Supporting Information

Structural regulation of three Fe-Co cyanometallate complexes: reactant ratio issue

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Table S1. Selected Bond lengths [Å] and angles [deg] for **1**.

Co(1)-N(10)	2.187(3)	Fe(2)-C(18)	1.923(4)
Co(1)-N(11)	2.120(3)	Fe(2)-C(22)	1.905(4)
Co(1)-N(15)	2.143(3)	Fe(2)-C(36)	1.914(5)
Co(1)-N(13)	2.162(3)	Fe(1)-N(3)	1.986(4)
Co(1)-N(9)	2.084(4)	Fe(1)-N(5)	1.971(4)
Co(1)-N(17)	2.045(3)	Fe(1)-N(1)	1.973(4)
Fe(2)-N(20)	1.959(3)	Fe(1)-C(16)	1.904(4)
Fe(2)-N(24)	1.983(4)	Fe(1)-C(32)	1.935(4)
Fe(2)-N(22)	1.983(3)	Fe(1)-C(27)	1.915(6)
N(11)-Co(1)-N(10)	73.48(12)	C(22)-Fe(2)-C(18)	86.74(16)
N(11)-Co(1)-N(15)	82.19(12)	C(22)-Fe(2)-C(36)	86.80(18)
N(11)-Co(1)-N(13)	83.35(12)	C(36)-Fe(2)-N(20)	92.59(18)
N(15)-Co(1)-N(13)	81.87(13)	C(36)-Fe(2)-N(22)	91.77(18)
N(9)-Co(1)-N(10)	80.58(13)	C(36)-Fe(2)-C(18)	87.8(2)
N(9)-Co(1)-N(13)	84.74(13)	N(5)-Fe(1)-N(3)	87.02(16)
N(17)-Co(1)-N(10)	91.14(12)	N(5)-Fe(1)-N(1)	89.15(15)
N(17)-Co(1)-N(15)	88.35(13)	N(1)-Fe(1)-N(3)	89.21(17)
N(17)-Co(1)-N(9)	90.97(14)	C(16)-Fe(1)-N(5)	88.38(16)
N(20)-Fe(2)-N(24)	88.72(15)	C(16)-Fe(1)-C(32)	89.41(17)
N(20)-Fe(2)-N(22)	88.50(14)	C(16)-Fe(1)-C(27)	84.93(19)
N(22)-Fe(2)-N(24)	88.98(15)	C(32)-Fe(1)-N(3)	88.86(17)
C(18)-Fe(2)-N(24)	90.88(17)	C(32)-Fe(1)-N(1)	93.46(16)
C(18)-Fe(2)-N(22)	93.21(16)	C(27)-Fe(1)-N(5)	95.82(18)
C(22)-Fe(2)-N(20)	91.56(15)	C(27)-Fe(1)-N(1)	89.87(19)
C(22)-Fe(2)-N(24)	92.45(16)	C(27)-Fe(1)-C(32)	88.34(19)

Table S2. Selected Bond lengths [Å] and angles [deg] for **2**.

Co(1)-N(1)	2.1456(18)	Fe(1)-N(12)	1.9704(17)
Co(1)-N(8)	2.0545(18)	Fe(1)-N(14)	1.9617(17)
Co(1)-N(16)A	2.1071(18)	Fe(1)-N(9)	1.9936(18)
Co(1)-N(5)	2.1402(17)	Fe(1)-C(16)	1.916(2)
Co(1)-N(4)	2.1366(18)	Fe(1)-C(26)	1.919(2)
Co(1)-N(7)	2.1874(18)	Fe(1)-C(27)	1.913(2)
N(1)-Co(1)-N(7)	148.27(7)	N(12)-Fe(1)-N(9)	88.15(7)
N(8)-Co(1)-N(1)	109.22(7)	N(14)-Fe(1)-N(12)	88.99(7)
N(8)-Co(1)-N(16)A	89.10(7)	N(14)-Fe(1)-N(9)	88.58(7)
N(8)-Co(1)-N(5)	164.62(7)	C(16)-Fe(1)-N(12)	89.68(8)
N(8)-Co(1)-N(4)	91.74(7)	C(16)-Fe(1)-N(14)	92.21(8)
N(8)-Co(1)-N(7)	97.85(7)	C(16)-Fe(1)-N(9)	177.68(8)
N(16)A-Co(1)-N(1)	85.17(7)	C(16)-Fe(1)-C(26)	88.69(9)
N(16)A-Co(1)-N(5)	101.05(7)	C(26)-Fe(1)-N(12)	177.16(8)

