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Supporting Information for

A Chiral Spin Crossover Metal-Organic Framework

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Materials and Physical Measurements

The reagents and solvents used were all commercially available and used without further purification.

The C, H, and N microanalyses were carried out with an ElementarVario-ELCHNS elemental analyzer. PXRD intensities for bulk samples were measured at room temperature and high temperature under N_2 atmosphere on a Bruker D8 Advance diffratometer (Cu K_α, $\lambda = 1.54056$Å) by scanning over the range 5-50 with step of 0.3°/s. The calculated patterns were generated with Mercury. The FT-IR spectra were recorded from KBr pellets in the range from 4000 to 400 cm- with a Bruker-EQUINOX 55 FT-IR spectrometer. Magnetic susceptibility measurements were performed on a Quantum Design MPMS-XL7 SQUID instrument, and diamagnetic corrections were made with Pascal's constant. The samples were sealed in parafilm to avoid any displacement of the crystallites. DSC measurement was carried out by using a Netzsch DSC 204 instrument under nitrogen atmosphere at a scan rate of 5 K min^{-1} in both heating and cooling modes. ^{57}Fe Mössbauer spectra of the **1**·solv sample were collected in the transmission geometry at 60 K, room temperature (300 K), and 400 K employing a Mössbauer spectrometer operating at a constant-acceleration mode and equipped with a 50 mCi^{57}Co(Rh) source. For a low-temperature Mössbauer measurement, the sample was placed inside the chamber of the closed-helium cycle system. For a high-temperature Mössbauer measurement, the sample was place inside the oven. For both low-temperature and high-temperature Mössbauer measurements, the γ-rays source was kept at room temperature. Velocity calibration of the spectrometer was carried out using a metallic α-iron at room temperature and all isomer shift values are given relative to this standard. TG-DTA coupled to a Mass Spectrometer (STA449 F3 Jupiter-QMS 403C aedo) was used, and the thermogravimetric analysis performed under the flowing N_2 atmosphereat a scan rate of 10 K min^{-1}. Diffraction intensities data was collected on a Rigaku R-AXIS SPIDER IP diffractometer using Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods, and all non-hydrogen atoms were refined anisotropically through least-squares on F^2 using the SHELXTL program.[1] Hydrogen atoms on organic ligands were generated by the riding mode. Some of the severely disordered guest molecules for both 1 and 2 were removed by SQUEEZE from the PLATON software[2] in structural refinement. Further details for these compounds are summarized in Table S1. The picture of coordination environment and framework pictures were produced using Diamond 3.1.[3] The Solid-state circular dichroism (CD) spectra were recorded on a Jasco J-810 spectropolarimeter. For each sample, the spectrum was scanned at least three times and accumulated over the wavelength range of 700–230 nm at a temperature of 293 K. For variable-temperature CD spectra, a Jasco CDF-426S thermo controller was used from 278 K to 373 K.

1. *SHELXTL 6.10*, Bruker Analytical Instrumentation, Madison, Wisconsin, USA, 2000.
2. Spek, A. L. *J. Appl. Crystallogr*. 2003, **36**, 7.
3. W. T. Pennington, *J. Appl. Crystallogr.*, 1999, **32**, 1028.

