(F_o^2-F_c^2)^2/(n-p)]1/2$, where n is the number of reflections and p the number of parameters. [b]$R_1 = \Sigma \| F_o | - | F_c \| / \Sigma | F_o |$, $wR_2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Table S1. Crystal data and structure refinement information for $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$.

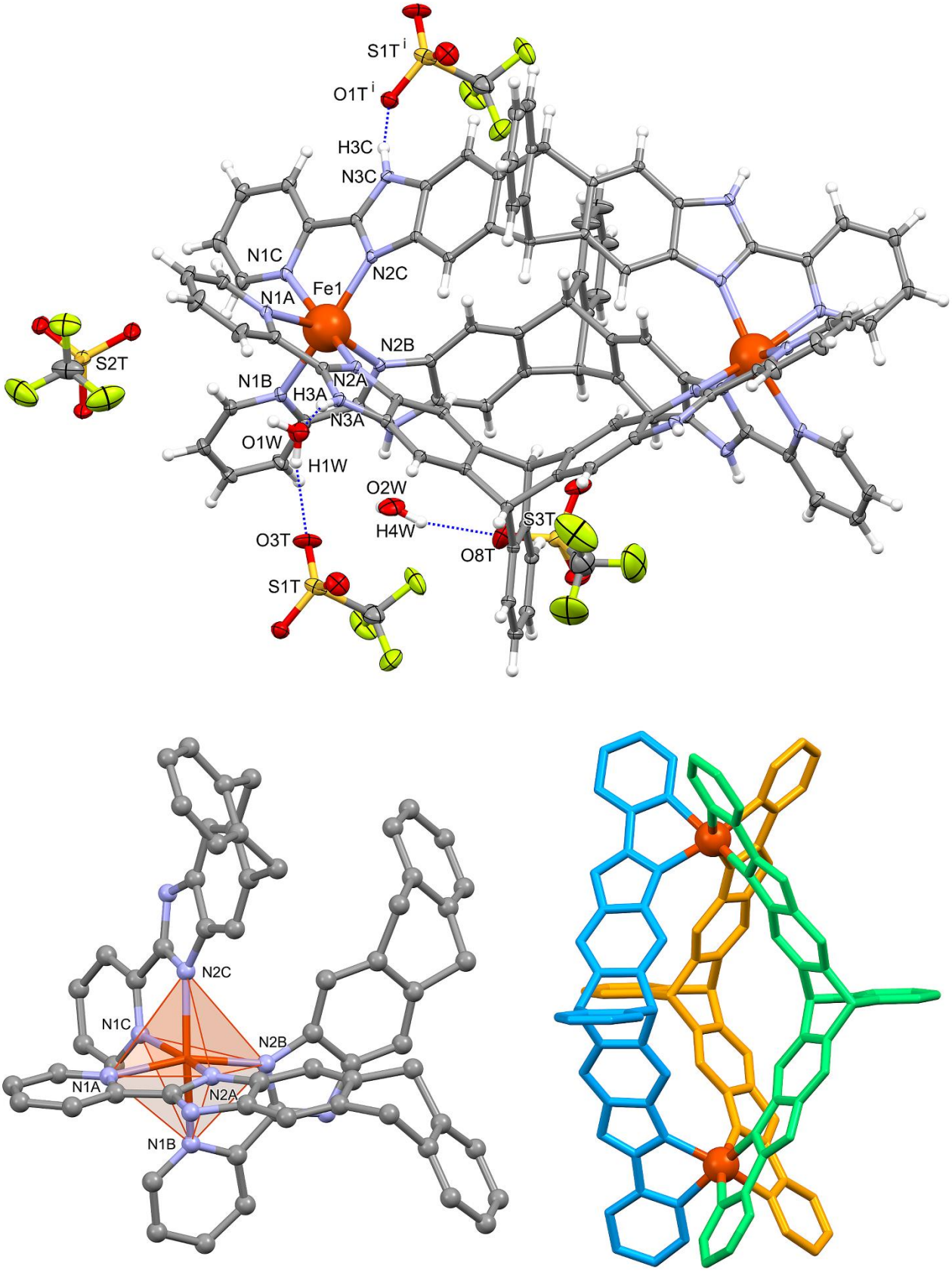


Figure S19. Top: ortep view of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ with ellipsoids at the 20% probability level. Disorder and solvent (except for water molecules forming H bonds) have been removed for clarity.

Half of the iron complex is generated by symmetry with coordinates x, ½-y, z. H bonds are shown as blue dotted lines. Symmetry code i = 1+x, y, z. Bottom: Coordination environment around Fe(II) and view of the complex with the three ligands highlighted in cyan, green and yellow.

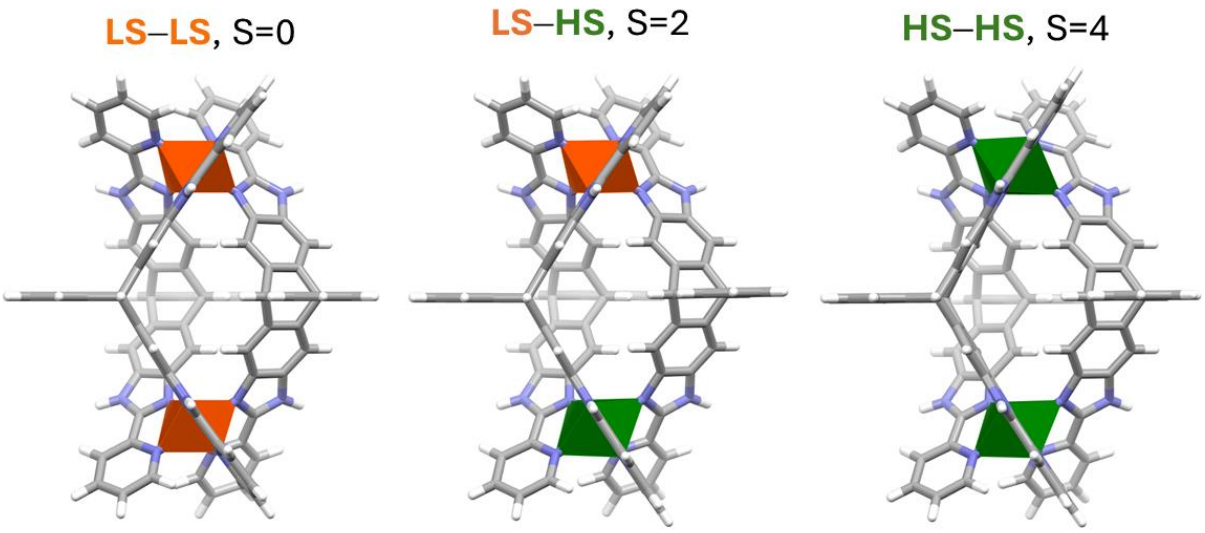
Donor-H	**Donor···Acceptor**	**H···Acceptor**	**Donor-H···Acceptor**
O1W-H1W 0.80	O1W···O3T 2.862(1)	H1W···O3T 2.08	O1W-H1W··O3T 166
O2W-H4W 0.84	O2W···O8T 2.955(1)	H4W···O8T 2.15	O2W-H4W··O8T 161
N3A-H3A 0.88	N3A···O1W 2.780(1)	H3A···O1W 1.92	N3A-H3A···O1W 165
N3B-H3B 0.88	N3B···O2W 2.737(1)	H3B···O2W 1.88	N3B-H3B···O2W 163
N3C-H3C 0.88	N3C···O1T^{i} 2.979(1)	H3C···O1T^{i} 2.15	N3C-H3C···O1T^{i} 157

i: 1+x, y, z.

Table S2. Geometrical parameters (Å, °) of the H-bonding network in $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$.

6. Computational study

The molecular structure of the diiron complex was optimized using Gaussian 16[S10] at the level of theory UB3LYP/LANL2DZ. The calculations were performed by using 32 cores and 100 Gb of RAM, at the CINECA supercomputer facility. Minima were checked to have no imaginary frequencies.



Spin	Relative difference in energy (kcal/mol)	distance Fe–Fe (Angstrom)
LS-LS (S=0)	0	10.862
HS-LS (S=2)	12.5	10.870
HS-HS (S=4)	25	10.871

Table S3. Calculated energy differences and Fe–Fe distance for the optimized structures shown in the figure above.[S11] Further information is reported in the main text (see Table 1) and in Appendix 1.