N(16)A-Co(1)-N(4)	169.63(7)	C(26)-Fe(1)-N(14)	93.40(8)
N(16)A-Co(1)-N(7)	78.88(7)	C(26)-Fe(1)-N(9)	93.44(8)
N(5)-Co(1)-N(1)	83.35(7)	C(27)-Fe(1)-N(12)	93.17(8)
N(5)-Co(1)-N(7)	73.18(7)	C(27)-Fe(1)-N(14)	177.43(8)
N(4)-Co(1)-N(1)	84.80(7)	C(27)-Fe(1)-N(9)	90.10(8)
N(4)-Co(1)-N(5)	80.36(7)	C(27)-Fe(1)-C(16)	89.21(9)
N(4)-Co(1)-N(7)	111.21(7)	C(27)-Fe(1)-C(26)	84.48(9)

Symmetry transformations used to generate equivalent atoms: A -x+1,-y+1,-z+1

Table S3. Selected Bond lengths [Å] and angles [deg] for **3**.

Co(1)-N(5)	2.150(6)	Fe(1)-N(16)	1.954(6)
Co(1)-N(1)	2.166(6)	Fe(1)-N(13)	1.969(6)
Co(1)-N(3)	2.127(5)	Fe(1)-N(11)	1.977(5)
Co(1)-N(8)	2.054(5)	Fe(1)-C(17)	1.922(8)
Co(1)-N(7)	2.114(5)	Fe(1)-C(16)	1.901(6)
Co(1)-N(9)A	2.099(7)	Fe(1)-C(18)	1.920(6)
N(5)-Co(1)-N(1)	110.7(2)	N(16)-Fe(1)-N(13)	88.4(3)
N(3)-Co(1)-N(5)	80.7(2)	N(16)-Fe(1)-N(11)	88.8(2)
N(3)-Co(1)-N(1)	73.2(2)	N(13)-Fe(1)-N(11)	88.2(2)
N(8)-Co(1)-N(5)	87.8(2)	C(17)-Fe(1)-N(16)	179.1(2)
N(8)-Co(1)-N(1)	89.0(2)	C(17)-Fe(1)-N(13)	91.1(3)
N(8)-Co(1)-N(3)	153.5(2)	C(17)-Fe(1)-N(11)	91.9(3)
N(8)-Co(1)-N(7)	116.0(2)	C(16)-Fe(1)-N(16)	91.4(3)
N(8)-Co(1)-N(9)A	95.4(2)	C(16)-Fe(1)-N(13)	92.7(2)
N(7)-Co(1)-N(5)	83.2(2)	C(16)-Fe(1)-N(11)	179.1(3)
N(7)-Co(1)-N(1)	152.4(2)	C(16)-Fe(1)-C(17)	87.9(3)
N(7)-Co(1)-N(3)	86.4(2)	C(16)-Fe(1)-C(18)	87.3(3)
N(9)A-Co(1)-N(5)	168.5(2)	C(18)-Fe(1)-N(16)	92.5(3)
N(9)A-Co(1)-N(1)	80.4(2)	C(18)-Fe(1)-N(13)	179.1(3)
N(9)A-Co(1)-N(3)	100.6(2)	C(18)-Fe(1)-N(11)	91.8(2)
N(9)A-Co(1)-N(7)	85.5(2)	C(18)-Fe(1)-C(17)	88.0(3)

Symmetry transformations used to generate equivalent atoms: A x,-y+3/2,z-1/2 B x,-y+3/2,z+1/2

Table S4. Continuous Shape Measure (CSM) parameters for **1**-**3**.

