Table S1. Summary of crystallographic data for complexes **1b**, **2a**, **2b**, **3a**, and **4**.

	1b	**2a**	**2b**	**3a**	**4**
Formula	$C_{78}H_{76}FeN_3O_3$	$C_{52}H_{50}ClFeN_2O_4$	$C_{52}H_{50}ClFeN_2O_2$	$C_{49}H_{34}Cl_5Fe_2N_2O_2$	$C_{68}H_{82}FeN_2Na_2O_6$
F_w	1159.27	858.24	826.24	971.73	1125.19
cryst syst	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
space group	P2(1)/c	P2(1)/c	P2(1)/c	P-1	P-1
a (Å)	12.410(4)	13.511(3)	16.5932(13)	13.3556(8)	10.3920(10
b (Å)	20.623(6)	19.197(4)	13.0580(10)	14.2676(8)	12.6130(10)
c (Å)	25.136(7)	17.181(3)	20.9718(17)	14.3243(8)	13.3290(10)
α (deg)	90	90	90	63.6670(10)	115.4240(10)
β (deg)	102.669(6)	108.80(3)	107.015(2)	66.6300(10)	108.3540(10)
γ (deg)	90	90	90	68.4790(10)	90.8050(10)
v (Å^3)	6277(3)	4218.8(15)	4345.1(6)	2184.3(2)	1474.8(2)
Z	4	4	4	2	1
μ (mm^{-1})	0.293	0.471	0.451	1.013	0.325
R_{int}	0.0539	0.1306	0.0824	0.0186	0.0325
GOOF	0.993	1.086	1.000	1.022	1.010
*R*1	0.0526	0.0635	0.0598	0.0553	0.0533
w*R*2	0.1233	0.1686	0.0965	0.1383	0.1228

Table S2 Selected experimental bond lengths (Å) of **2a** and **2b** and the corresponding calculated parameters of **2a** and **2b** obtained from B3LYP/DFT calculations

Bonds	Exptl (av)	Calcd	Exptl (av)	Calcd
	2a	**2a**	**2b**	**2b**
Fe–O	1.961	1.881	1.947	1.879
Fe–N	2.050	1.979	2.043	1.979
Fe–Cl	2.255	2.277	2.238	2.275
C–O	1.284	1.289	1.282	1.289
C–N	1.329	1.345	1.344	1.346
C–C	1.434	1.430	1.443	1.431

