Supporting Information for

Article

Diverse Magnetic Properties of Two New Binuclear Complexes Affected by [FeN_6] Octahedral Distortion: Two-Step Spin Crossover Versus Antiferromagnetic Interactions

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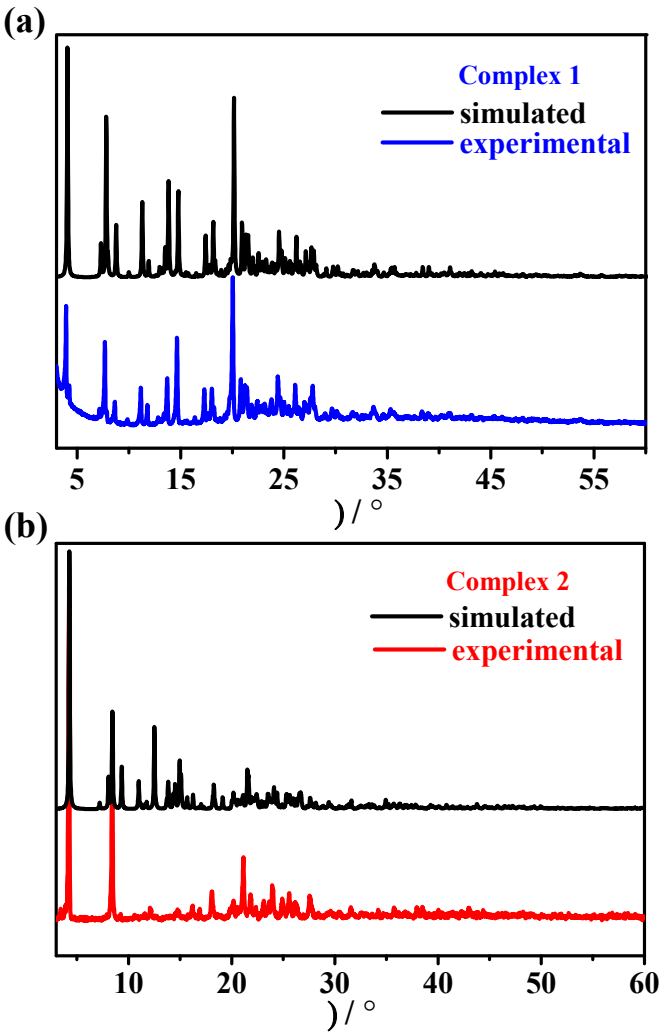

Figure S1. PXRD for complexes **1** (top) and **2** (bottom) at room temperature.

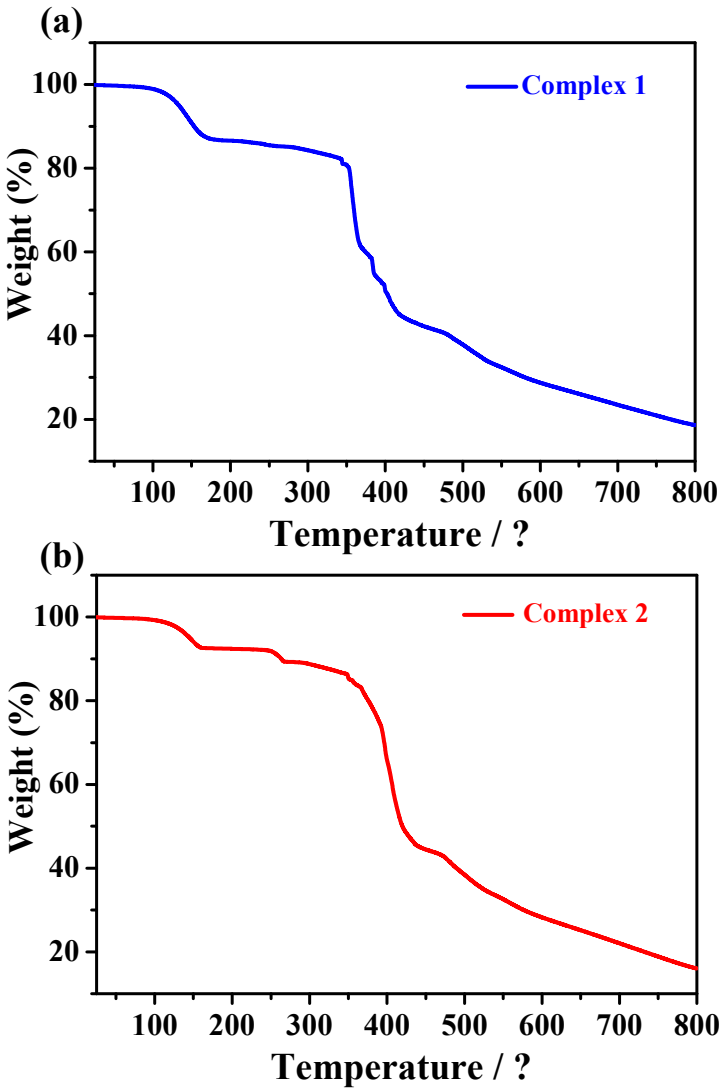

Figure S2. TG curves of complexes **1** (top) and **2** (bottom).

