Supporting materials

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A. Synthesis of 1D chain coordination polymer

A solution containing 0.249 g (1.5 mmol) of atrz dissolved in 15 mL of water and warmed to 60°C was added to a solution containing 0.128 g (0.5 mmol) of $Fe(BF_4)_2 \cdot 6H_2O$ and a small amount of ascorbic acid dissolved in 15 mL of water. Yellow crystals were obtained by slow evaporation at room temperature within one day. Anal. Calcd for $C_{12}H_{24}N_{24}B_2F_8O_6Fe$: C, 17.34; H, 2.91; N, 40.48. Found: C, 17.10; H, 2.88; N, 40.57.

B. Structural information of 1D chain coordination polymer

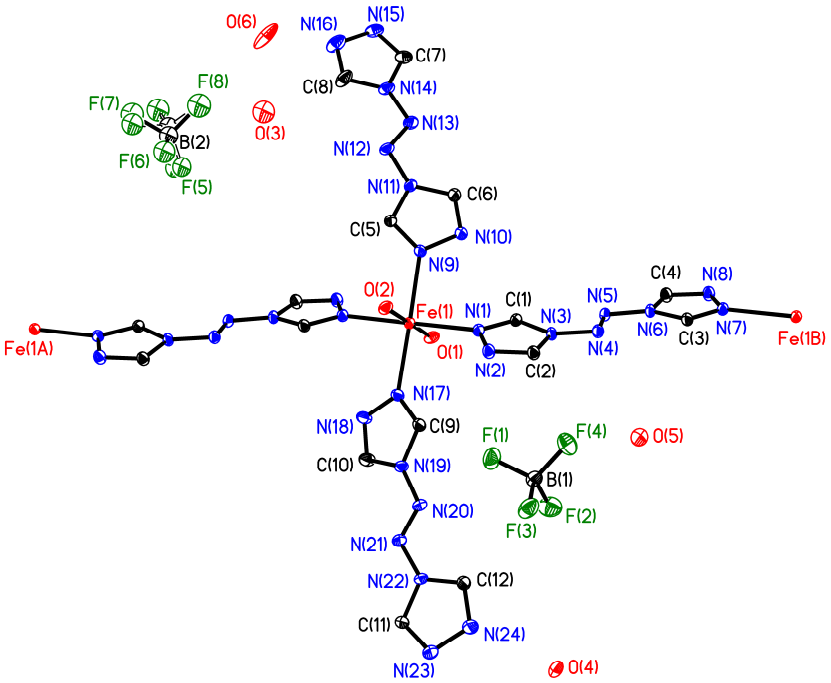

Figure S1. Molecular structure of $[Fe(\mu\text{-atrz})(atrz)_2(H_2O)_2](BF_4)_2 \cdot 4H_2O$ at 150 K, ellipsoids are drawn with 30 % probability. Hydrogen atoms are omitted.

Table S1. Crystallographic detail of $[Fe(\mu\text{-atrz})(atrz)_2(H_2O)_2](BF_4)_2\cdot 4H_2O$

Temperature	150 K
Formula	$C_{12}H_{22}B_2F_8FeN_{24}O_{5.32}$
Formula weight	817.14
Crystal system	Triclinic
Space group	*P*-1
a (Å)	11.2939(2)
b (Å)	11.4812(2)
c (Å)	13.0931(2)
α (deg)	112.1212(9)
β (deg)	95.5478(11)
γ (deg)	91.2584(11)
V (Å^3)	1562.27(5)
Z	2
D_{calc} (g/cm^3)	1.737
μ (mm^{-1})	0.603
Crystal size	0.20 x 0.15 x 0.08
F(000)	825
Reflections collected	32512
Unique reflections/ observed.(I > 2σ(I))	7169/4498
Max and min transmission	0.95, 0.89
R_1, wR_2[a] (I > 2σ(I))	0.0599, 0.1542
R_1, wR_2[a] (all data)	0.1070, 0.1750
Goodness of fit on F^2	1.070
Parameters / restraints	464 / 20
Largest diff. peak and hole	1.055 and -0.860 e.Å^{-3}