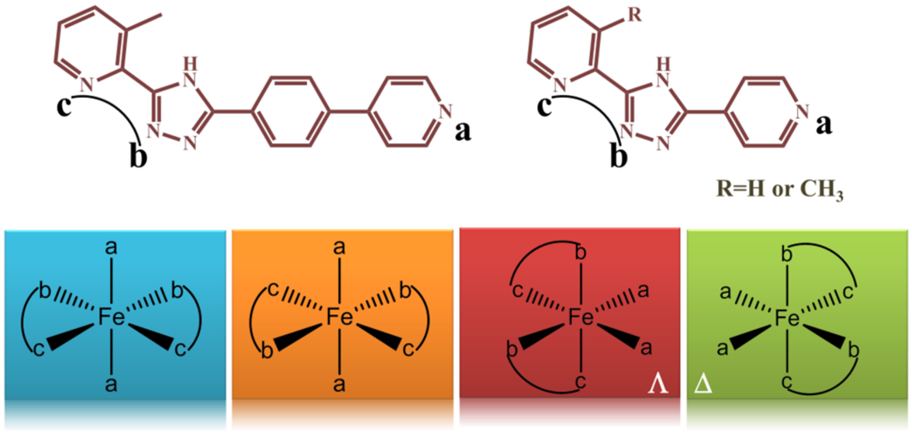
Synthesis of 1·solv

Single crystals of **1**·solv were solvothermally prepared: $FeCl_2 \cdot 4H_2O$ (0.010g, 0.05mmol), Hmptpy (0.031g, o.1mmol) and triethylamine (0.010g, 0.1mmol) in the mixed solution of ethanol (12ml) & DMF (2ml) was sealed in a 20ml Teflon-lined reactor and heated at 160°C for 2day before cooled to room temperature at 5°C/h^{-1}. Subsequently, dark red crystals of **1**·solv were obtained in 31% yield based on Fe. Those crystals are suitable for single crystal X-ray diffraction analysis but are quite difficult to be purified. Thus we made a slight modification by adding a small amount of ethylene glycol (2ml) in order to obtain pure bulk samples. Thus gave a higher yield of **1**·solv (63%) but much smaller crystals. Both TG-MS analysis and PXRD shows structural composition analysis and solvent in the structure are the same in spite of the adding of ethylene glycol. Without the addition of glycol, amorphous impurities may exist. IR data (KBr, cm^{-1}): 3905 w, 3753 w, 3450 m, 3103 w, 3061 w, 2924 w, 1607 s, 1562 w, 1516 s, 1459 s,1419 s, 1396 s,1344 w, 1189 m, 1140 m, 1105 m, 1053 m, 1028 m,806 s, 782 w, 747 s, 707 s; elemental analysis calcd (%) for 1: C 65.78, H 4.81, N 19.27; found: C 65.68, H 4.72, N 19.32.

Desolvated process for 1

Desolvated sample **1** was got by heating the **1**·solv to 500 K at a rate of 10 K min^{-1} and then maintained at this temperature for one hour under the flowing N_2 atmosphere.

Scheme S1 Up: Schematic drawing of the ligand: Hmptpy and 2,4-R-Hbpt. Down: all the possibilities of the coordination mode of Fe in formula Fe(mptpy)$_2$, two of which (in red and green) are potentially chiral.



Some reasonable methods were taken to solve the question of the guest molecules, such as TG-MS and elemental analysis to determine the proportion of the guest molecules. As shown in Figure S1, EtOH and DMF are both contend in the framework, the total weight proportion is about 6.7%. With the help of elemental analysis (found %: C 65.68, H 4.72, N 19.32.), we calculate that there are 1 EtOH and 0.2 DMF in the formula.

