Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

A Spin Crossover $Fe^{II}_4L_6$ Cage Based on Pyridyl- Hydrazone Sites

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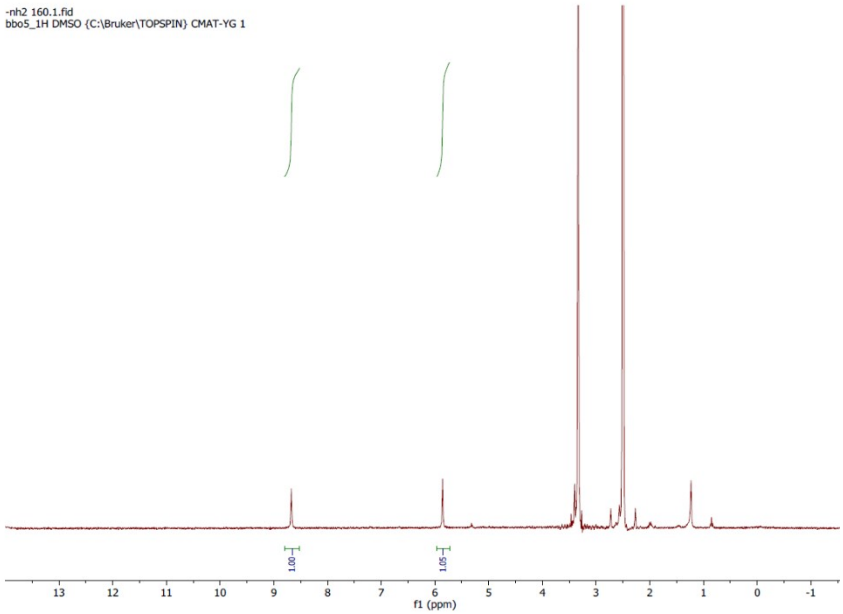
Contents

General information

All chemicals were used as purchased without further purification. NMR spectra were recorded on a Bruker AVANCE 300MHz spectrometer and referenced to the residual solvent signal: 2.50 ppm for dimethyl sulfoxide. Elemental analyses (C, H, and N) were carried out by MEDAC Ltd, UK. Thermogravimetric analyses (TGAs) were performed in $N_{2(g)}$ (100 mL min^{-1}) at a heating rate of 10 ^{o}C min^{-1} from 25 ^{o}C to 850 ^{o}C with Mettler Toledo TGA/SDTA 851e analyzer. High resolution electrospray ionization mass spectra (HRMS) were recorded on a Q-Exactive ThermoFisher spectrometer. Scanning electron microscopy (SEM) with energy-dispersive X-ray spectroscopy (EDS) were performed SEM JEOL 7600F. Fourier transformed infrared spectroscopy (FT-IR) were recorded on a Equinox 55 (Bruker) equipped with an ATR modulus and an MCT detector. Diffuse reflectance spectra (DRS) were performed with a PerkinElmer Lambda 9 UV/vis/NIR spectrophotometer equipped with a 60 mm integrating sphere and converted into absorption spectra by using the Kubelka−Munk function, using $BaSO_4$ as a reference. Magnetic susceptibility for non-solvated cage **1** (single crystals annealed at 400 K in the SQUID cavity) was measured on a Quantum design MPMS3 SQUID magnetometer in the order 400 K→2 K→400 K→2 K→400 K (two cycles) under an applied field of 5000 Oe. Magnetic data were corrected for the sample holder and diamagnetic contributions. Mössbauer data were recorded with a ^{57}Co source embedded in a Rh matrix using an alternating constant acceleration Wissel Mössbauer spectrometer operated in the transmission mode and equipped with a Janis closed-cycle helium cryostat. The spectra were fitted with the Mfit program (E. Bill, Max-Planck Institute for Chemical Energy Conversion, Mülheim/Ruhr, Germany) and isomer shift values are given with respect to α-Fe at room temperature.

Synthesis of *N*, *N*-diaminonaphthalene-1,4,5,8-tetracarboxydi-imide

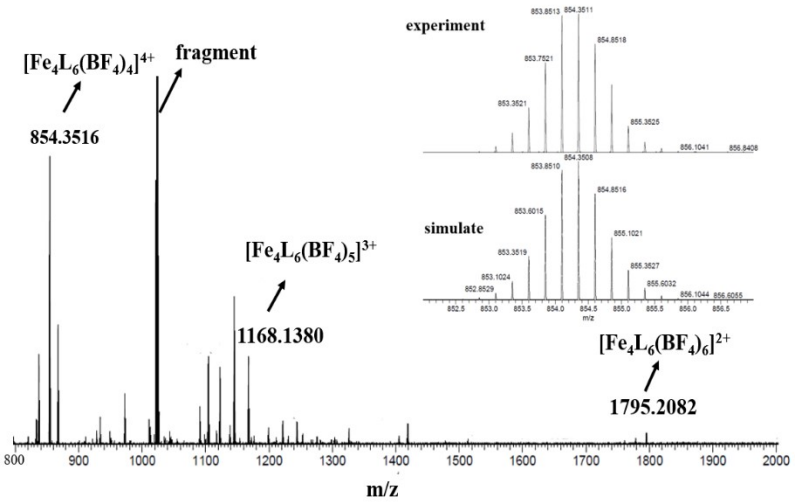
To naphthalene-l,4,5,8-tetracarboxylicacid dianhydride (3.73 mmol, 1.0 g) was added an excess of hydrazine hydrate (60 mmol, 3.0 g) in acetone (30 mL). This was an exothermic reaction accompanied by the formation of a black solid. The solution was filtered, and the solid was washed with acetone. During the washing process, the colour of the solid changed to light brown. Finally, the product was heated at 160 °C under vacuum overnight to ensure complete cyclization. Yield: 0.81 g (73%).^{1}H NMR (DMSO-d6, 300 MHz, ppm) δ: 5.85 (s, 4H), 8.67 ppm (s, 4H). Elemental analysis (%) calcd. for $C_{14}H_8N_4O_4$: C 56.76%, H 2.72%, N 18.91%; found: C 56.69%, H 2.73%, N 18.58%.