7. ^{1}H-NMR Studies

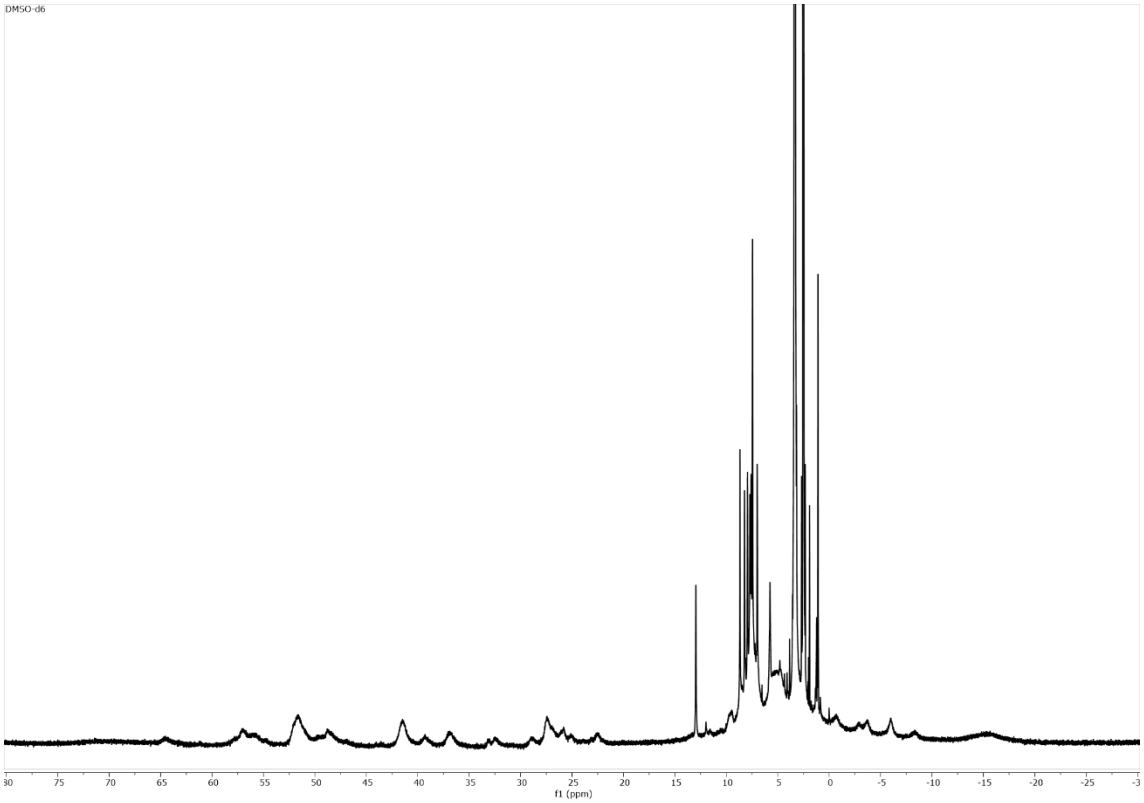


Figure S20 Paramagnetic ^{1}H-NMR spectrum of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in DMSO-d_6 at 298 K. As observed by other authors,[S12] the complex showed good solubility in DMSO but rapidly decomposed, as confirmed by the emergence of signals attributed to the free ligand in the diamagnetic region of the spectrum.

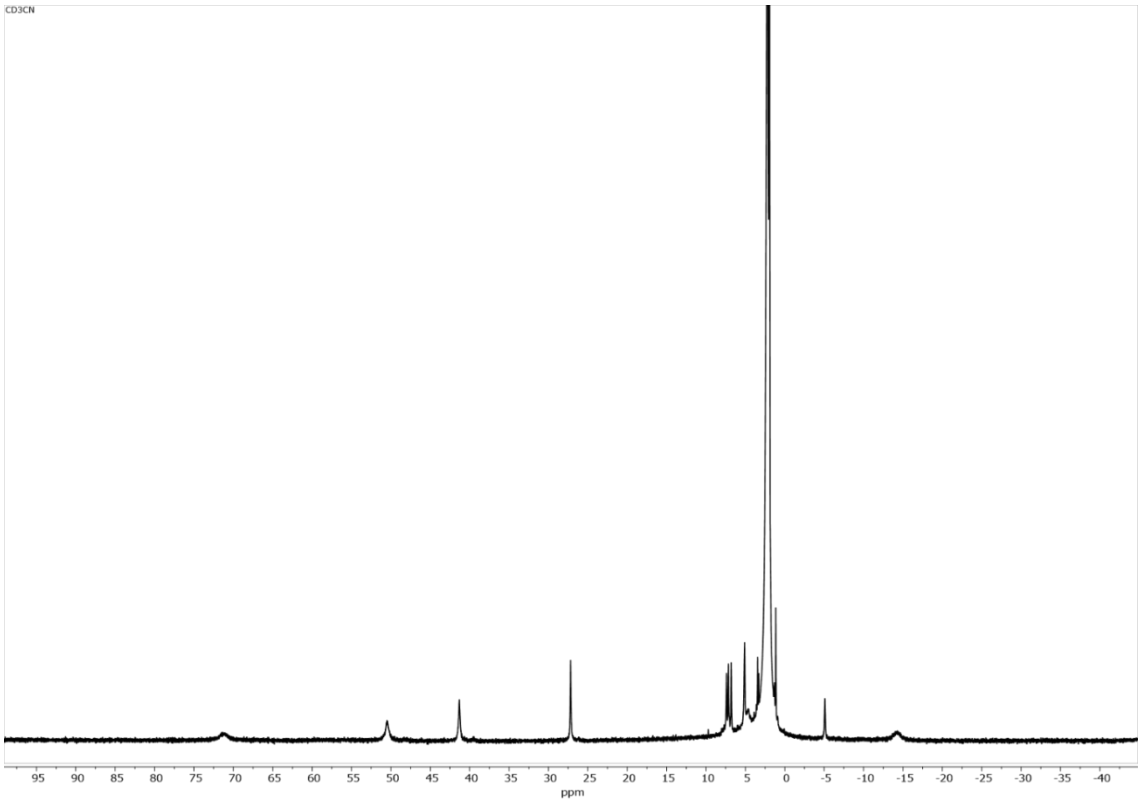


Figure S21 Paramagnetic ^{1}H-NMR spectrum of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3CN at 298 K.

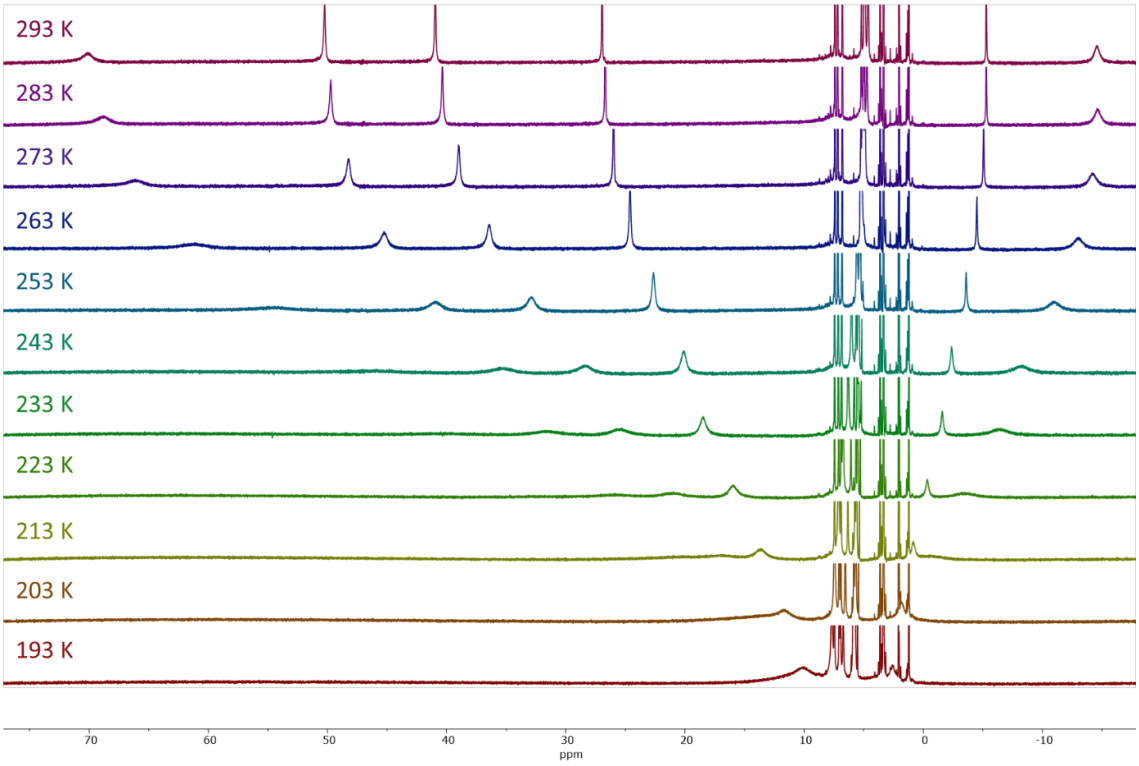


Figure S22 Stacked spectra, obtained by variable temperature ^{1}H-NMR, from 193 to 293 K for complex $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD.