Compound, Metal center	CSM parameters					Determined coordinnation geometry
	Six- coordinated coordination sphere					
	Hexagon (D_{6h})	Pentagonal pyramid (C_{5v})	Octahedron (O_h)	Trigonal prism (D_{3h})	Johnson pentagonal pyramid (C_{5v})	
1_Co	32.317	19.024	**4.709**	4.743	23.264	Octahedron (O_h)
2_Co	29.906	18.706	**3.393**	6.775	22.478	
3_Co	32.629	18.915	**3.908**	5.864	22.723	

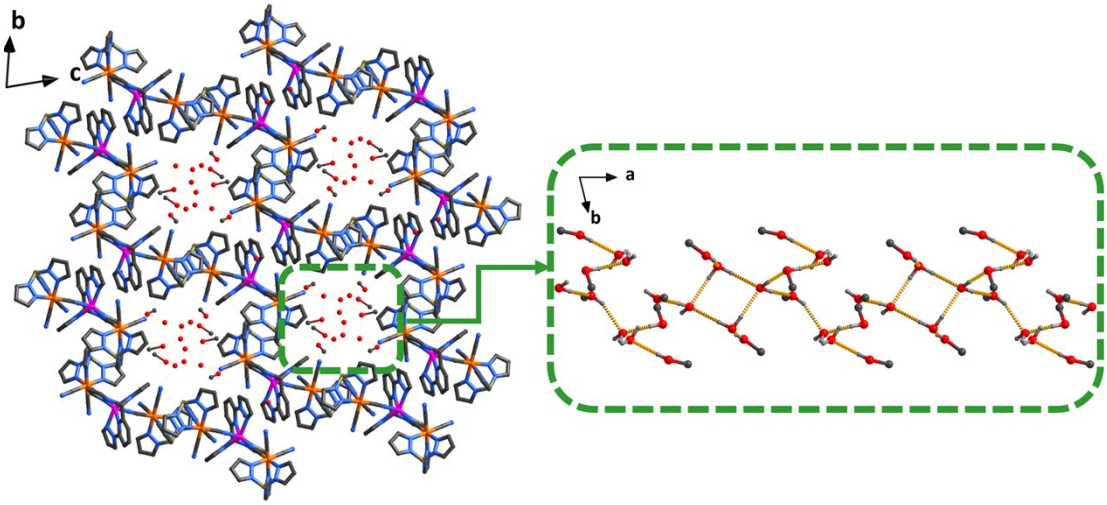

Figure S1. The packing diagram of **1**. Colour codes: Co, pink; Fe, orange; B, yellow; N, blue; O, red; C, grey. All hydrogen atoms, counterions and partial lattice solvents are omitted for clarity. Insert is the hydrogen bond network formed through MeOH and H_2O.

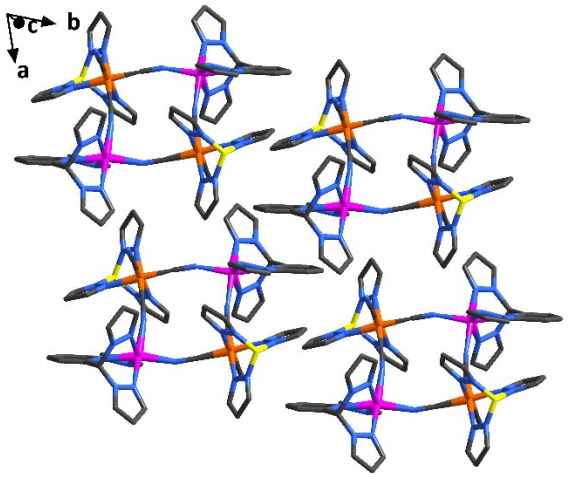

Figure S2. The packing diagram of **2**. Colour codes: Co, pink; Fe, orange; B, yellow; N, blue; O, red; C, grey. All hydrogen atoms, lattice solvents and counterions are omitted for clarity.