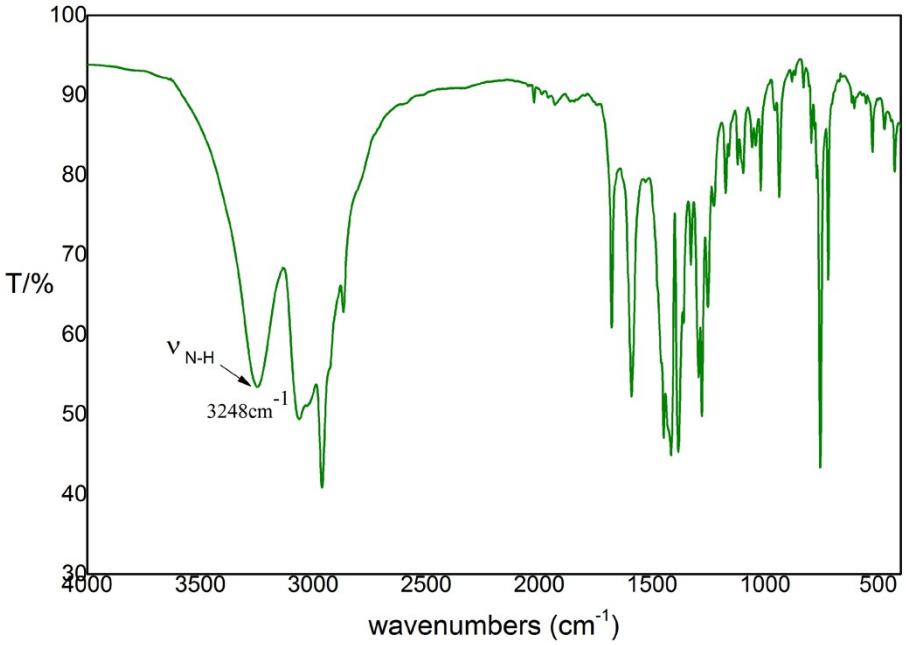

Figure S1. IR spectrum of **1b.**

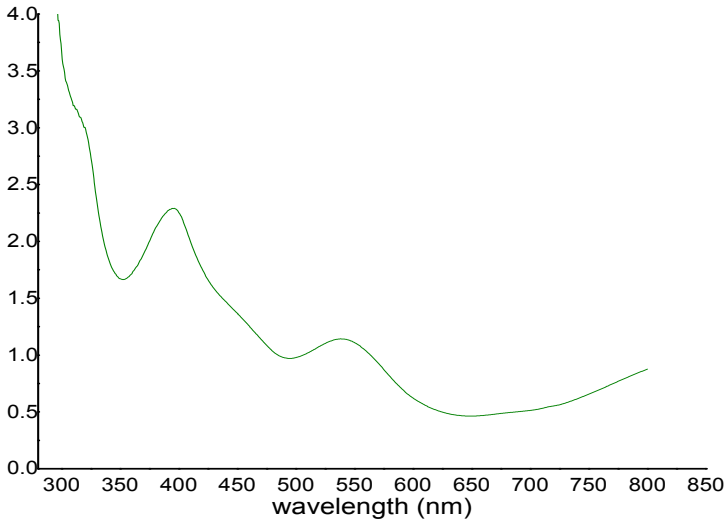

Figure S2. UV spectrum of **1b.**

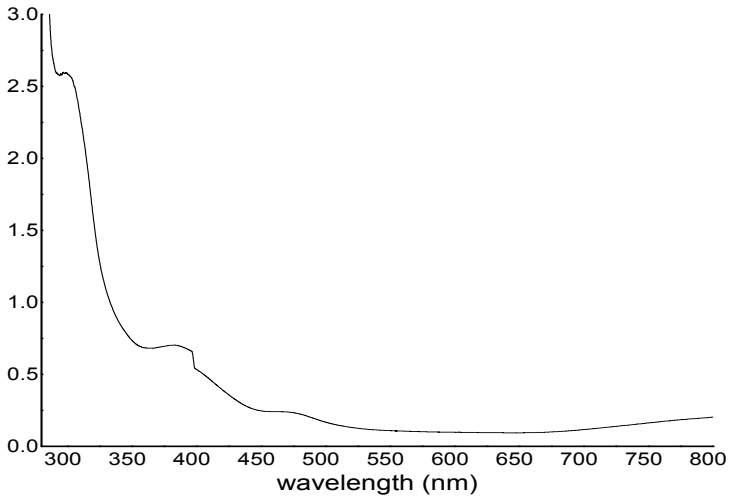