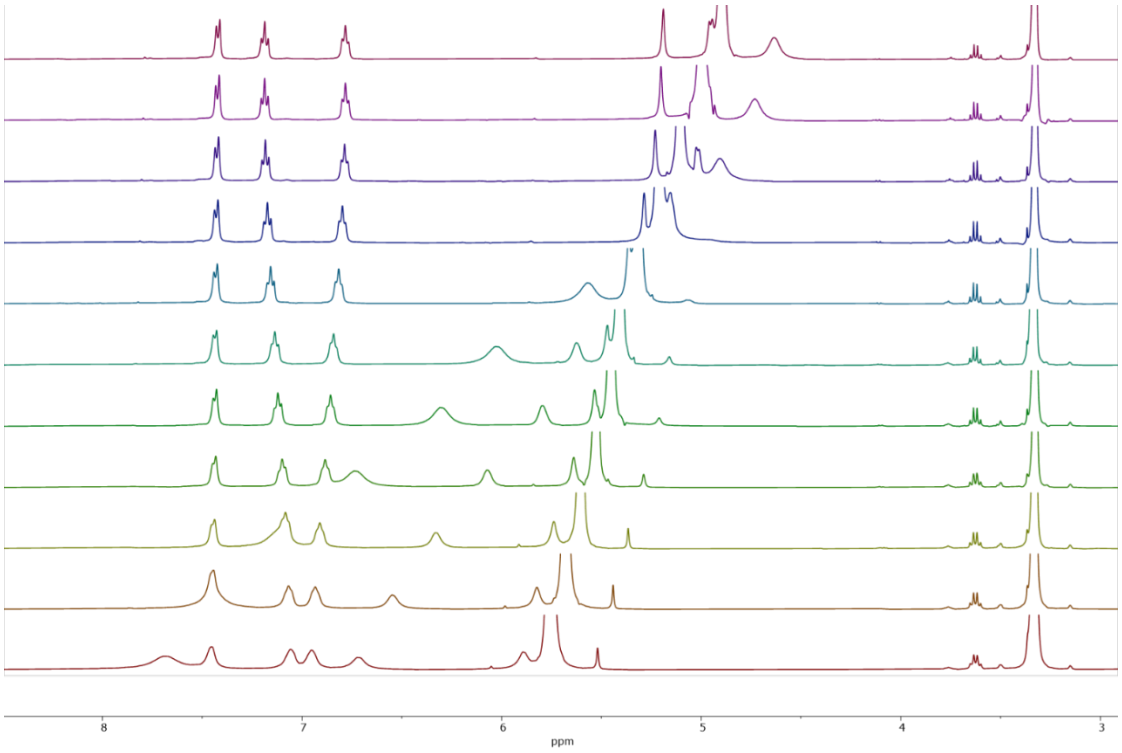


Figure S23 Stacked spectra, obtained by variable temperature ^{1}H-NMR experiment, from 193 to 293 K for complex $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD (diamagnetic region).

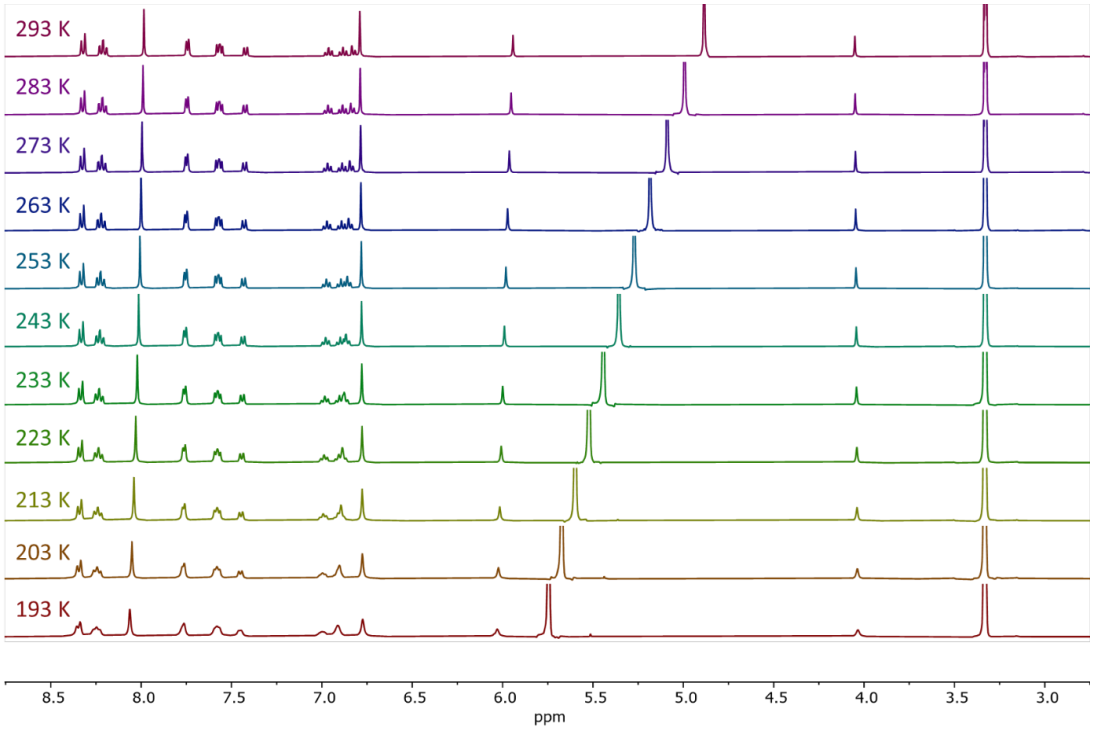


Figure S24 Stacked spectra, obtained by variable temperature ^{1}H-NMR experiment, from 193 to 293 K for complex $[Zn_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD.

8. Evans Method

For the Evans method,[S13-S14] a paramagnetic solution of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ (2.5 mM) in CD_3OD was prepared.

The inner tube was loaded with 50 μL of the paramagnetic solution and 5 μL of $CHCl_3$ to obtain a final concentration of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ of 2.3 mM. The outer tube was loaded with 500 μL of CD_3OD and 50 μL of $CHCl_3$.

The difference, in Hz, between the chemical shift of the $CHCl_3$ peak in the paramagnetic solution (inner tube) and that of $CHCl_3$ in deuterated methanol (outer tube) at a certain temperature is defined as Δf (Figure S25 and Table S4). This value was used to calculate the molar susceptibility of the complex at that temperature by the equation (S1):

$$\chi_m = \frac{3\Delta f}{4\pi c F} \qquad \text{S1}$$

Where "*c"* is the concentration of the paramagnetic solution in mmol·L^{-1} and "F" is the spectrometer frequency in MHz (400 MHz). We decided to calculate the χ_m for each iron centre and therefore the value of the concentration "*c*" was 4.6 mmol·L^{-1}

The χ_m (cm^{3}mol^{-1}) values obtained at each temperature were then multiplied for the relative T (K) to obtain the molar magnetic susceptibility $\chi_m T$ (cm^{3}mol^{-1}K). Experimental $\chi_m T$ values were plotted against T and finally modelled with the regular solution model (Equation S2).[S13-S14] The modelling to equation S2 was carried out in SigmaPlot 11.0® from Systat Software Inc.

$$\chi_m T(T) = \frac{\chi_m T(\max)}{1+e^{\left(\frac{\Delta H}{RT}-\frac{\Delta S}{R}\right)}} \qquad \text{S2}$$

Where "$\chi_m T(T)$" is the multiplication between the temperature T and the molar magnetic susceptibility at that temperature, "$\chi_m T(max)$" is a constant set to 3.7 cm^{3}mol^{-1}K (molar magnetic susceptibility of high spin iron (II) centre) and "*R*" is the ideal gas constant (8.314 Jmol^{-1}K^{-1}).

The parameters obtained from the fit are the thermodynamic enthalpy and entropy values associated with the SCO event, *i.e* ΔH (kJ K mol^{-1}) and ΔS (J mol^{-1}).The SCO transition temperature "$T_{1/2}$" (K) was calculated form $\Delta H/\Delta S$.

Note that the Evans method has an intrinsic error of 5-10% in the determination of $\chi_m T$(T) due to instrument instability in the temperature setting of ± 1 K.