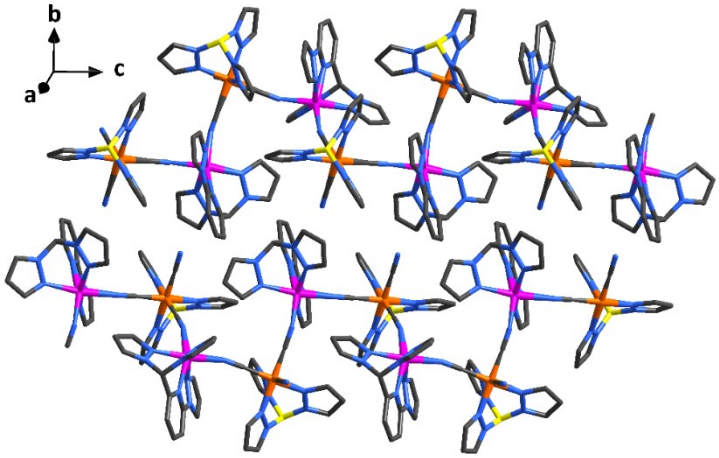

Figure S3. The packing diagram of **2**. Colour codes: Co, pink; Fe, orange; B, yellow; N, blue; O, red; C, grey. All the fluorine and hydrogen atoms, lattice solvents and counterions are omitted for clarity.

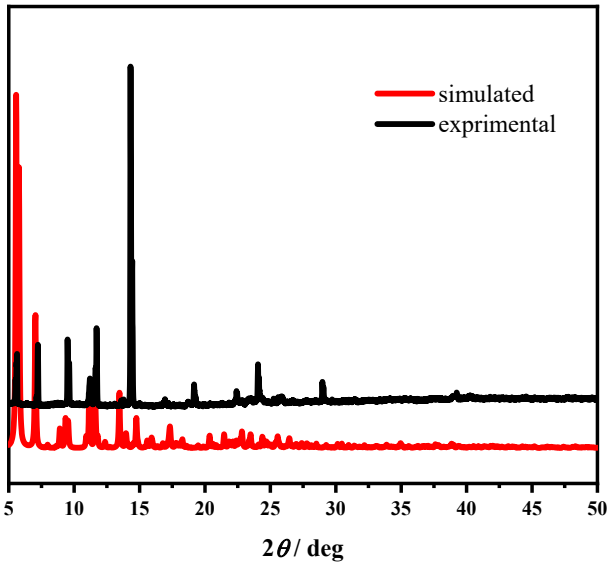

Figure S4. The powder X-ray diffraction for **1**. The red line is calculated from the single crystal data.

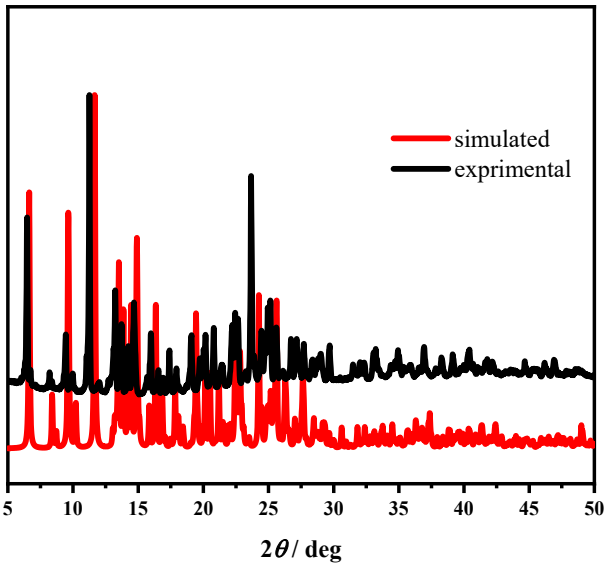

Figure S5. The powder X-ray diffraction for **2**. The red line is calculated from the single crystal data.