Figure S3. UV spectrum of **2a.**

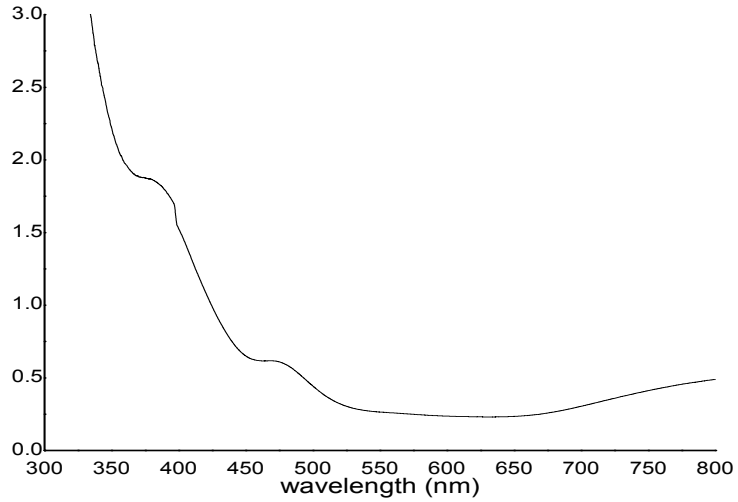

Figure S4. UV spectrum of **2b.**

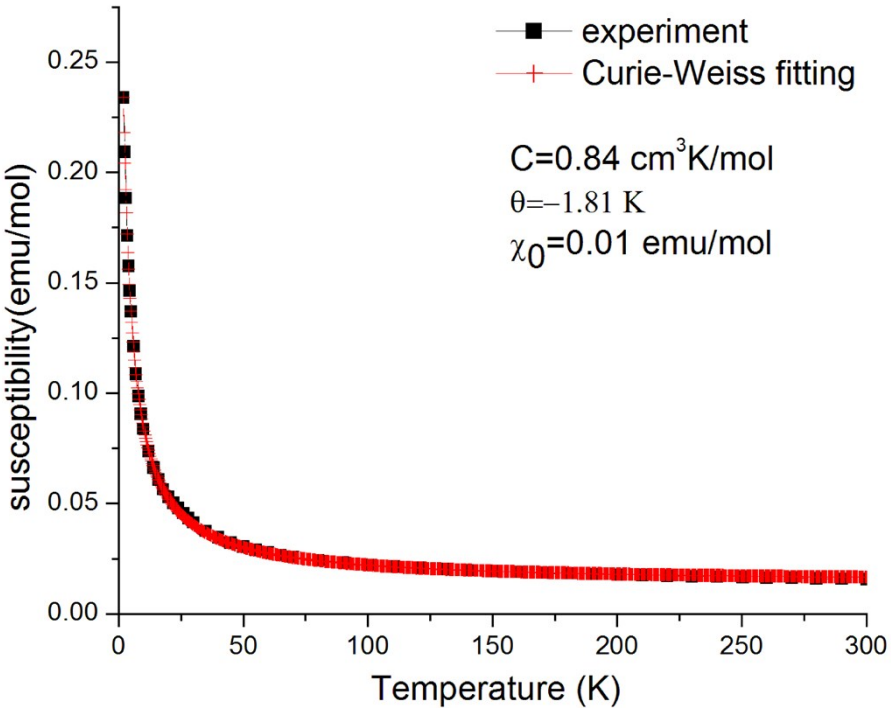

Figure S5. Simulation of the magnetic susceptibility of **1a**.