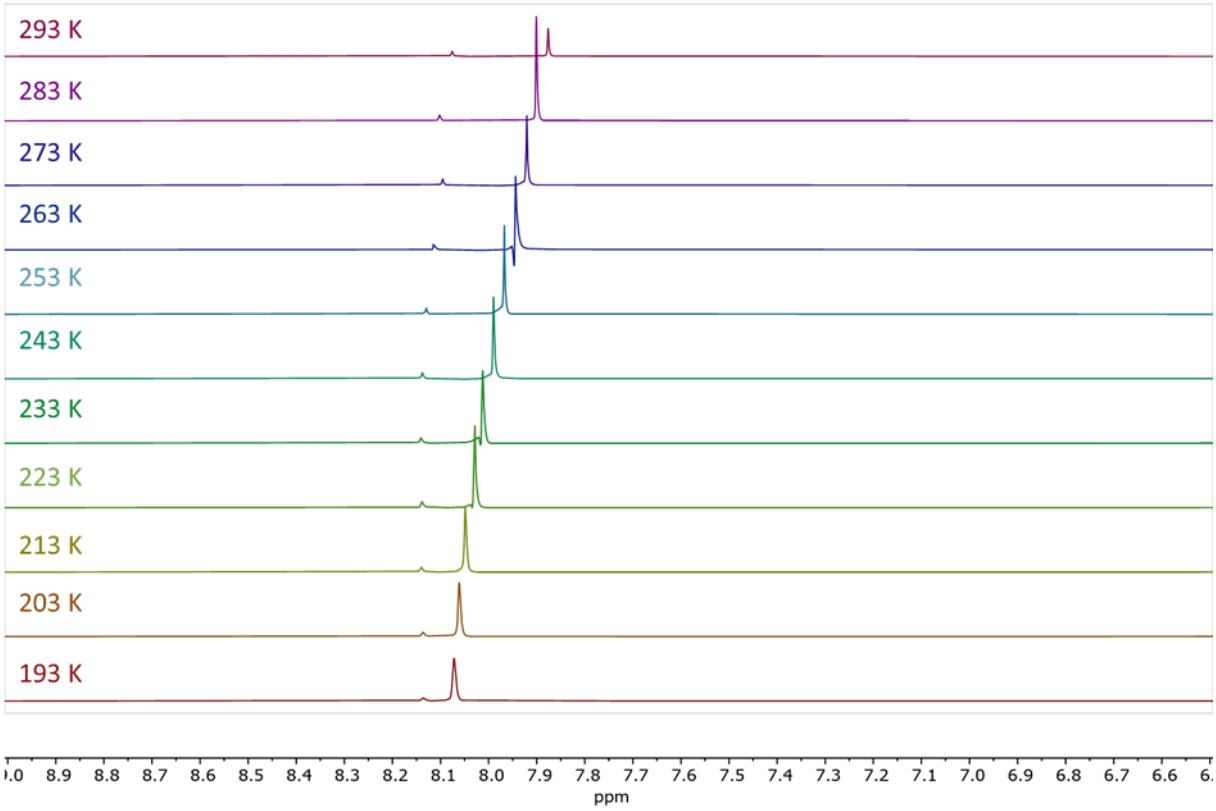


Figure S25 Stacked ^{1}H-NMR spectra of complex $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD obtained for the Evans method from 193 to 293 K ($CHCl_3$ signals).

T (K)	**Δf *(Hz)***	**$\chi_m T$ (cm^3 K mol^{-1})**
193	25.5	0.642
203	30.2	0.799
213	36.6	1.02
223	44.0	1.28
233	51.5	1.56
243	59.3	1.88
253	65.1	2.15
263	68.4	2.36
273	69.8	2.48
283	70.4	2.60
293	70.0	2.67

Table S4 Experimental data from Evans experiment for a 2.3 mM solution of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in CD_3OD (4.6 mM in Fe(II)).

ΔH (kJ K mol^{-1})	ΔS (J mol^{-1})	$T_{1/2}$ (K)
12.9 (0.4)	52.9 (0.5)	243 (7)

Table S5 Thermodynamic values of the SCO event obtained by fitting experimental Evans data with the equation S2. $T_{1/2}$ obtained by $\Delta H/\Delta S$. Errors are reported in brackets.

9. VT-UV-vis $[Fe_2(L)_3](CF_3SO_3)_4$

The UV-vis. spectra of a methanol solution of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ (0.075 mM) were recorded from 193 K to 313 K. The resulting VT-UV-vis data were then modelled using the regular solution model (Equation S3).[S14] The decreasing absorbance at 528 nm with increasing temperature can be correlated to the increasing population of the Fe(II) High Spin (HS) state. In thermal equilibrium state, the extinction coefficient "ε" can be defined as a function of temperature (Equation S3).

$$\varepsilon(T) = \frac{\varepsilon_0}{1+e^{\left(\frac{-\Delta H}{RT}+\frac{\Delta S}{R}\right)}} \qquad \text{S3}$$

Where "$\varepsilon(T)$" is the molar extinction coefficient as a function of temperature, "ε_0" is the extinction coefficient for a fully Low Spin state (*i.e.* %HS = 0) and "*R*" is the ideal gas constant (8.314 $Jmol^{-1}K^{-1}$).

The value of "ε_0" can be estimated from the linear correlation between the %HS derived from the Evans method and the extinction coefficient obtained from the VT-UV-vis. experiment (see chapter 8).

T (K)	**$\varepsilon \cdot 10^3$@528 nm** ***(L cm^{-1} mol^{-1})***	**$\varepsilon \cdot 10^3$@528 nm per Fe(II)** ***(L cm^{-1} mol^{-1})***
193	9.4	4.7
203	8.7	4.4
213	8.0	4.0
223	7.2	3.6
233	6.3	3.2
243	5.6	2.8
253	4.9	2.5
263	4.3	2.2
273	3.8	1.9
283	3.4	1.7
293	2.9	1.5
303	2.6	1.3
313	2.4	1.2

Table S6 Experimental data from VT UV-vis. experiment for a 0.075 mM solution of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in methanol (0.15 mM in Fe(II)).

9.1 Estimation of ε_0 from %HS *vs* ε

The VT-UV-vis spectra were recorded from 193 K to 313 K with a 10 K increasing rate in methanol. The extinction coefficient ε values observed at 528 nm are due to the LS state and can be correlated with the %HS obtained by the Evans method.[S13] %HS from the Evans method data was calculated assuming $\chi_M T(max)$ = 3.7 K cm^3 mol^{-1} for the fully High Spin state. Plotting %HS *vs* ε (per Fe(II) ion) gave the linear relationship noted in the insert in Figure S26. The linear equation %HS = m*ε+q was then used to calculate the ε_0 expected for the fully LS state (*i.e.* %HS = 0).

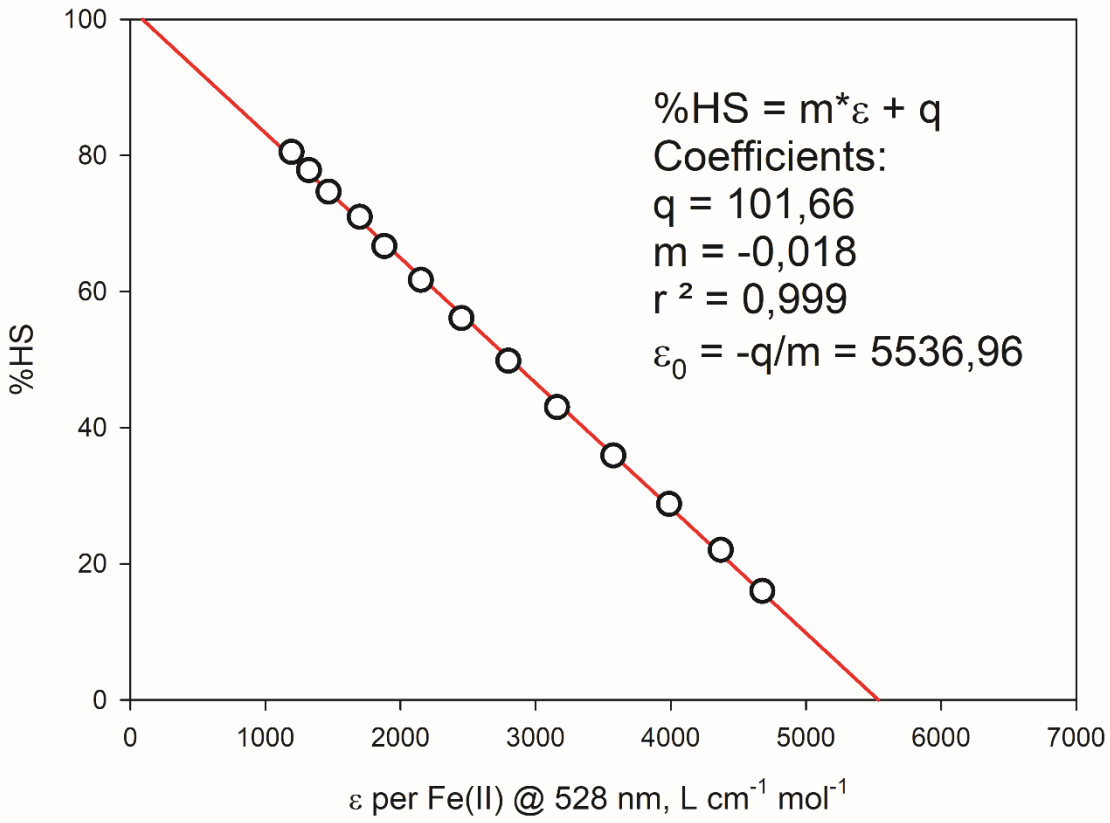


Figure S26 Plot of %HS (obtained from Evans method) *vs* extinction coefficient per metal ion (obtained from VT-UV-vis. studies) of 528 nm band of complex in 0.075 mM methanol solution (R^2 = 0.999).

The parameters obtained from the fit are the thermodynamic enthalpy and entropy values associated with the SCO event, *i.e* ΔH and ΔS. The SCO transition temperature ($T_{1/2}$) was calculated form ΔH/ΔS.