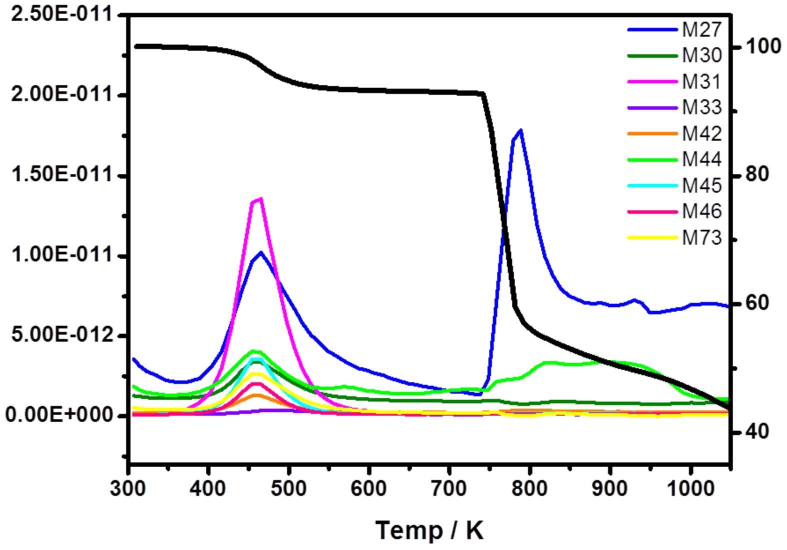


Figure S1 Thermogravimetric-mass spectroscopy analysis of **1**·solv; the *x* axis represents temperature and the double *y* axis represents the percentage of mass lost (left) and the intensity in arbitrary units (right).

Table S1 Crystal Data and Structure Refinements for **1**·solv.

compound	**1**-P	**1**-P	**1**-P	**1**-M
space group	$P3_112$	$P3_112$	$P3_112$	$P3_212$
crystal syst	trigonal	trigonal	trigonal	trigonal
temp/K	150(2)	293(2)	373(2)	293(2)
formula	$C_{38}H_{28}FeN_{10}$	$C_{38}H_{28}FeN_{10}$	$C_{38}H_{28}FeN_{10}$	$C_{38}H_{28}FeN_{10}$
M / (g mol^{-1})	680.55	680.55	680.55	680.55
a/Å	10.8557(7)	11.0080(11)	11.1911(11)	11.0431(10)
c/Å	25.463(2)	25.490(4)	25.406(4)	25.478(5)
V/Å^3	2598.7(3)	2674.9(5)	2755.6(5)	2690.8(6)
Z	3	3	3	3
μ/mm^{-1}	0.478	0.464	0.451	0.462
reflns collected	8873	7451	7562	8370
unique reflns	3397	2812	3419	3432
R_{int}	0.0912	0.1212	0.1464	0.1147
Final R_1 values ($I > 2\sigma(I)$)	0.0606	0.0564	0.1265	0.0798
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1294	0.1037	0.2141	0.1960
Goodness of fit on F^2	1.132	0.950	1.071	1.079
Flack parameter	0.00(4)	0.06(4)	0.05(7)	0.08(5)

Table S2 Fe-N bond lengths (Å) and parameters Σ (°) for **1**·*n*solv.

1-P	Fe-N$_{cis}$	Fe-N$_{trz}$	Fe-N$_{pychelate}$	Fe-N$_{averange}$	Σ
150K	2.040	1.989	2.035	2.021	49.5
293K	2.096	2.026	2.109	2.077	56.7
373K	2.167	2.089	2.238	2.165	74.9
1-M	Fe-N$_{cis}$	Fe-N$_{trz}$	Fe-N$_{pychelate}$	Fe-N$_{averange}$	Σ
293K	2.090	2.058	2.134	2.094	60.9

Variable-temperature CD patterns of 1-P in KCl pellets is taken from 278K to 373K. No distinct changes are observed at the appropriate temperatures. Its range at negative peak 355 nm depends on temperature are also putted in the supporting information (Figure S2). Chirality in this SCO-MOFs owe to intrinsic chiral *qtz* topology derives from *trans*-Fe or *cis*-Fe chiral building block (Scheme 1).