^{1}H NMR spectrum for *N*,*N*-diaminonaphthalene-1,4,5,8-tetracarboxydi-imide

Synthesis of cage 1

N,*N*-diaminonaphthalene-1,4,5,8-tetracarboxydi-imide (37 mg, 0.125 mmol), 2-formylpyridine (23.8 μL, 0.25 mmol) and $Fe(BF_4)_2 \cdot 6H_2O$ (28.1 mg, 0.083 mmol) were added to a Schlenk flask with acetonitrile (40 mL). The reaction mixture was stirred under $Ar_{(g)}$ at 65 °C overnight and then cooled to room temperature. The resulting purple solution was filtered and vapor-diffused with diethyl ether. After one-week, dark purple crystals suitable for X-ray crystallography were obtained. Yield: 25.4 mg (30%). Elemental analysis for crystals washed by diethyl ether and dried (%) calcd. for $C_{156}H_{84}N_{36}O_{24}Fe_4B_8F_{32} \cdot 7H_2O$, C, 48.16%; H, 2.54%; N, 12.96%; found C, 48.04%; H, 2.66%; N, 12.77%. ESI-HRMS calculated for $[Fe_4L_6(BF_4)_4]^{4+}$, *m/z* : 854.3516; $[Fe_4L_6(BF_4)_5]^{3+}$, *m/z* : 1168.1380; $[Fe_4L_6(BF_4)_6]^{2+}$, *m/z* : 1795.2082.



ESI-HRMS spectrum of cage **1**. The inset shows the isotope pattern for $[Fe_4L_6(BF_4)_4]^{4+}$ with the simulated distribution.

Single-crystal X-ray diffraction analyses

The structural analysis at 120 K was performed on MAR345 image plate using Mo-Kα radiation (λ = 0.71073Å), generated by an Incoatec IμS generator equipped with Montel Mirrors. Prior to data collection the crystals were flash frozen at 120 K. CrysAlis^{PRO} was used for data integration and reduction and the implemented absorption correction was applied. The structures were solved by SHELXT and showed 2 cage systems in the asymmetric unit along with the BF_4 counter anions and solvent atoms of which some were only partially occupied. Refinement was done by full-matrix least squares on F^2 using SHELXL2018/3. The crystals of cage **1** were quite small and unstable. Because diethyl ether was used as anti-solvent, crystals readily redissolved into the mother liquid (acetonitrile) when exposed to air and the diethyl ether evaporates. In order to be able to manipulate the crystals prior to data collection, a solvent transfer to tetrahydrofuran was performed to ensure that the necessary time was available to separate and harvest the crystals. Although more data was collected in the low temperature measurements, the final resolution limit was set at 1.10 Å, beyond which the crystal diffracted poorly. Despite the lower diffraction limit, all BF_4 anions could be located as well as acetonitrile and THF solvent molecules. Geometry restraints were applied to the BF_4 and solvent molecules as well as similarity restraints on 3 ligands of the second cage. The electron density inside this cavity was taken into account by the SQUEEZE procedure in PLATON. Final crystallographic data and refinement values for cage **1** are listed in Table S1. CCDC **2191810** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures

SHELXT:

Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3-8.

Crysalis^{PRO}:

Rigaku (2015). *CrysAlisPro Software System*, Version 1.171.38.41. Rigaku Oxford Diffraction

PLATON SQUEEZE:

Spek, A. L. (2015). *Acta Cryst.* C**71**, 9-18.

Table S1. Crystal data and structure refinement details for cage **1** in 120 K.