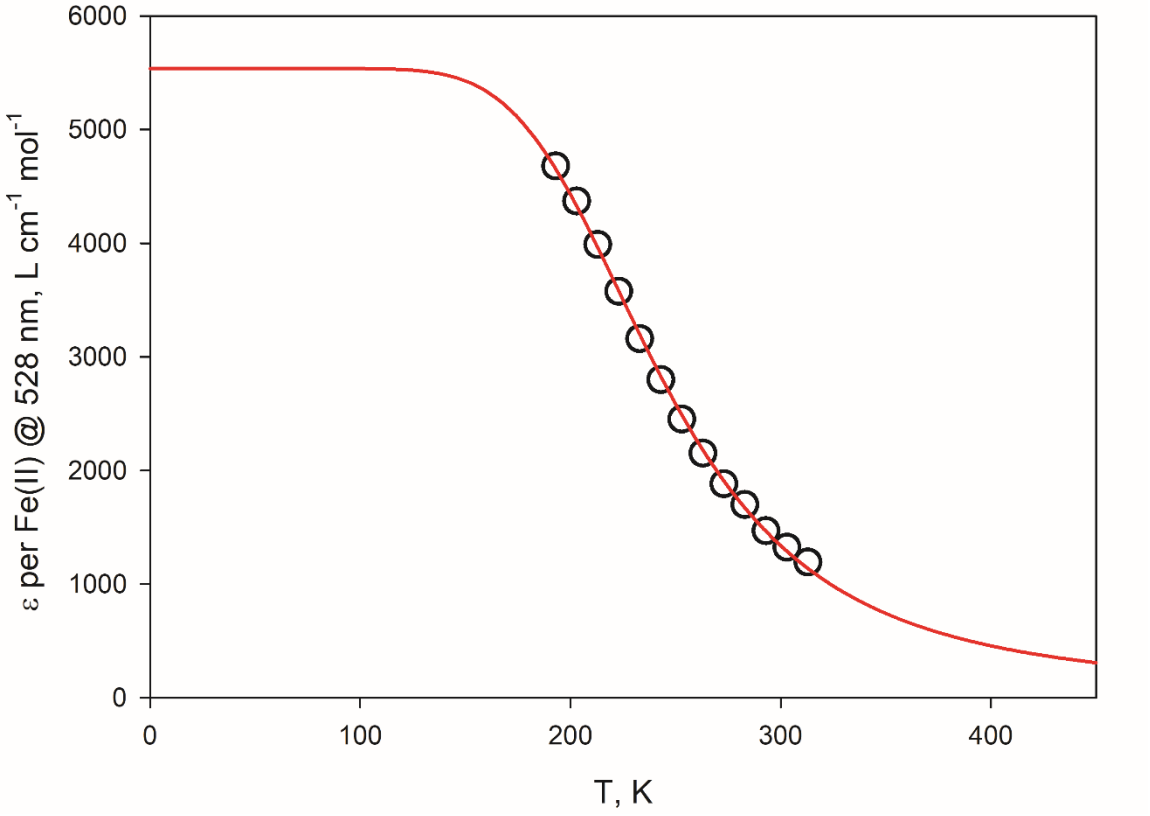


Figure S27 Plot of ε *vs* T for a 0.075 mM solution (0.15 mM in Fe(II)) of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in methanol from VT UV-vis. studies (l = 1 cm). Black dots: experimental data; Red curve: fitted model from equation S3. Thermodynamic values reported in table S7.

Δ*H* (kJ K mol^{-1})	**Δ*S* (J mol^{-1})**	***T*$_{1/2}$ (K)**
12.6 (0.4)	52 (1)	242 (9)

Table S7 Thermodynamic values of the SCO event obtained by fitting experimental VT UV-vis. data with the equation S3 constraining ε_0 value to $5.5 \cdot 10^3$ Lcm^{-1}mol^{-1}. $T_{1/2}$ obtained by ΔH/ΔS. Errors are reported in brackets.

To decrease the dependence of the thermodynamic values obtained by VT-UV-vis method compared to those obtained by Evans method we also tried to fit the data from VT-UV-vis experiment with equation S3 without constraining the ε_0.

The obtained ε_0 value ($5.8 \cdot 10^3$ $Lcm^{-1}mol^{-1}$) is in good agreement with that obtained from the correlation of %HS (from Evans method) *vs* ε per metal ion (from VT-UV-vis studies) at 528 nm. Also the thermodynamic values (ΔH, ΔS and the resulting $T_{1/2}$) are very similar to those previously reported.

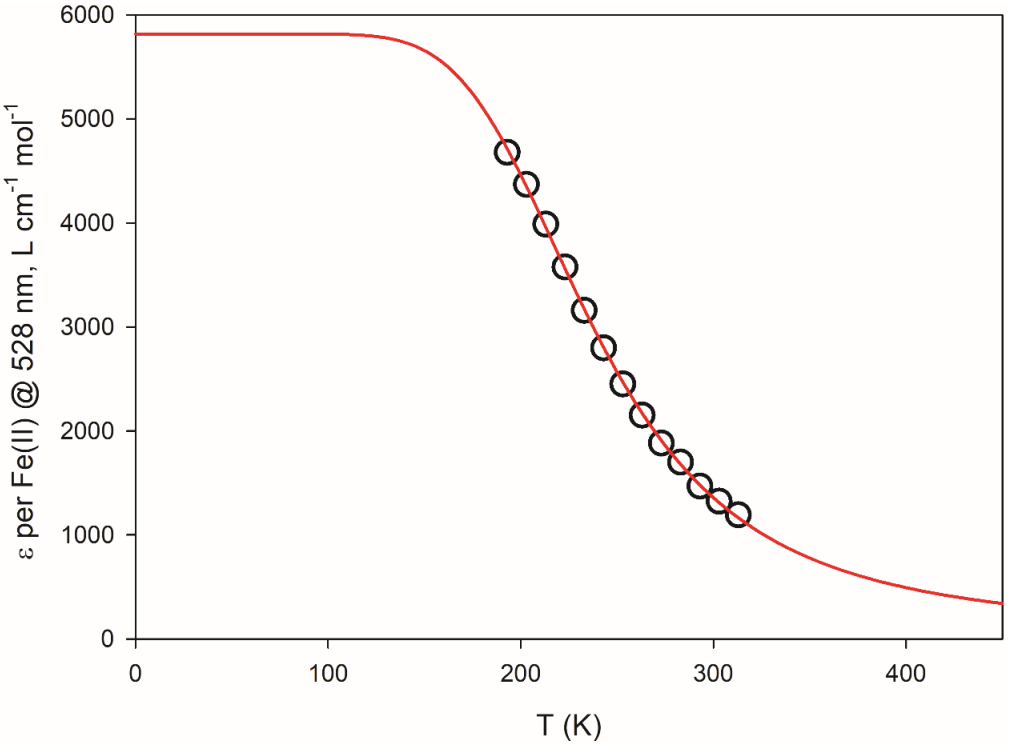


Figure S28 Plot of ε vs T for a 0.075 mM solution (0.15 mM in Fe(II)) of $[Fe_2(\mathbf{L})_3](CF_3SO_3)_4$ in methanol from VT UV-vis studies (l = 1 cm). Black dots: experimental data; Red curve: fitted model from equation S3. ε_0 and thermodynamic values reported in table S8.

ε_0 (L cm^{-1} mol^{-1})	**ΔH (kJ K mol^{-1})**	**ΔS (J mol^{-1})**	**$T_{1/2}$ (K)**
$5.8 \cdot 10^3$	11.9 (0.2)	49.5 (0.7)	240 (3)

Table S8 Molar absorbance of LS-LS species (ε_0) and thermodynamic values of SCO event obtained by fitting experimental VT UV-vis data with the equation S3 without constraining ε_0 value. $T_{1/2}$ obtained by ΔH/ΔS. Errors are reported in brackets.

10. Appendix 1

Cartesian coordinates (in Angstrom) for the optimized complexes.