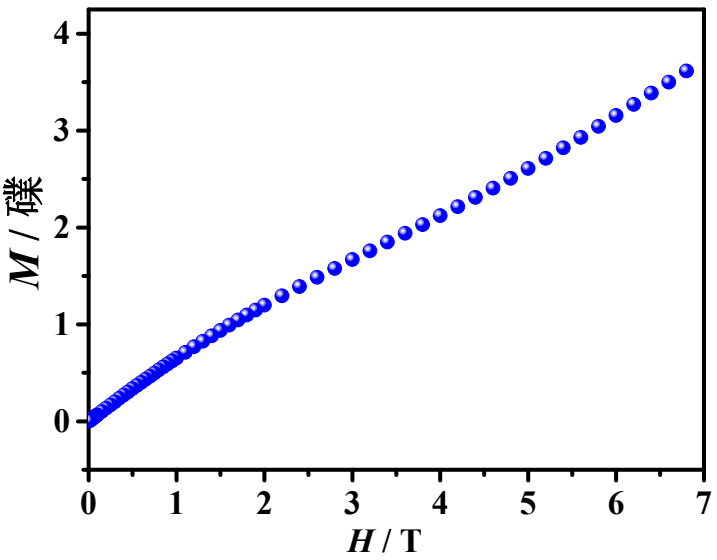

Figure S3. Plot of magnetization (*M*) vs. field (*H*) for complex **2**.

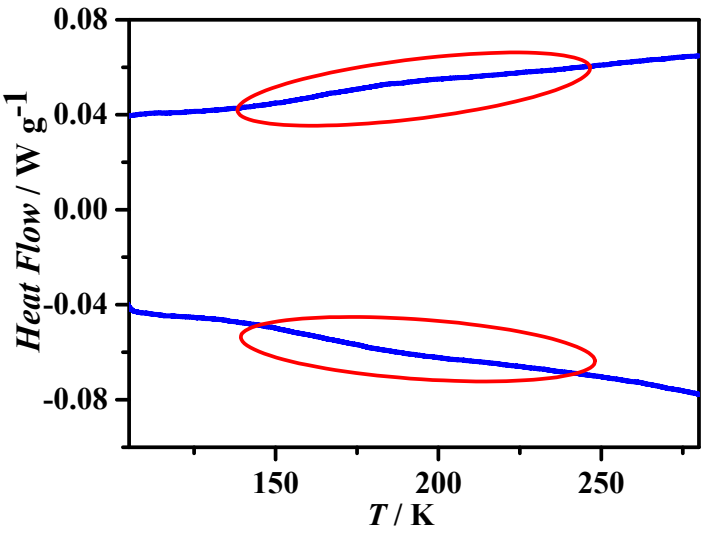

Figure S4. DSC curves for complex **1** in the heating and cooling modes.

Table S1. Selected crystallographic data for complex **1**.

Complex **1**			
Temperature (K)	100.00(10)	149.99(10)	299.9(2)
Empirical formula		C96H76Fe2N22O2S4	
Formula weight		1809.72	
Crystal system		triclinic	
Space group		*P*-1	
a (Å)	7.9613(4)	7.9229(3)	8.0625(4)
b (Å)	12.2941(7)	12.3251(4)	12.4506(6)
c (Å)	22.5759(13)	22.7521(9)	23.0585(8)
α (°)	81.117(5)	81.092(3)	81.650(4)
β (°)	80.286(5)	80.398(4)	80.018(4)
γ (°)	86.964(4)	86.615(3)	87.305(4)
V (Å^3)	2151.0(2)	2162.95(14)	2254.91(18)
Z	1	1	1
ρ_{calc} (g·cm^{-3})	1.397	1.389	1.333
F (000)	938.0	938.0	938.0
μ (mm^{-1})	4.136	4.114	3.946
GOF on F^2	1.054	1.057	1.241
R_1, wR_2 (I>2σ (l))	0.0716/0.1767	0.0576/0.1392	0.0844/0.3572
R_1, wR_2 (all data)	0.1064/0.1922	0.0932/0.1567	0.1862/0.4077
CCDC number	2182046	2181920	2182048

$^aR_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $^bwR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

Table S2. Selected crystallographic data for complex **2**.

Complex **2**			
Temperature (K)	100	γ (°)	90
Empirical formula	$C_{92}H_{66}Cl_4Fe_2N_{20}S_4$	V (Å^3)	4737.13(19)
Formula weight	1833.38	Z	2
Crystal system	monoclinic	ρ_{calc} (g·cm^{-3})	1.285
Space group	$P2_1/n$	$F(000)$	1884.0
a (Å)	8.6220(2)	μ (mm^{-1})	4.755
b (Å)	42.2912(9)	GOF on F^2	1.121
c (Å)	13.5723(3)	R_1, wR_2 (I>2σ (l))	0.0842, 0.2525
α (°)	90	R_1, wR_2 (all data)	0.0961, 0.2689
β (°)	106.823(2)	CCDC number	2182052

$^aR_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $^bwR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$