Formula	$C_{156}\,H_{84}\,Fe_4N_{36}O_{24}\cdot 8(BF_4)\cdot 3.64\,(C_4H_8O)\cdot 2(C_2H_3N)\cdot$[+solvent]
Formula weight	4067.97
λ (Å)	MoK_α (0.71073)
Crystal system	Triclinic
Space group	*P*-1
T (K)	120
a (Å)	22.121(2)
b (Å)	22.881(3)
c (Å)	38.937(3)
α (°)	93.602(3)
β (°)	91.560(7)
γ (°)	96.891(8)
V (Å^3)	19515(3)
Z	4
ρ_{calc} (g.cm^{-3})	1.385
Absorption coefficient (mm^{-1})	0.396
θ range (°)	2.815 to 19.027
F(000)	8254
Crystal size (mm)	0.38×0.15×0.03
Reflections collected	56550
Independent reflections	29971 [$R_{(int)}$ = 0.1112]
Completeness to θ_{max}	94.9%
Data/restraints/parameters	29971/16405/5333
Goodness of fit on F^2	1.422
$R_1{}^a, wR_2{}^b$ *(I>2σ(I))*	0.1377, 0.288
$R_1{}^a, wR_2{}^b$ *(all data)*	0.2296, 0.3247
Δρ max and min (e.Å^{-3}.)	1.017 and -0.732

Table S2. Fe−N bond lengths for cage **1** in 120 K.

Fe(II) centre	Average Fe-N bond length (Å)	Spin-state
Fe01	1.99	LS
Fe02	1.98	LS
Fe03	2.00	LS
Fe04	1.98	LS
Fe05	2.00	LS
Fe06	2.00	LS
Fe07	2.00	LS
Fe08	1.99	LS

Fig. S1 Morphology of single crystals of **1** under a microscope.

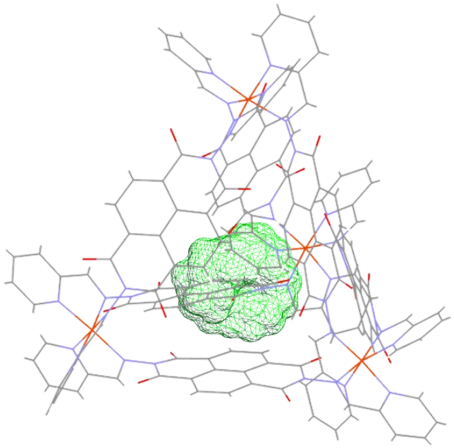


Fig. S2 Image of the internal cavity/void volume (green mesh) of the cage. The solvent accessible volume of the cage was determined with the PLATON software using the VOID CALC option, and its corresponding figure was generated with Chem3D Pro 12.0.

VOID CALC:

Spek, A. L. Single-crystal structure validation with the program PLATON. *J. Appl. Crystallogr*. 2003, **36** (1), 7–13.

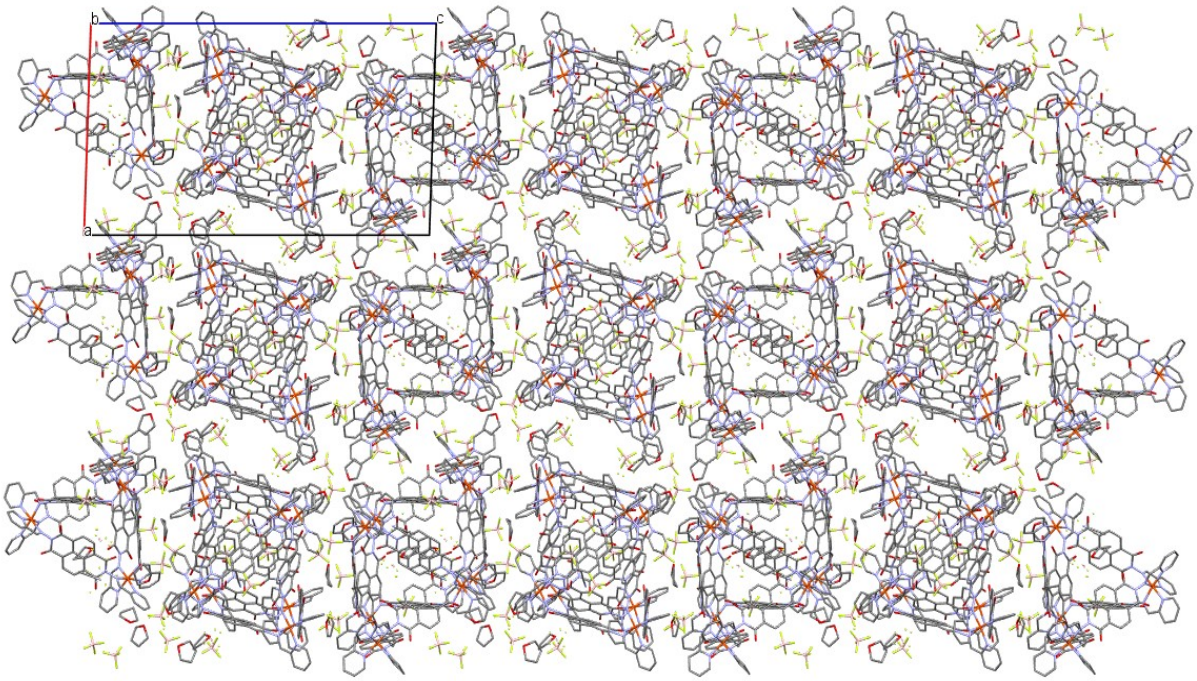


Fig. S3 crystal packing diagram of cage **1**, viewed along b axis. Fe: red, C: grey, N: blue, O: red, F: yellow, B: pink, H: white. All H atoms have been removed for clarity.