Singlet (charge +4)

C	6.14633600	2.07088700	1.89327400
C	4.98087000	1.37795700	2.41732000
C	3.22610600	0.71064700	3.64216300
C	2.21271800	0.53025300	4.60345300
C	1.21684100	-0.38841300	4.28493200
C	1.22557000	-1.10958300	3.04378000
C	2.24495000	-0.94809600	2.10866700
C	3.27060200	-0.02022500	2.41518800
C	0.00000000	-0.72160500	5.15893900
C	-1.21684100	-0.38841300	4.28493200
C	-1.22557000	-1.10958300	3.04378000
C	0.00000000	-2.02740300	2.89149600
C	-2.21271800	0.53025300	4.60345300
C	-3.22610600	0.71064800	3.64216300
C	-3.27060200	-0.02022400	2.41518800
C	-2.24495000	-0.94809600	2.10866700
C	-4.98087000	1.37795700	2.41732000
C	-6.14633600	2.07088800	1.89327300
C	0.00000000	-2.24765200	5.34356300
C	0.00000000	-2.93385600	6.56308500
C	-0.00000100	-5.05097000	5.33464000
C	-0.00000100	-4.35303500	4.10593000
C	0.00000000	-2.95368100	4.11893100
N	6.54884500	1.57077600	0.67545200
N	4.39183300	0.41610600	1.68172400
N	4.32162000	1.58141700	3.60823800
N	-4.39183200	0.41610700	1.68172400
N	-6.54884500	1.57077700	0.67545200
N	-4.32162000	1.58141700	3.60823800
C	-7.61799200	2.14890600	0.06859000

C	-8.32082300	3.22590500	0.63477700
C	-6.80322700	3.14469300	2.51851800
C	0.00000000	-4.34656900	6.55385700
C	6.14741000	-2.67403700	0.84686500
C	4.98149200	-2.78203700	-0.01453500
C	3.22637300	-3.51027200	-1.20352200
C	2.21281000	-4.25327000	-1.83924500
C	1.21680800	-3.51878700	-2.47613300
C	1.22558800	-2.08332700	-2.48180500
C	2.24511200	-1.35358500	-1.87540800
C	3.27084900	-2.08226300	-1.22443300
C	0.00000000	-4.10999600	-3.20093200
C	-1.21680900	-3.51878700	-2.47613300
C	-1.22558800	-2.08332700	-2.48180500
C	0.00000000	-1.49343200	-3.20125900
C	-2.21281100	-4.25326900	-1.83924500
C	-3.22637400	-3.51027200	-1.20352200
C	-3.27084900	-2.08226300	-1.22443300
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C	-4.98149300	-2.78203700	-0.01453500
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C	0.00000000	-2.10221400	-7.04058600
C	0.00000000	-2.09504000	-4.61642300
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N	4.39221400	-1.66447000	-0.48043600
N	4.32216400	-3.91553000	-0.43251600
N	-4.39221500	-1.66447000	-0.48043700
N	-6.54995900	-1.36921600	1.02157200
N	-4.32216500	-3.91552900	-0.43251600
C	-7.61977700	-1.13217900	1.82461600
C	-8.32323800	-2.16058300	2.47423300
C	-6.80491800	-3.75202700	1.46420000

C	0.00000000	-3.51028300	-7.03844200
C	6.14642500	0.60475000	-2.73996800
C	4.98070500	1.40477300	-2.40217200
C	3.22589200	2.79903800	-2.43727400
C	2.21262200	3.72169500	-2.76213800
C	1.21678900	3.90573300	-1.80739900
C	1.22552100	3.19213100	-0.56188400
C	2.24482000	2.30160500	-0.23374200
C	3.27036700	2.10237700	-1.19054200
C	0.00000000	4.82920300	-1.95634200
C	-1.21678800	3.90573200	-1.80739900
C	-1.22552100	3.19213100	-0.56188400
C	0.00000000	3.51973700	0.30895200
C	-2.21262100	3.72169400	-2.76213900
C	-3.22589100	2.79903700	-2.43727500
C	-3.27036700	2.10237700	-1.19054300
C	-2.24482100	2.30160500	-0.23374200
C	-4.98070400	1.40477100	-2.40217300
C	-6.14642400	0.60474800	-2.73996800
C	0.00000000	5.75280700	-0.72758600
C	-0.00000100	7.15203500	-0.74390400
C	-0.00000100	7.14816300	1.70378400
C	-0.00000100	5.73511100	1.71453500
C	0.00000000	5.04597200	0.49655900
N	6.54922700	-0.19931500	-1.69768400
N	4.39161500	1.24895900	-1.20134100
N	4.32143300	2.33406000	-3.17418700
N	-4.39161400	1.24895800	-1.20134200
N	-6.54922700	-0.19931500	-1.69768300
N	-4.32143100	2.33405800	-3.17418900
C	-7.61872600	-1.01354800	-1.89460000
C	-8.32161400	-1.06184600	-3.11036600
C	-6.80340400	0.60925600	-3.98248500
C	-0.00000100	7.85113100	0.48373800

C	0.00000000	-1.38558900	-5.82268500
H	0.00000000	-4.05172500	-7.98017800
H	0.00000000	-1.56619900	-7.98577200
H	2.20281600	-5.33924300	-1.82881000
H	2.24326400	-0.27029600	-1.87744500
H	-2.20281700	-5.33924300	-1.82881000
H	-2.24326500	-0.27029600	-1.87744500
H	-0.00000100	-4.90182100	3.16650500
H	-0.00000100	-6.13754300	5.34170300
H	0.00000000	-4.89257000	7.49295800
H	0.00000000	-2.39566900	7.50776200
H	2.24287000	-1.49027100	1.17080600
H	2.20268900	1.08128700	5.53930100
H	2.24281800	1.76143800	0.70527500
H	2.20267500	4.25620000	-3.70752300
H	-0.00000100	5.19651200	2.65983900
H	-0.00000100	7.70049300	-1.68265700
H	-0.00000100	7.69810600	2.64093500
H	-0.00000100	8.93741800	0.48640000
H	-2.20267400	4.25619800	-3.70752400
H	-2.24281900	1.76143800	0.70527500
C	-7.90951900	-0.23633400	-4.17298100
H	-8.43518200	-0.25086500	-5.12250300
H	-6.46495500	1.25162800	-4.78991800
H	-7.92446700	-1.63042100	-1.06031800
C	-7.91135700	-3.49373500	2.29117600
H	-8.43744200	-4.30853400	2.77847800
H	-6.46665600	-4.77258900	1.31199700
H	-7.92539700	-0.10114900	1.94123300
H	-9.17318700	-1.91711300	3.10257200
C	-7.90900300	3.73291200	1.88128400
H	-7.92353000	1.73525200	-0.88303000
H	-9.17024100	3.64929900	0.10968000
H	-8.43461600	4.56247400	2.34354500

H	-6.46500300	3.52237900	3.47877500
H	-2.24287000	-1.49027000	1.17080600
H	-2.20268900	1.08128700	5.53930100
C	6.80322800	3.14469200	2.51851800
C	7.90900400	3.73291200	1.88128400
H	6.46500300	3.52237800	3.47877500
C	8.32082400	3.22590400	0.63477800
C	7.61799300	2.14890500	0.06859100
H	8.43461600	4.56247400	2.34354600
H	7.92353100	1.73525200	-0.88302900
H	9.17024200	3.64929800	0.10968100
C	6.80340600	0.60925900	-3.98248400
C	7.90952000	-0.23633100	-4.17298000
C	8.32161400	-1.06184500	-3.11036700
H	8.43518400	-0.25086200	-5.12250200
C	7.61872600	-1.01354900	-1.89460100
H	9.17129600	-1.72799100	-3.21424400
H	6.46495800	1.25163200	-4.78991600
H	7.92446600	-1.63042300	-1.06032000
C	6.80491600	-3.75202700	1.46420000
C	7.91135600	-3.49373600	2.29117600
C	8.32323900	-2.16058500	2.47423200
C	7.61977800	-1.13218000	1.82461400
H	7.92539900	-0.10115000	1.94123000
H	9.17318800	-1.91711400	3.10257000
H	8.43744100	-4.30853500	2.77847800
H	6.46665400	-4.77259000	1.31199800
H	0.00000000	-0.29763900	-5.82961700
H	0.00000000	-5.31034000	-5.82364600
H	0.00000000	-0.17918300	6.10770300
H	0.00000000	-2.57438700	1.94476100
H	0.00000000	-5.20286200	-3.20421900
H	0.00000000	-0.40006700	-3.20303300
H	0.00000000	2.97383400	1.25626800

H	0.00000000	5.37913400	-2.90077200
H	-9.17129700	-1.72799100	-3.21424300
Fe	-5.43127200	0.00045700	-0.00016600
Fe	5.43127200	0.00045700	-0.00016600
H	-4.58129000	2.63729000	-4.10407100
H	-4.58141800	2.23488200	4.33600700
H	-4.58208300	-4.87232900	-0.22971000
H	4.58141800	2.23488100	4.33600700
H	4.58129200	2.63729300	-4.10407000
H	4.58208200	-4.87232900	-0.22970900

Triplet (charge +4)

C	-6.19751600	-2.84048000	-0.67705900
C	-5.00641500	-2.86664000	0.17234300
C	-3.22851500	-3.56230300	1.36026600
C	-2.19988300	-4.27701500	2.00504900
C	-1.19350800	-3.51397500	2.59197300
C	-1.20683600	-2.07916700	2.54667900
C	-2.23782100	-1.37711600	1.92678500
C	-3.26903200	-2.13629200	1.32190800
C	0.03910200	-4.07322800	3.31577800
C	1.24154100	-3.49854900	2.55430500
C	1.24506100	-2.06325400	2.51700100
C	0.02403900	-1.45864000	3.23141700
C	2.23081400	-4.24768000	1.92426900
C	3.23304300	-3.51997700	1.25406600
C	3.27682400	-2.09181700	1.23786700
C	2.25657800	-1.34760300	1.88019500
C	4.96810800	-2.82189200	0.01905700
C	6.11752900	-2.73793300	-0.86647100
C	0.05619300	-3.42657100	4.71025000
C	0.07724800	-4.10141800	5.93589000
C	0.07939400	-1.94213100	7.08833400
C	0.05829000	-1.26559700	5.84791500