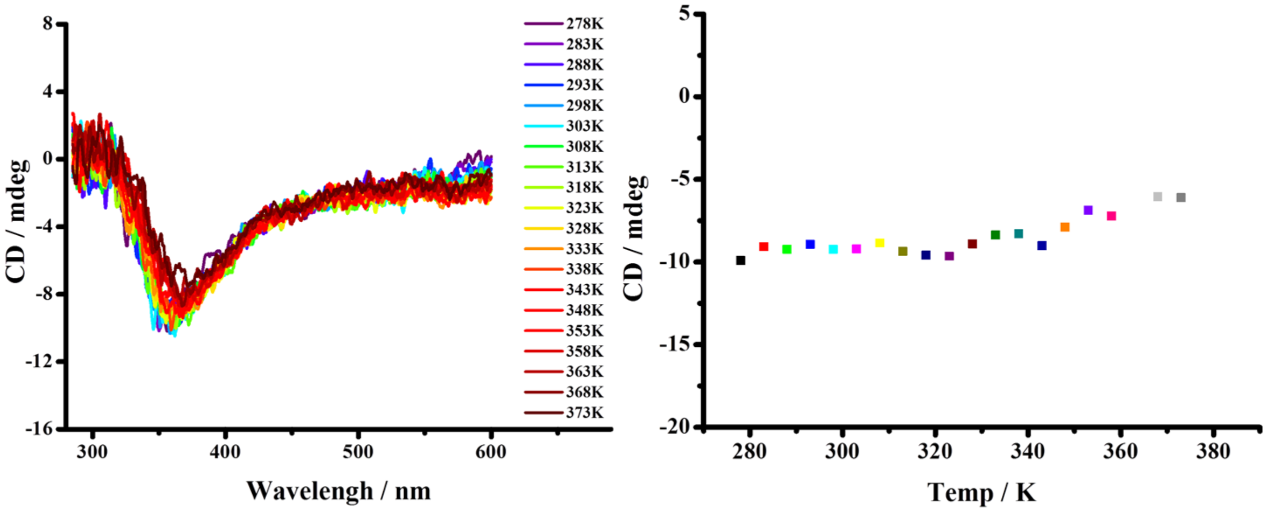


Figure S2 Variable-temperature CD patterns of **1**·solv in KCl pellets from 278K to 373K (left) as well as its range at 355 nm depends on temperature (right). No distinct changes are observed at the appropriate temperatures.