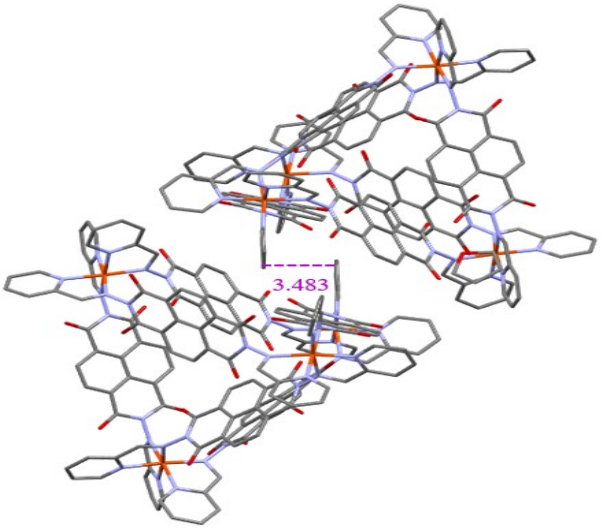


Fig. S4 Diagram showing π–π interactions. Fe: red, C: grey, N: blue, O: red. All H atoms and BF_4^- anions have been removed for clarity.

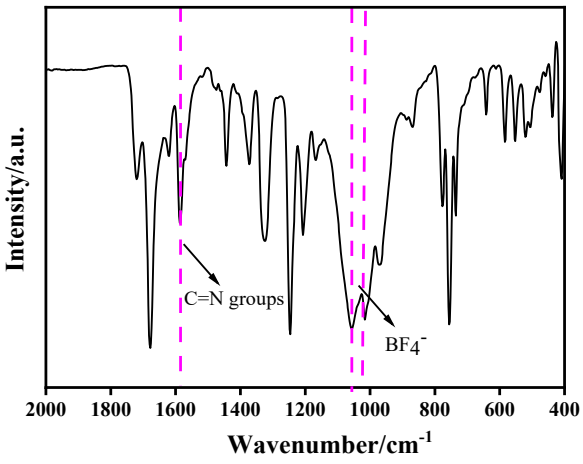


Fig. S5 FT-IR of cage **1** recorded at room temperature.

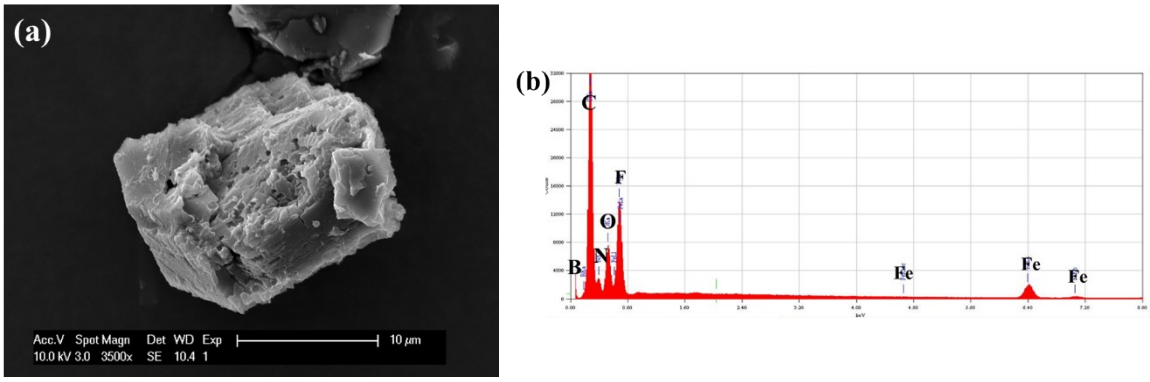


Fig. S6. SEM image (a) and EDS spectrum (b) for cage **1**.

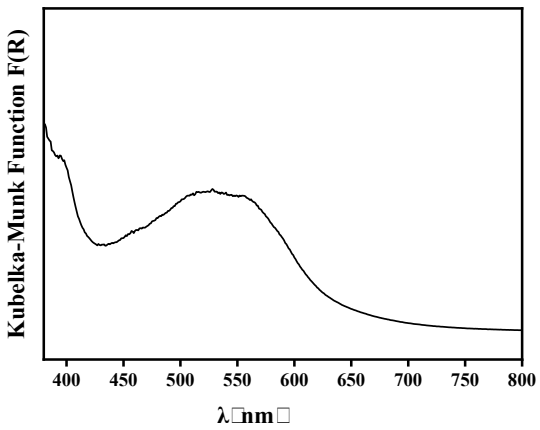


Fig. S7. Ultraviolet−visible diffuse reflectance spectroscopy of cage **1** recorded at room temperature.