C	0.04670100	-2.01370600	4.66532100
N	-6.67354900	-1.58012500	-0.92736600
N	-4.39716900	-1.73928800	0.57947300
N	-4.34338400	-3.98848700	0.62885300
N	4.38736300	-1.69247100	0.46741400
N	6.52092000	-1.43923700	-1.07942400
N	4.31636900	-3.94429900	0.47622200
C	7.57540000	-1.22540500	-1.90904600
C	8.26186000	-2.27135900	-2.54862800
C	6.75863700	-3.83268900	-1.47161100
C	0.08886400	-3.34945100	7.13181500
C	-6.06063000	0.89529800	2.77566400
C	-4.88696500	1.67308800	2.40056100
C	-3.10947200	3.04500100	2.40355300
C	-2.07480500	3.95273700	2.70287300
C	-1.07597300	4.08550800	1.74147400
C	-1.10741500	3.34728400	0.51012900
C	-2.14207600	2.46495400	0.21118800
C	-3.16078000	2.30956700	1.18076300
C	0.17017900	4.97320300	1.86936100
C	1.35663100	4.00856300	1.72893100
C	1.33620300	3.27746500	0.49377700
C	0.11770000	3.63011400	-0.37517000
C	2.35063400	3.80340600	2.68158500
C	3.33056100	2.84241900	2.36451400
C	3.34321500	2.12560900	1.12848000
C	2.32064900	2.34643600	0.17415900
C	5.04384500	1.39671800	2.33440600
C	6.19993100	0.58021400	2.66509900
C	0.19114400	5.87735500	0.62661600
C	0.23251500	7.27607500	0.62104300
C	0.21260000	7.23462800	-1.82612100
C	0.16081500	5.15214800	-0.58630300
N	-6.46332500	0.01103000	1.79941200

N	-4.28916000	1.46986200	1.21126200
N	-4.22103300	2.62115800	3.14552600
N	4.43748300	1.23884600	1.14249100
N	6.58117100	-0.23366500	1.62219500
N	4.41884200	2.35579900	3.09857800
C	7.64519500	-1.05721600	1.81045400
C	8.36198200	-1.10688900	3.01797100
C	6.87080000	0.58297300	3.90015600
C	0.24341900	7.95593100	-0.61722600
C	-6.35691800	1.97371300	-2.04622500
C	-5.14881300	1.29003000	-2.49260200
C	-3.35412700	0.62079300	-3.66317500
C	-2.32976200	0.41892600	-4.60883700
C	-1.31386200	-0.45817800	-4.24002700
C	-1.31472700	-1.11976700	-2.96615600
C	-2.33523500	-0.92420800	-2.03857800
C	-3.37902200	-0.03584600	-2.39552200
C	-0.09690300	-0.82451700	-5.10005000
C	1.12736600	-0.46457700	-4.24694300
C	1.14139500	-1.13975400	-2.98041600
C	-0.09228300	-2.03550200	-2.78067600
C	2.13325700	0.42682000	-4.60991700
C	3.16497200	0.62065200	-3.67046200
C	3.21884100	-0.07464400	-2.42331400
C	2.17971100	-0.96909800	-2.06832700
C	4.95446000	1.28980800	-2.49677400
C	6.13873600	1.97786900	-2.00901200
C	-0.10476700	-2.35776500	-5.22204800
C	-0.11383400	-3.09399100	-6.41192300
C	-0.12360200	-5.15835800	-5.09686100
C	-0.11449400	-4.41004900	-3.89814200
C	-0.10519300	-3.01256000	-3.96897600
N	-6.75456200	1.58935700	-0.78995000
N	-4.52029300	0.40247100	-1.69423000

N	-4.48541500	1.44425300	-3.68835500
N	4.36278100	0.35888600	-1.72451300
N	6.55337200	1.50157700	-0.78549900
N	4.27663700	1.47200400	-3.68092300
C	7.63756700	2.08060300	-0.20724500
C	8.34489600	3.13537800	-0.80869000
C	6.79961800	3.02816600	-2.66886400
C	-0.12314400	-4.50513600	-6.34418300
C	0.17104900	5.82228800	-1.81479800
H	0.27485700	9.04158900	-0.63708800
H	0.21992100	7.77002700	-2.77161400
H	-2.04852200	4.51261100	3.63310300
H	-2.16104200	1.90056200	-0.71496700
H	2.36431100	4.35117800	3.61930500
H	2.29440900	1.79358500	-0.75688400
H	0.05056500	-0.17802500	5.81966700
H	0.08797500	-1.37586300	8.01569100
H	0.10480700	-3.85983900	8.09062000
H	0.08422300	-5.18787500	5.97602200
H	-2.24701600	-0.29326500	1.88807800
H	-2.18532800	-5.36244300	2.03974100
H	-2.32885500	-1.42162200	-1.07648300
H	-2.33117300	0.91763900	-5.57364500
H	-0.11514000	-4.91926700	-2.93671700
H	-0.11380200	-2.59551300	-7.37813400
H	-0.13122200	-6.24429200	-5.05911900
H	-0.13021000	-5.08972500	-7.25975300
H	2.11953400	0.94502200	-5.56430800
H	2.18340500	-1.48116600	-1.11370400
C	7.92158200	3.61736100	-2.06127300
H	8.45051900	4.42918600	-2.55045200
H	6.45195000	3.38757300	-3.63276700
H	7.95104700	1.68539500	0.74971100
C	7.97010000	-0.27327500	4.08190600

H	8.50618400	-0.28947500	5.02555400
H	6.54777200	1.23202600	4.70855400
H	7.93557900	-1.68056300	0.97554500
H	9.20668200	-1.78042800	3.11462800
C	7.84902100	-3.59826400	-2.32642900
H	7.88310400	-0.19888400	-2.05548000
H	9.09984200	-2.04592200	-3.19937600
H	8.36223800	-4.42624300	-2.80515900
H	6.41966100	-4.84801700	-1.28907900
H	2.25321600	-0.26416900	1.85287900
H	2.22403300	-5.33355200	1.94397100
C	-6.80641900	-3.98897300	-1.21879400
C	-7.93669700	-3.83860000	-2.04117700
H	-6.41591600	-4.98182900	-1.01671600
C	-8.42308500	-2.54388900	-2.30179600
C	-7.76128400	-1.44467100	-1.72540100
H	-8.42473000	-4.70911500	-2.46831100
H	-8.11408400	-0.43429400	-1.89785000
H	-9.29280800	-2.38635000	-2.93058600
C	-7.05976300	2.94161800	-2.78631800
C	-8.20316500	3.53226600	-2.21906700
C	-8.60943200	3.13927400	-0.92963800
H	-8.76377400	4.28124000	-2.76978200
C	-7.85743300	2.16443200	-0.25006600
H	-9.48579300	3.57332800	-0.46058600
H	-6.73444200	3.23685700	-3.77937100
H	-8.14426400	1.83470700	0.74170200
C	-6.72241900	0.99075700	4.01246600
C	-7.82336500	0.15622800	4.26847300
C	-8.22880000	-0.75382600	3.27465500
C	-7.52688200	-0.79469900	2.05892900
H	-7.82137400	-1.47562000	1.27204400
H	-9.07204900	-1.41777200	3.43130500
H	-8.34950400	0.21342300	5.21612400

H	-6.39118100	1.69699100	4.76775900
H	0.14571300	5.26974500	-2.75161700
H	0.25548800	7.83864900	1.55110800
H	0.04694600	-5.16539200	3.35428400
H	0.01653300	-0.36587600	3.19840000
H	0.19280900	5.53720600	2.80516000
H	0.09502300	3.07015400	-1.31392200
H	-0.09065100	-2.54276300	-1.81213500
H	-0.09841600	-0.32166500	-6.07035700
H	9.20642500	3.56109700	-0.30565700
Fe	5.43336700	-0.04224800	-0.05918700
Fe	-5.43541100	0.07790600	0.05994500
H	4.53443300	2.10023000	-4.43130500
H	4.57213700	-4.90590500	0.29176100
H	4.69770600	2.66649600	4.02047100
H	-4.61591000	-4.95085000	0.47566900
H	-4.76369600	2.04262000	-4.45569400
H	-4.48077800	2.95840900	4.06389400

Quintuplet (charge +4)

C	-6.16997500	-2.85314000	-0.85901500
C	-4.99373900	-2.91099600	0.00894300
C	-3.23580000	-3.65310000	1.19818800
C	-2.21924300	-4.39323400	1.83346500
C	-1.21867100	-3.65458700	2.46004900
C	-1.22593800	-2.21872400	2.46053900
C	-2.24751900	-1.49193300	1.85334500
C	-3.27330100	-2.22654500	1.21011300
C	-0.00000900	-4.24298400	3.18508500
C	1.21865400	-3.65458900	2.46005000
C	1.22592400	-2.21872600	2.46054000
C	-0.00000700	-1.62711400	3.17774300
C	2.21922500	-4.39323800	1.83346700
C	3.23578500	-3.65310500	1.19819200