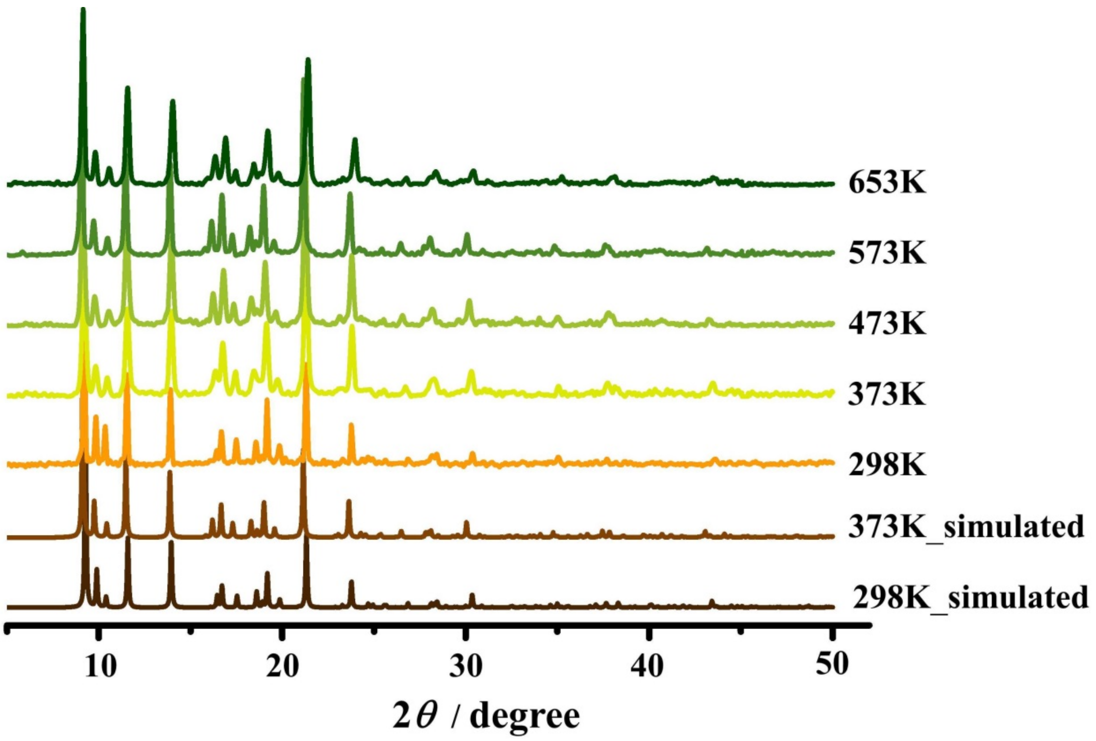


Figure S3 Variable-temperature PXRD patterns of **1**·solv as well as its simulated PXRD pattern.

Table S3 Values of the Mössbauer hyperfine parameters of **1**·solv, derived from the fitting procedure of the low-temperature, room-temperature, and high-temperature Mössbauer spectra, where δ is the isomer shift, ΔE_Q is the quadrupole splitting, Γ is the linewidth, and RA is the relative spectral area of individual spectral components.

Temperature (K)	**Component**	**δ ± 0.01 (mm/s)**	**ΔE_Q ± 0.01 (mm/s)**	**Γ ± 0.01 (mm/s)**	**RA ± 1 (%)**	**Assignment**
60	Doublet	0.46	0.83	0.44	100	LS Fe^{2+}
300	Doublet	0.42	0.93	0.27	55	LS Fe^{2+}
	Doublet	0.93	2.04	0.31	45	HS Fe^{2+}
400	Doublet	0.33	0.61	0.37	35	LS Fe^{2+}
	Doublet	0.83	1.42	0.31	65	HS Fe^{2+}

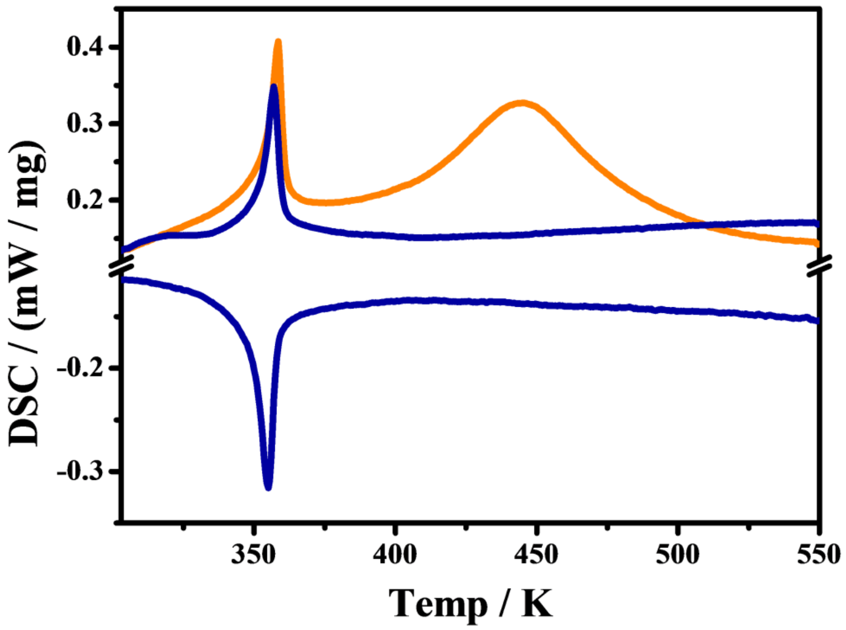


Figure S4 DSC for **1**·solv (in orange) and **1** (in royal) for the second step spin transition.