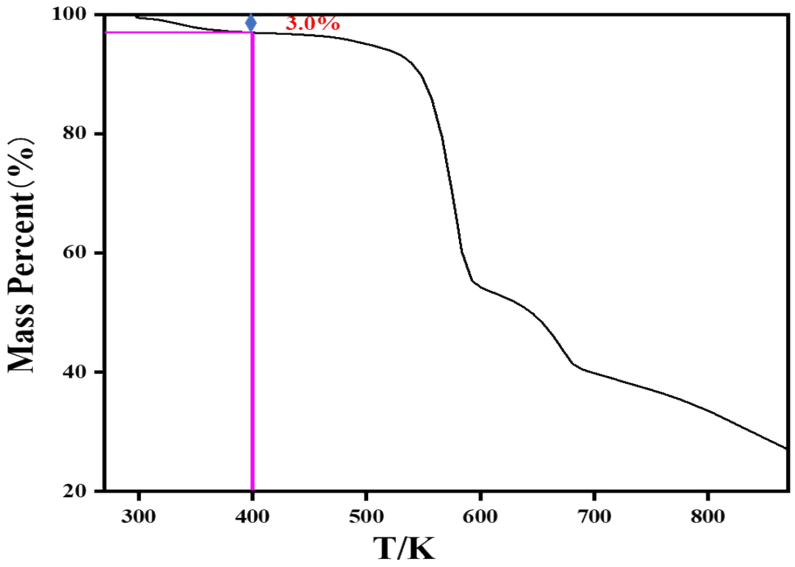


Fig. S8. TGA curve of cage **1** and the abscissa of the magenta line is 400 K. The mass loss of c.a. 3.0% from room temperature to 400 K, which is attributed to the release of 7 water molecules, matching well elemental analysis result (3.2 %).

Table S3. ^{57}Fe Mössbauer parameters for cage **1** at 80 K.

Sample	Spin State Fe(II)	A/A_{tot} (%)	Mössbauer parameters		
			δ (mm s^{-1})	ΔE_Q (mm s^{-1})	$\Gamma/2$
Cage **1**	LS (red)	62	0.45	0.36	0.34
	HS-1 (blue)	38	1.17	3.12	0.52

DFT section

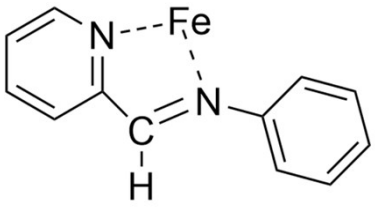
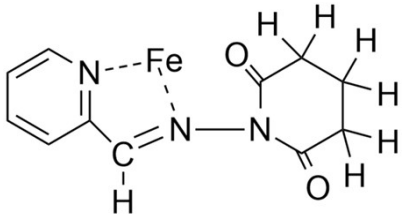
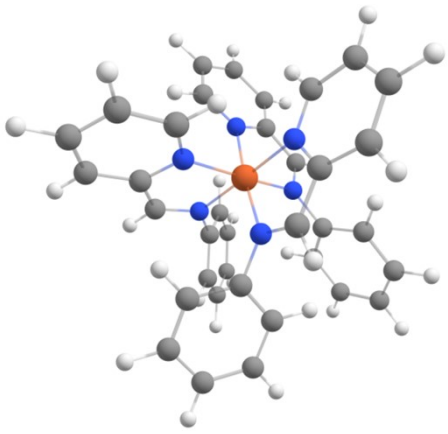
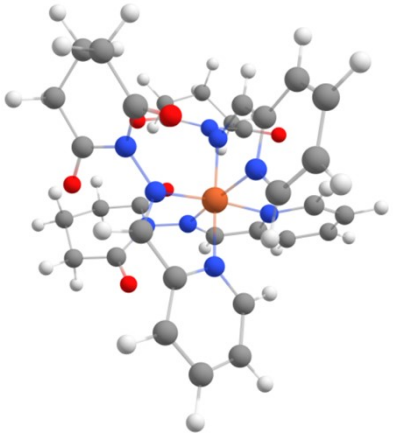
Computational details:

The ORCA 4.1.2 program was used for all calculations.[1,2] Due to the size of the systems in the DFT calculations we only considered one iron centre with a simplified ligand structure as shown in Table S4. All ligands retained the essential traits of the original ligands in order to ensure the resemblance to the original ligand field. Two model systems were studied: the model of the compound known from the literature, which exists in the LS state and does not undergo SCO, and a model of our synthesized compound that does undergo SCO behaviour with changes in temperature.

Geometry optimization was performed at the BP86/def2-SVP level of theory.[3–5] RI density fitting approximation was integrated with the def2/J auxiliary basis set.[6] Relativistic effects and dispersion interactions were taken into account by including the zeroth-order relativistic approximation (ZORA)[7,8] and Grimme's Becke-Johnson damped dispersion correction (D3(BJ)).[9,10] Following the geometry optimization, all of the structures were characterized by harmonic vibration analysis at the same level of theory, which revealed no imaginary vibrational frequencies. These second derivative calculations were performed to ensure that the located stationary points are minima on the potential energy surface and to obtain the thermal correction for Gibbs Free Energy at 2 K, 298.15 K, and 400 K respectively. Geometries were optimized in both the high spin (quintet)and low spin (singlet) states.