C	3.27328800	-2.22655100	1.21011700
C	2.24750700	-1.49193700	1.85334900
C	4.99372700	-2.91100400	0.00894900
C	6.16996300	-2.85314900	-0.85900800
C	-0.00000900	-3.63770300	4.59820300
C	-0.00001000	-4.34834500	5.80360500
C	-0.00000900	-2.22400800	7.01920800
C	-0.00000800	-1.51119400	5.79907600
C	-0.00000800	-2.22407700	4.59491100
N	-6.64414300	-1.58476500	-1.06968500
N	-4.39007500	-1.80014100	0.46681700
N	-4.33970000	-4.05007000	0.43473000
N	4.39006400	-1.80014800	0.46682300
N	6.64413100	-1.58477400	-1.06968000
N	4.33968600	-4.05007700	0.43473500
C	7.71864200	-1.42136300	-1.88054600
C	8.36820700	-2.49891900	-2.50919600
C	6.76723900	-3.98123100	-1.45416900
C	-0.00001000	-3.63199500	7.02126900
C	-6.11933200	0.72407900	2.74810400
C	-4.95734700	1.54026700	2.42262100
C	-3.21969300	2.96085900	2.49532400
C	-2.21656500	3.88932900	2.83671300
C	-1.21737700	4.09222800	1.88773700
C	-1.21954300	3.40132500	0.62888200
C	-2.22140900	2.49678200	0.28965300
C	-3.23923100	2.27096900	1.24536900
C	0.00000700	5.01368200	2.05636400
C	1.21739100	4.09222600	1.88773600
C	1.21955500	3.40132300	0.62888200
C	0.00000600	3.75450200	-0.23676800
C	2.21657900	3.88932600	2.83671200
C	3.21970500	2.96085500	2.49532200
C	3.23924200	2.27096500	1.24536700

C	2.22142000	2.49677900	0.28965100
C	4.95735700	1.54026100	2.42262000
C	6.11934100	0.72407200	2.74810100
C	0.00000800	5.96372200	0.84825600
C	0.00000900	7.36228900	0.89493100
C	0.00000800	7.41136000	-1.55215500
C	0.00000700	5.28362600	-0.39078800
N	-6.49447300	-0.12020300	1.72624600
N	-4.34222000	1.39855500	1.23325600
N	-4.32509900	2.47698100	3.20985000
N	4.34223000	1.39854900	1.23325400
N	6.49447800	-0.12021300	1.72624400
N	4.32511100	2.47697600	3.20984700
C	7.54942500	-0.95202000	1.93335900
C	8.26807600	-0.97798000	3.13970300
C	6.79806300	0.75143900	3.97899500
C	0.00000900	8.08775700	-0.31717800
C	-6.34441400	1.99780800	-2.04679800
C	-5.11807100	1.34631400	-2.49266900
C	-3.29059100	0.74259200	-3.64930400
C	-2.24890000	0.58009100	-4.58405100
C	-1.22424700	-0.28994400	-4.22148500
C	-1.23054400	-0.97625800	-2.96092900
C	-2.26955100	-0.82301500	-2.04624700
C	-3.32552900	0.05128600	-2.40055300
C	0.00000100	-0.63458800	-5.08054600
C	1.22424900	-0.28994400	-4.22148400
C	1.23054500	-0.97625800	-2.96092900
C	0.00000000	-1.88010700	-2.77935000
C	2.24890100	0.58009100	-4.58405000
C	3.29059300	0.74259100	-3.64930200
C	3.32553000	0.05128500	-2.40055200
C	2.26955200	-0.82301600	-2.04624600
C	5.11807200	1.34631200	-2.49266700

C	6.34441700	1.99780500	-2.04679800
C	0.00000100	-2.16669300	-5.22593300
C	0.00000100	-2.88512400	-6.42658200
C	0.00000000	-4.96884700	-5.14233100
C	0.00000000	-4.23839400	-3.93252300
C	0.00000000	-2.84005400	-3.98254600
N	-6.75889100	1.56715500	-0.81118500
N	-4.48846200	0.44621600	-1.70948900
N	-4.43613600	1.54679000	-3.67130000
N	4.48846300	0.44621400	-1.70948700
N	6.75889800	1.56714900	-0.81118700
N	4.43613800	1.54678900	-3.67129800
C	7.87795900	2.11024800	-0.27202200
C	8.63069800	3.09797800	-0.93215800
C	7.04696700	2.98082700	-2.76704500
C	0.00000100	-4.29721900	-6.37980100
C	0.00000700	5.99901500	-1.59353600
H	0.00001000	9.17385600	-0.29662500
H	0.00000800	7.98152100	-2.47711200
H	-2.21394300	4.41314800	3.78807800
H	-2.21603100	1.96845500	-0.65751200
H	2.21395900	4.41314400	3.78807700
H	2.21604000	1.96845200	-0.65751300
H	-0.00000700	-0.42322200	5.80272300
H	-0.00000900	-1.68530700	7.96289400
H	-0.00001100	-4.17049900	7.96471600
H	-0.00001100	-5.43554100	5.81173300
H	-2.25403500	-0.40698200	1.85285500
H	-2.20906100	-5.47927000	1.83163600
H	-2.26960800	-1.34405300	-1.09678800
H	-2.24600300	1.09960000	-5.53783400
H	0.00000000	-4.76161400	-2.97865500
H	0.00000200	-2.37235600	-7.38529100
H	0.00000000	-6.05526900	-5.12077700

H	0.00000100	-4.86813100	-7.30400000
H	2.24600500	1.09960000	-5.53783200
H	2.26960800	-1.34405500	-1.09678800
C	8.20754300	3.53814200	-2.20075400
H	8.76821100	4.29801200	-2.73627900
H	6.70828400	3.31321700	-3.74377200
H	8.17720100	1.74393800	0.70322000
C	7.88918500	-0.11037300	4.18078400
H	8.42817900	-0.10572600	5.12290500
H	6.48701600	1.42612900	4.77083100
H	7.82387900	-1.59949700	1.11186900
H	9.10362200	-1.66019800	3.25316800
C	7.88359900	-3.80183300	-2.28946800
H	8.07134000	-0.40613500	-2.02064100
H	9.22751400	-2.31890800	-3.14621200
H	8.36235900	-4.65636500	-2.75742700
H	6.37784500	-4.98032700	-1.28320700
H	2.25402600	-0.40698600	1.85285900
H	2.20904200	-5.47927400	1.83163800
C	-6.76725000	-3.98122200	-1.45417800
C	-7.88361000	-3.80182300	-2.28947600
H	-6.37785500	-4.98031800	-1.28321800
C	-8.36821900	-2.49890900	-2.50920200
C	-7.71865500	-1.42135400	-1.88055000
H	-8.36236900	-4.65635400	-2.75743700
H	-8.07135300	-0.40612600	-2.02064400
H	-9.22752700	-2.31889800	-3.14621800
C	-7.04696700	2.98082800	-2.76704600
C	-8.20754100	3.53814400	-2.20075200
C	-8.63069100	3.09798400	-0.93215300
H	-8.76821100	4.29801300	-2.73627700
C	-7.87794900	2.11025500	-0.27201700
H	-9.52031300	3.50575700	-0.46446900
H	-6.70828800	3.31321500	-3.74377500

H	-8.17718800	1.74394800	0.70322700
C	-6.79805100	0.75144600	3.97899900
C	-7.88917400	-0.11036400	4.18078900
C	-8.26807000	-0.97796900	3.13970800
C	-7.54942100	-0.95200800	1.93336200
H	-7.82387800	-1.59948300	1.11187100
H	-9.10361600	-1.66018500	3.25317400
H	-8.42816600	-0.10571700	5.12291100
H	-6.48700100	1.42613400	4.77083500
H	0.00000700	5.48135100	-2.55036700
H	0.00000900	7.89019800	1.84537800
H	-0.00001000	-5.33584600	3.19174300
H	-0.00000600	-0.53367100	3.17649500
H	0.00000800	5.54294000	3.01251000
H	0.00000500	3.22955700	-1.19577300
H	0.00000000	-2.40181200	-1.81858800
H	0.00000100	-0.11735000	-6.04326900
H	9.52032100	3.50575100	-0.46447500
Fe	5.43525900	0.03655700	0.00942900
Fe	-5.43525700	0.03656500	0.00942800
H	4.71178300	2.16201800	-4.42615400
H	4.61022600	-5.00568600	0.24121900
H	4.60372200	2.77262800	4.13700100
H	-4.61024200	-5.00567800	0.24121400
H	-4.71178100	2.16201900	-4.42615700
H	-4.60371000	2.77263400	4.13700400

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