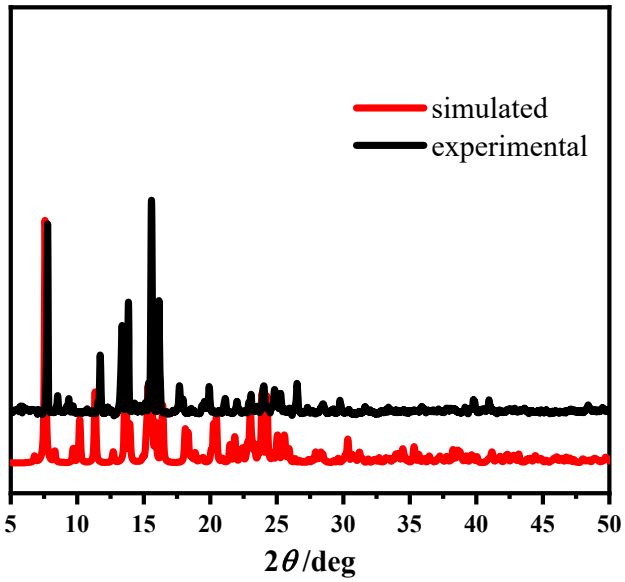

Figure S6. The powder X-ray diffraction for 3. The red line is calculated from the single crystal data.

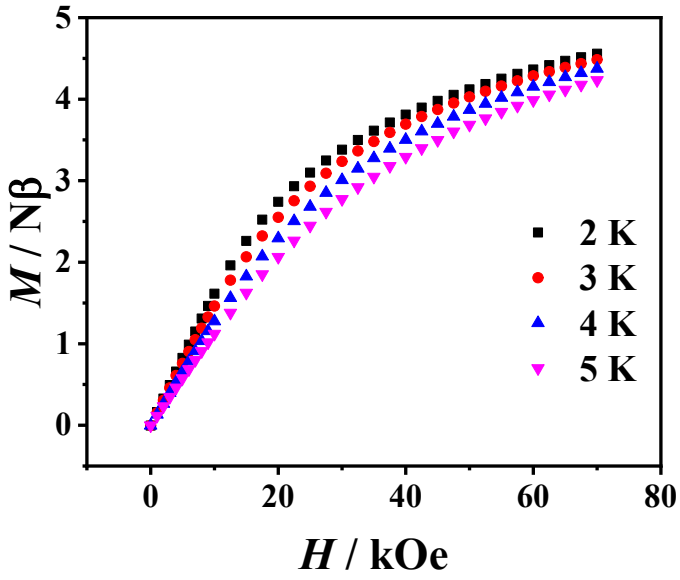

Figure S7. Field dependence of the magnetization for 1 between 2 and 5 K. Solid lines are guides for eye.

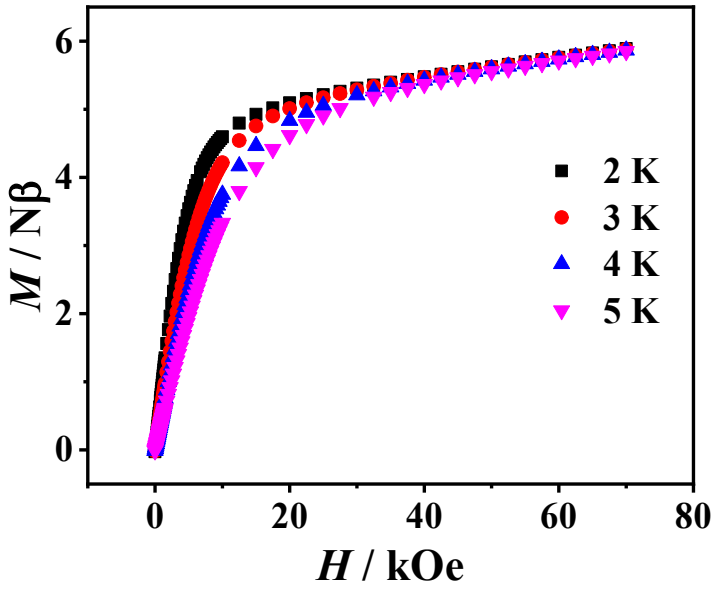

Figure S8. Field dependence of the magnetization for **2** between 2 and 5 K. Solid lines are guides for eye.