As it is well-established that calculated energy gap between the various spin-states strongly depends on the contribution of HF-exchange included, final single point energies were obtained with the pure BP86 functional (no HF exchange), and hybrid B3LYP (20% admixture of HF exchange), and B3LYP* (15% of functionals. The spin-state splittings obtained with the three functionals were in very good accordance with the trends established in the literature, and as previous research suggested the B3LYP* functional may yield the best spin-state energetics.[11,12] For this reason these data are included in the manuscript and results with the other functionals are only included in the SI. The single-point calculations used the larger basis set def2-TZVP[3–5] and also included the treatment of scalar relativistic effects via the ZORA[7,8] formalism and dispersion corrections (D3(BJ))[9,10].

Table S4. Calculated relative energies and Gibbs free energies at 2 K, 298.15 K and 400 K (in kcal/mol) of the high spin (quintet) species compared to the low spin state (singlet) using various functionals and the def2-TZVP basis set.

	Model of non-SCO compound				Model of SCO compound			
Ligand used in the calculations (calculations were done using three ligands)								
3D structure								
Functional	**ΔE**	**ΔG (2K)**	**ΔG (298.15K)**	**ΔG (400K)**	**ΔE**	**ΔG (2K)**	**ΔG (298.15K)**	**ΔG (400K)**
BP86	33.6	30.3	27.2	25.8	27.7	25.1	22.4	21.2
B3LYP	2.5	-0.8	-3.9	-5.3	-3	-5.6	-8.3	-9.5
B3LYP*	**10.7**	**7.4**	**4.3**	**2.9**	**5.2**	**2.7**	**-0.1**	**-1.3**

XYZ Coordinates of located stationary points:

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Model of non-SCO compound, S = 1

Fe	8.548949	14.988314	18.555203
N	8.983477	14.119564	16.847722
N	9.439175	16.472914	17.702623
C	8.742319	12.838890	16.490105
H	8.217929	12.211873	17.217018

C	9.130526	12.322148	15.244760
C	9.794517	13.153661	14.326821
H	10.105455	12.772213	13.347751
C	10.055371	14.482289	14.692120
H	10.577746	15.168319	14.015737
C	9.643864	14.934292	15.957679
C	9.870138	16.261840	16.484577
H	10.376656	17.047264	15.907077
C	9.666217	17.766391	18.278505
C	8.591402	18.665185	18.425391
H	7.596866	18.394891	18.057169
C	8.821458	19.926779	18.994757
H	7.992433	20.637349	19.091412
C	10.113199	20.287894	19.422051
H	10.286571	21.273721	19.868122
C	11.182026	19.391852	19.252529
H	12.193798	19.675396	19.563916
C	10.967290	18.130537	18.674125
H	11.796059	17.429823	18.537990
N	6.826365	15.665389	17.913705
N	8.018785	15.952921	20.142116
C	6.286953	15.507965	16.684508
H	6.862177	14.922253	15.961798
C	5.043670	16.056726	16.336038
C	4.321580	16.797302	17.287475
H	3.347564	17.232801	17.037895
C	4.877522	16.972694	18.563024

H	4.358372	17.548412	19.337682
C	6.130559	16.401809	18.844734
C	6.844870	16.529335	20.095586
H	6.440240	17.083414	20.953843
C	8.784041	16.080907	21.348672
C	9.413326	17.305169	21.643039
H	9.312488	18.149574	20.955962
C	10.172978	17.422425	22.818016
H	10.664549	18.374734	23.047499
C	10.295089	16.333674	23.697778
H	10.884049	16.431952	24.616714
C	9.637388	15.123089	23.409744
H	9.699909	14.283679	24.111887
C	8.881528	14.990284	22.234837
H	8.335423	14.064957	22.026989
N	10.155768	14.226088	19.316126
N	7.761616	13.360249	19.314297
C	11.467468	14.806254	19.282515
C	12.002224	15.377462	20.452394
H	11.421083	15.368408	21.378246
C	13.278802	15.960822	20.411644
H	13.694291	16.406921	21.322421
C	14.021336	15.964648	19.218998
H	15.019493	16.416328	19.192788
C	13.491494	15.362275	18.062444
H	14.083323	15.329391	17.140373
C	12.213734	14.782647	18.087923

H 11.815473 14.276454 17.203232

C 10.013757 13.068459 19.908269

H 10.866741 12.541173 20.357516

C 8.667768 12.539976 19.944994

C 8.285561 11.337799 20.564241

H 9.044024 10.716558 21.053927

C 6.933645 10.964819 20.549234

H 6.605388 10.034339 21.025899

C 6.010115 11.812321 19.914177

C 6.459996 12.996726 19.311076

H 5.759042 13.667224 18.805512

H 4.652469 15.898145 15.325227

H 4.943569 11.564927 19.880742

H 8.909266 11.276407 15.005379

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Model of non-SCO compound, S=5