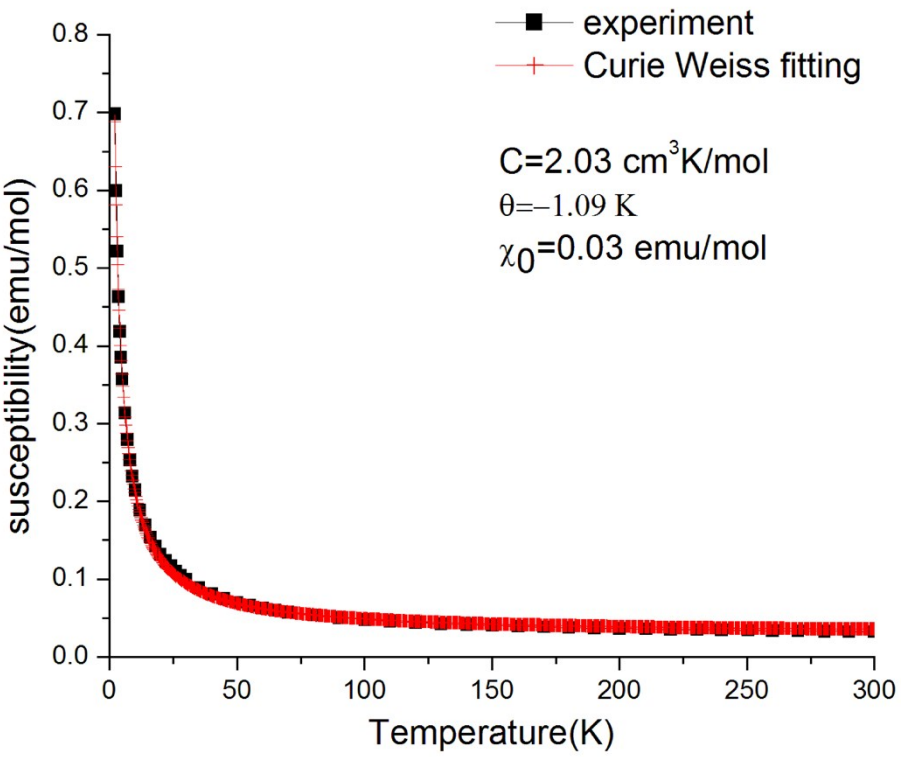

Figure S6. Simulation of the magnetic susceptibility of **1b**.

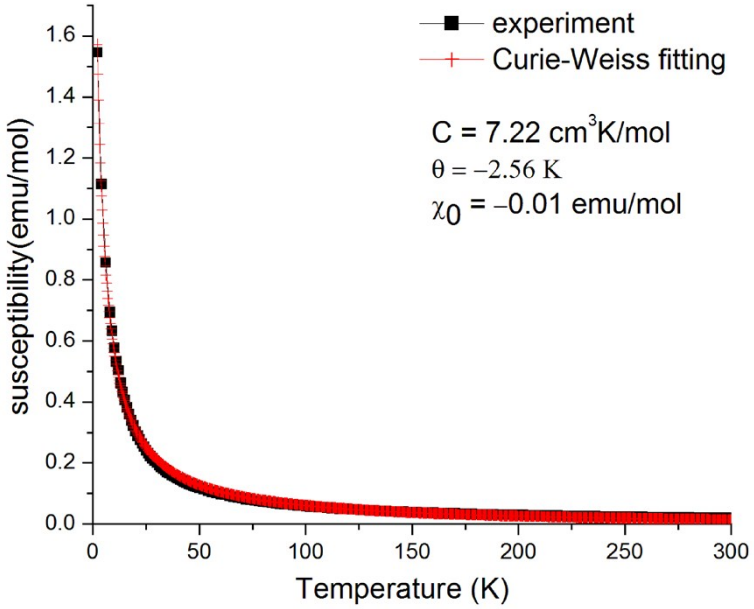

Figure S7. Simulation of the magnetic susceptibility of **2a**.

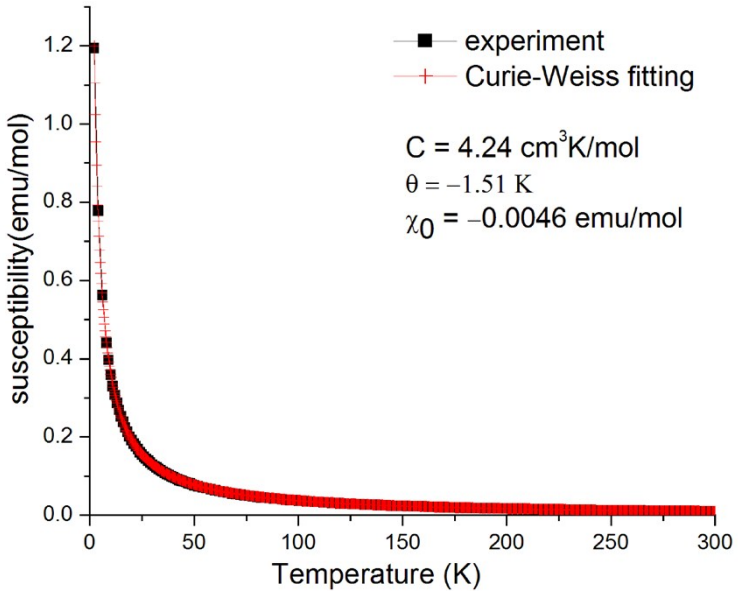

Figure S8. Simulation of the magnetic susceptibility of **2b**.