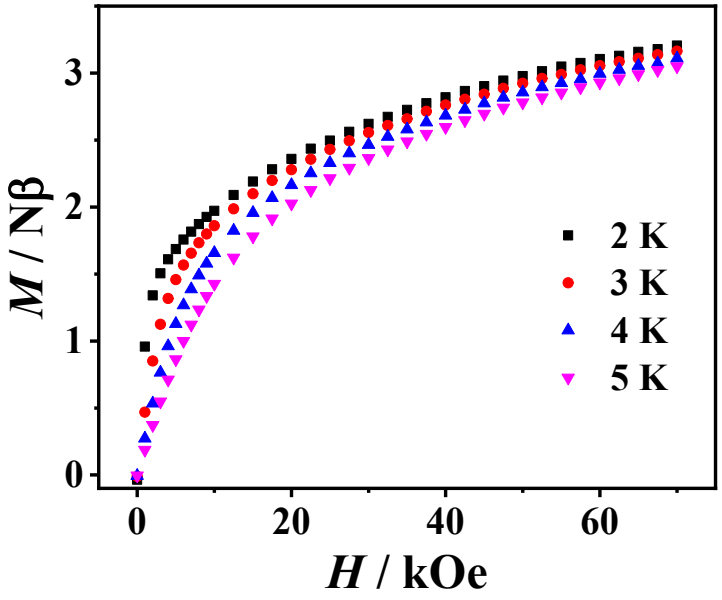

Figure S9. Field dependence of the magnetization for **3** between 2 and 5 K. Solid lines are guides for eye.

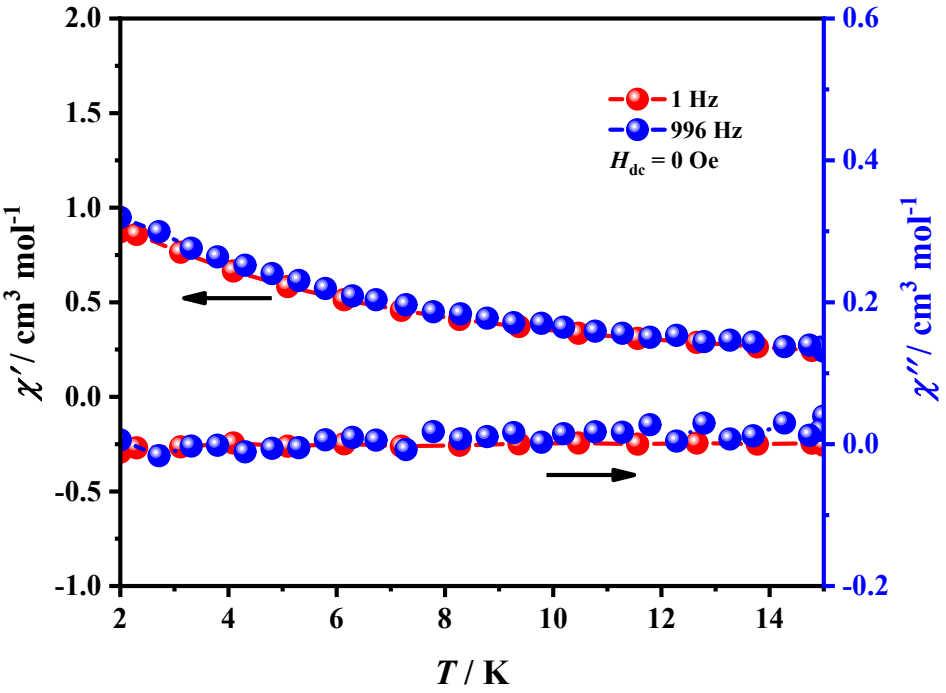

Figure S10. Temperature dependence of the in-phase (□′) and out-of-phase (□″) ac susceptibility for **1** at zero dc field. The lines are guides to the eyes.