Fe 8.417468 15.038786 18.656421

N 9.079412 14.204831 16.763309

N 9.504545 16.680042 17.745716

C 8.830302 12.979688 16.266416

H 8.002604 12.424595 16.725170

C 9.579124 12.423612 15.215895

C 10.636682 13.168280 14.666344

H 11.241715 12.760663 13.848454

C 10.900451 14.446700 15.179642

H 11.713469 15.063174 14.779568

C	10.099419	14.937923	16.227442
C	10.278801	16.278713	16.781646
H	11.033635	16.944756	16.330587
C	9.612622	17.988495	18.275209
C	8.432410	18.743407	18.456905
H	7.474203	18.328449	18.131250
C	8.509018	20.041352	18.979518
H	7.596274	20.638562	19.088506
C	9.753718	20.583962	19.351411
H	9.808702	21.594920	19.770761
C	10.927820	19.832393	19.166924
H	11.899745	20.255264	19.446239
C	10.865242	18.543589	18.618329
H	11.774852	17.947762	18.488466
N	6.466087	15.808667	18.106162
N	7.825108	16.079656	20.381898
C	5.849176	15.687742	16.918583
H	6.371610	15.098655	16.154017
C	4.601983	16.281260	16.658592
C	3.979595	17.019154	17.679622
H	3.003261	17.488322	17.511689
C	4.628038	17.154772	18.918183
H	4.176966	17.732029	19.733619
C	5.881890	16.542627	19.098785
C	6.675655	16.685852	20.320164
H	6.300910	17.307761	21.149250
C	8.716104	16.294162	21.462503

C 9.168092 17.598406 21.761791

H 8.806587 18.447637 21.171297

C 10.127283 17.779219 22.769965

H 10.492257 18.788504 22.991989

C 10.615923 16.675978 23.491563

H 11.360103 16.823582 24.282305

C 10.144443 15.380859 23.202567

H 10.509799 14.523526 23.779256

C 9.210310 15.182161 22.178503

H 8.830660 14.181708 21.948451

N 10.120601 13.987978 19.383483

N 7.574748 13.164458 19.264404

C 11.454859 14.445402 19.253605

C 11.853205 15.625894 19.916599

H 11.137126 16.166752 20.542495

C 13.179687 16.063998 19.800969

H 13.500737 16.957154 20.349701

C 14.097254 15.364204 18.995268

H 15.130086 15.719118 18.903486

C 13.687844 14.206409 18.309323

H 14.396806 13.663137 17.673878

C 12.372812 13.738736 18.442768

H 12.039476 12.845228 17.900272

C 9.887897 12.735050 19.669832

H 10.707521 12.043624 19.923468

C 8.514491 12.262603 19.689208

C 8.160562 10.971173 20.130415

H 8.941324 10.276797 20.461976

C 6.808930 10.603610 20.145692

H 6.505739 9.607860 20.488587

C 5.849034 11.538885 19.717695

C 6.276119 12.803590 19.286483

H 5.554145 13.554240 18.944322

H 4.132877 16.163131 15.675810

H 4.781110 11.294931 19.715538

H 9.331250 11.425564 14.838140

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Model of the SCO compound S=1

Fe 17.838162 -0.165111 24.640145

N 18.592829 -1.482239 23.399713

C 19.883890 -1.852231 23.276963

H 20.602508 -1.389578 23.957258

C 20.308901 -2.785584 22.320163

H 21.371304 -3.045427 22.263664

C 19.372874 -3.361788 21.447442

H 19.684598 -4.087776 20.688440

C 18.029405 -2.981515 21.564880

H 17.257425 -3.394588 20.906109

C 17.674480 -2.040172 22.546283

C 16.338078 -1.545508 22.753650

H 15.489407 -1.923613 22.173422

N 16.199453 -0.614598 23.669625

N 14.907452 -0.066250 23.726895

C	14.146844	-0.326376	24.917952
O	14.617208	-1.051965	25.772801
C	12.751130	0.247972	24.951599
C	12.513499	1.416961	23.996641
C	12.989063	1.056618	22.591930
C	14.382081	0.479635	22.516495
O	15.030472	0.421434	21.479676
N	19.603852	0.200844	25.414705
C	20.158772	-0.369759	26.501782
H	19.593399	-1.168104	26.989278
C	21.409517	0.026614	27.000297
H	21.812933	-0.472291	27.887944
C	22.118736	1.053656	26.359507
H	23.094444	1.381229	26.734876
C	21.548149	1.655296	25.230039
H	22.057830	2.463306	24.693642
C	20.291695	1.210453	24.787234
C	19.593399	1.729963	23.640333
H	20.037254	2.467918	22.960591
N	18.393292	1.236527	23.433573
N	17.856223	1.586430	22.179891
C	16.800012	2.533153	22.162207
O	16.318263	2.919392	23.216020
C	16.364849	3.035270	20.803429
C	17.337248	2.727965	19.662712
C	17.763058	1.255738	19.729733
C	18.454853	0.949532	21.033009