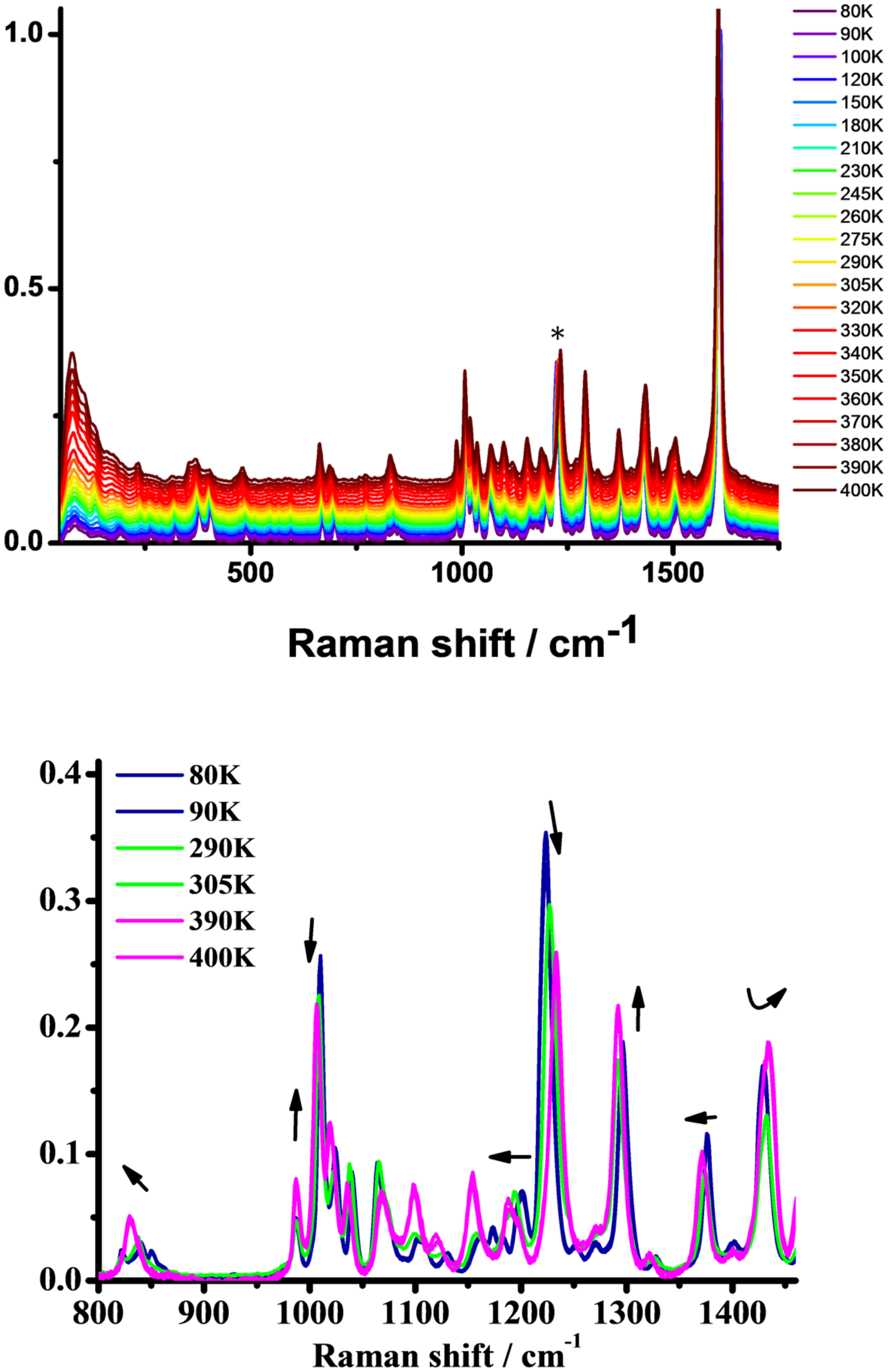


Figure S5 Variable temperature Raman spectra of **1**·solv with excitation of 632.8 nm radiation. Above: Full spectra in the range of 50-1700 cm^{-1}; below: spectra in the range of 800-1480 cm^{-1}.