$R_F = \Sigma||F_o - F_c||/\Sigma|F_o|$; $R_w(F^2) = [\Sigma w|F_o^2 - F_c^2|^2/\Sigma w(F_o^4)]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (deg) of $[Fe(\mu\text{-atrz})(atrz)_2(H_2O)_2](BF_4)_2\cdot 4H_2O$ and torsion angle of atrz ligand

Bond	Distance (Å)
Fe(1)–O(1)	2.053(2)
Fe(1)–O(2)	2.070(3)
Fe(1)–N(1)	2.195(3)
Fe(1)–N(7)	2.206(3)
Fe(1)–N(9)	2.207(3)
Fe(1)–N(17)	2.218(3)
Angle	Degree (˚)
O(1)–Fe(1)–O(2)	179.42(10)
N(1)–Fe(1)–N(9)	91.02(11)
N(9)–Fe(1)–N(7)	88.36(11)
N(1)–Fe(1)–N(17)	90.40(11)
N(7)–Fe(1)–N(17)	90.20(11)
O(1)–Fe(1)–N(1)	89.14(11)
O(2)–Fe(1)–N(1)	90.89(11)
O(1)-Fe(1)-N(7)	89.97(11)

O(2)-Fe(1)-N(7)	90.01(10)
O(1)-Fe(1)-N(9)	90.27(11)
O(2)-Fe(1)-N(9)	90.30(11)
O(1)-Fe(1)-N(17)	88.52(11)
O(2)-Fe(1)-N(17)	90.91(11)

Torsion angle	Degree (˚)
N(1)–N(2)···N(7)–N(8)	6.7 (3)
N(9)–N(10)···N(15)–N(16)	9.5 (3)
N(17)–N(18)···N(23)–N(24)	16.0 (3)

C. Synchrotron powder X-ray diffraction pattern measurement

The PXRD measurements were performed at beamline BL01C in NSRRC. The in-situ powder diffraction data were recorded on a Mar3450 image plate at the wavelength of 0.97946 Å, where two theta angle is calibrated based on the standard powder sample of CeO_2.

D. Magnetic measurement

The temperature dependent magnetic susceptibility was measured in RSO mode using the Quantum Design MPMS SQUID magnetometer under an applied magnetic field of 2000 Oe.

E. Thermogravimetric analyses (TGA) of 1D chain coordination polymer

A TGA measurement was taken in the range of (a) 25-150°C at a heating rate of 1°C/min; (b) 150-350°C at a heating rate of 5°C/min. The sample weight is 9.832 mg. The water content of the title compound established from the thermogravimetric analysis is ~ 5.7, which includes water molecules in coordination and in the lattice. The first weight loss should be related to the loss of water molecules in the lattice; and the second drop should attribute to the coordinated water molecules with a ratio of 4:2. However the steps are not that clearly separated, the total loss corresponds to ~ 5.7 water molecules. It is worth noticing that the water molecules in lattice are strongly H-bonded to the coordinated water molecules which may explain the two steps are not clearly separated. Furthermore, sample starts to loose water even at room temperature. It is clear that the sample is completely anhydrous beyond 100°C.

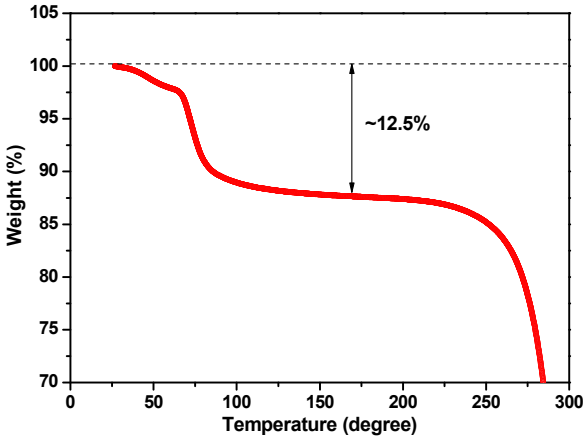

Figure S2. TGA analysis of $[Fe(\mu\text{-atrz})(atrz)_2(H_2O)_2](BF_4)_2 \cdot 4H_2O$; calculated water content should be 13.0%.