O	19.433037	0.240017	21.173203
N	17.436098	-1.543189	25.977845
C	17.542197	-2.879603	25.837677
H	17.931797	-3.253114	24.887007
C	17.184573	-3.772634	26.860500
H	17.290698	-4.849538	26.690724
C	16.702813	-3.273598	28.080512
H	16.420781	-3.952296	28.893026
C	16.580592	-1.885499	28.231885
H	16.193432	-1.442201	29.155744
C	16.941209	-1.053500	27.161374
C	16.814167	0.382516	27.163168
H	16.481374	0.950201	28.040554
N	17.115208	0.970124	26.033763
N	17.069292	2.370412	26.054501
C	15.788808	2.957013	25.809014
O	14.805663	2.241033	25.761790
C	15.774072	4.461722	25.696055
C	17.157981	5.072095	25.475096
C	18.129585	4.558904	26.539098
C	18.186964	3.049438	26.631924
O	19.085137	2.419407	27.162079
H	19.167662	4.900763	26.382092
H	17.845628	4.926548	27.546782
H	17.516962	4.796553	24.467222
H	17.101060	6.172765	25.509979
H	15.073789	4.697983	24.877417

H 15.309571 4.847804 26.626379

H 12.330312 0.290623 22.130299

H 12.970708 1.916751 21.900217

H 11.442237 1.677215 23.974736

H 13.063495 2.297145 24.366592

H 12.070826 -0.599403 24.724291

H 12.560231 0.519241 26.003253

H 15.387954 2.553320 20.608817

H 16.169086 4.115470 20.921190

H 16.858943 2.939485 18.692018

H 18.228806 3.380531 19.722388

H 16.870518 0.601989 19.666150

H 18.458191 0.969251 18.924381

82

Model of the SCO compound S=5

Fe 18.017544 -0.104352 24.443233

N 18.768951 -1.847867 23.358047

C 20.052004 -2.187699 23.167493

H 20.800788 -1.604455 23.715938

C 20.433535 -3.247694 22.325992

H 21.494155 -3.492781 22.203571

C 19.436497 -3.985279 21.668883

H 19.700456 -4.824144 21.014815

C 18.093250 -3.626593 21.859511

H 17.283987 -4.167417 21.355997

C 17.798530 -2.536864 22.697537

C	16.443252	-2.038031	22.870163
H	15.598783	-2.604089	22.455304
N	16.284592	-0.895337	23.476503
N	14.968690	-0.492897	23.671363
C	14.075226	-1.403763	24.359287
O	14.495436	-2.475347	24.751656
C	12.644336	-0.937948	24.469071
C	12.474750	0.579786	24.565329
C	13.264541	1.291651	23.462414
C	14.711474	0.873298	23.382190
O	15.636144	1.590661	23.015908
N	19.968198	0.184884	25.318643
C	20.436220	-0.359769	26.450574
H	19.800909	-1.115189	26.928378
C	21.672736	0.010611	27.010253
H	22.012029	-0.459020	27.940003
C	22.447966	0.984478	26.363832
H	23.413995	1.296268	26.776716
C	21.958204	1.561257	25.181291
H	22.522546	2.336519	24.650960
C	20.710774	1.140390	24.692686
C	20.121835	1.715754	23.487308
H	20.675829	2.477343	22.922188
N	18.957499	1.281302	23.101703
N	18.371437	1.912223	22.012808
C	18.116461	3.315654	22.135740
O	18.603669	3.941973	23.062637

C	17.204072	3.901096	21.087336
C	17.264274	3.157638	19.751189
C	16.958081	1.674704	19.972995
C	17.802464	1.031513	21.045124
O	18.030182	-0.162661	21.126163
N	17.361989	-1.445780	26.036580
C	17.481448	-2.785590	26.089587
H	18.141680	-3.248275	25.347782
C	16.805811	-3.570170	27.035825
H	16.934878	-4.657798	27.030893
C	15.969725	-2.941427	27.973585
H	15.423473	-3.528625	28.720186
C	15.852517	-1.546522	27.938124
H	15.219345	-1.010283	28.654362
C	16.559208	-0.828028	26.953267
C	16.480682	0.615282	26.850256
H	15.953187	1.184338	27.626457
N	17.062903	1.204457	25.837521
N	16.900653	2.597327	25.793545
C	15.570210	3.111242	25.773961
O	14.617405	2.350973	25.858262
C	15.440376	4.614281	25.695020
C	16.670177	5.327683	25.137189
C	17.927065	4.871111	25.877113
C	18.095934	3.372157	25.948669
O	19.145070	2.802177	26.186298
H	18.849968	5.260689	25.417435

H	17.923459	5.232559	26.926596
H	16.787465	5.108807	24.062352
H	16.549005	6.419641	25.231885
H	14.522067	4.818760	25.118056
H	15.223410	4.952325	26.730214
H	12.825132	1.072105	22.465828
H	13.250689	2.385703	23.584246
H	11.406134	0.840690	24.489141
H	12.830396	0.943164	25.543031
H	12.136816	-1.330576	23.562088
H	12.200112	-1.474039	25.324153
H	16.182174	3.838229	21.515243
H	17.459702	4.970103	20.999535
H	16.540770	3.593748	19.042466
H	18.264263	3.278168	19.294009
H	15.907244	1.547365	20.303227
H	17.081455	1.067401	19.060572

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