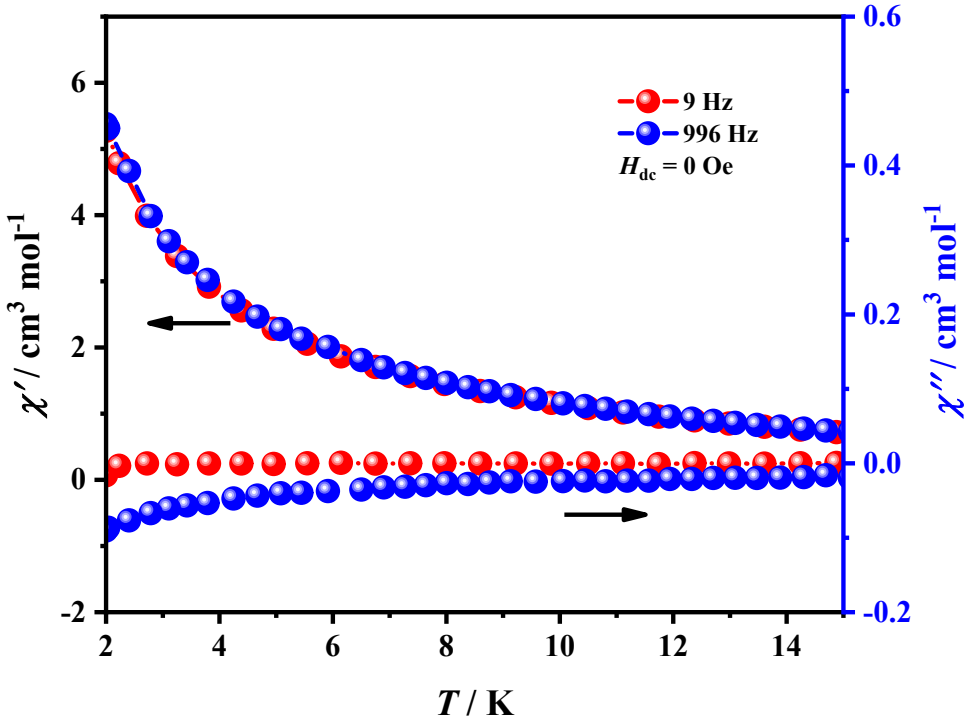

Figure S11. Temperature dependence of the in-phase (□′) and out-of-phase (□″) ac susceptibility for **2** at zero dc field. The lines are guides to the eyes.

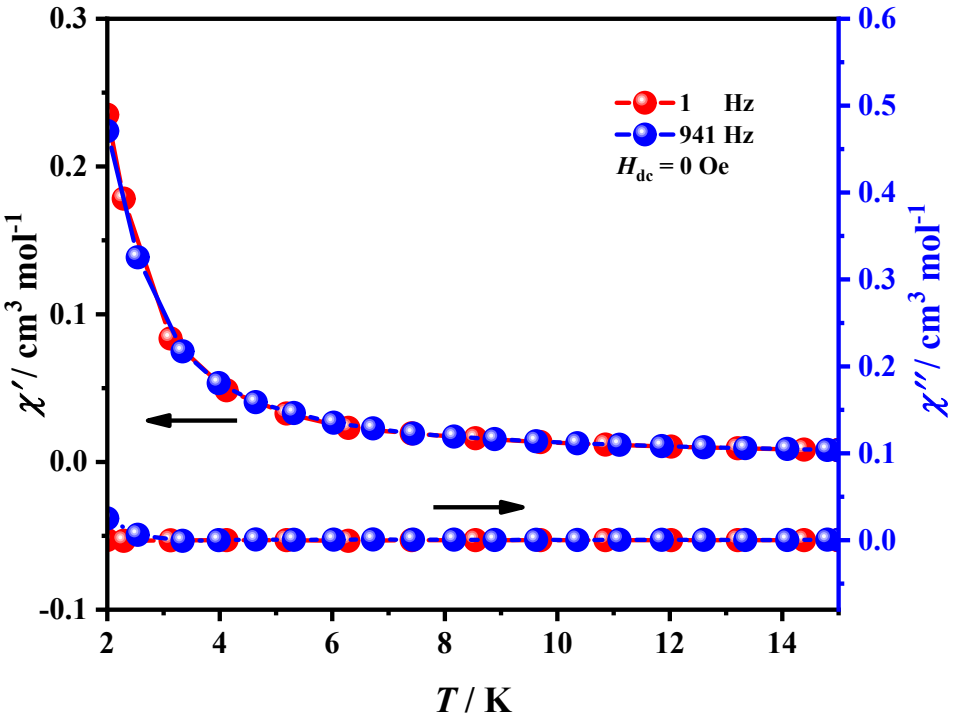

Figure S12. Temperature dependence of the in-phase (□′) and out-of-phase (□″) ac susceptibility for **3** at zero dc field. The lines are guides to the eyes.