Electronic Supplementary Information

Two-Step Magnetic Switching in a Mononuclear Iron(II) Complex around Room Temperature

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Table S1. Crystallographic data for **1** at 100 K, 230 K and 250 K.

Complex	100 K	230 K	250 K
Empirical formula	$C_{42}H_{22}F_6FeN_{10}S_2$	$C_{42}H_{22}F_6FeN_{10}S_2$	$C_{42}H_{22}F_6FeN_{10}S_2$
Formula weight	900.67	900.67	900.67
Temperature (K)	100.00(10)	230.01(10)	250.00(10) K
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Pbcn*	*Pbcn*	*Pbcn*
a (Å)	12.7527(5)	12.8121(4)	12.8112(5)
b (Å)	9.9764(3)	10.0581(4)	10.0738(4)
c (Å)	29.6380(15)	29.6866(9)	29.6623(11)
Volume (Å^3)	3770.7(3)	3825.6(2)	3828.1(2)
Z	4	4	4
μ (mm^{-1})	0.589	0.581	0.581
Reflections collected	12710	13988	13462
Unique reflections	3317	3367	4196
R_{int}	0.0390	0.0247	0.0226
$R_1/wR_2/S$ (all data)	0.0715/0.1454/1.036	0.0604/0.14491.068	0.0708/0.1497/1.037
Residual ρ (e Å^{-3})	1.731 and -0.269	1.414 and -0.250	1.371 and -0.245

Table S2. Crystallographic data for **1** at 270 K, 298 K and 420 K.

Complex	270 K	298 K	420 K
Empirical formula	$C_{42}H_{22}F_6FeN_{10}S_2$	$C_{42}H_{22}F_6FeN_{10}S_2$	$C_{42}H_{22}F_6FeN_{10}S_2$
Formula weight	900.67	900.67	900.67
Temperature (K)	270.00(10)	298.00(10) K	420.00(11) K
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Pbcn*	*Pbcn*	*Pbcn*
a (Å)	12.8042(6)	12.8371(6)	12.9544(8)
b (Å)	10.6288(6)	10.6474(5)	10.7221(8)
c (Å)	28.3592(14)	28.4181(13)	28.685(2)
Volume (Å^3)	3859.5(3)	3884.2(3)	3984.3(5)
Z	4	4	4
μ (mm^{-1})	0.576	0.572	0.558
Reflections collected	14799	15126	16606
Unique reflections	3398	3422	3510
R_{int}	0.0429	0.0303	0.0389
$R_1/wR_2/S$ (all data)	0.0636/ 0.17541.099	0.0877/0.1897/1.058	0.1099/0.2124/1.019
Residual ρ (e Å^{-3})	1.083 and -0.328	1.047 and -0.369	0.771 and -0.286

Table S3. Selected bond lengths (Å) and angles (°) for **1** at 100 K, 230 K, 250 K, 270 K, 298 K and 420 K.

100 K	
Fe1-N1 = 1.931(3) Å	N(1)-Fe(1)-N(2) = 92.54(12) °
Fe1-N2 = 1.972(3) Å	N(1)-Fe(1)-N(3) = 88.46(12) °
Fe1-N3 = 1.971(3) Å	N(2)-Fe(1)-N(3) = 82.60(12) °
230 K	
Fe1-N1 = 1.944(3) Å	N(1)-Fe(1)-N(2) = 88.57(12) °
Fe1-N2 = 1.975(3) Å	N(1)-Fe(1)-N(3) = 92.50(12) °
Fe1-N3 = 1.973(3) Å	N(2)-Fe(1)-N(3) = 82.44(11) °
250 K	
Fe1-N1 = 1.940(3) Å	N(1)-Fe(1)-N(2) = 174.62(10) °
Fe1-N2 = 1.975(3) Å	N(1)-Fe(1)-N(3) = 92.40(11) °
Fe1-N3 = 1.976(2) Å	N(2)-Fe(1)-N(3) = 82.38(10) °
270 K	
Fe1-N1 = 1.960(5) Å	N(1)-Fe(1)-N(2) = 90.62(15) °
Fe1-N2 = 2.032(3) Å	N(1)-Fe(1)-N(3) = 94.75(15) °
Fe1-N3 = 2.020(3) Å	N(2)-Fe(1)-N(3) = 80.66(13) °
298 K	
Fe1-N1 = 1.997(5) Å	N(1)-Fe(1)-N(2) = 171.21(15) °
Fe1-N2 = 2.087(3) Å	N(1)-Fe(1)-N(3) = 92.04(15) °
Fe1-N3 = 2.056(3) Å	N(2)-Fe(1)-N(3) = 79.44(12) °
420 K	
Fe1-N1 = 2.090(6) Å	N(1)-Fe(1)-N(2) = 167.05(17) °
Fe1-N2 = 2.214(4) Å	N(1)-Fe(1)-N(3) = 92.04(17) °
Fe1-N3 = 2.158(4) Å	N(2)-Fe(1)-N(3) = 75.44(14) °

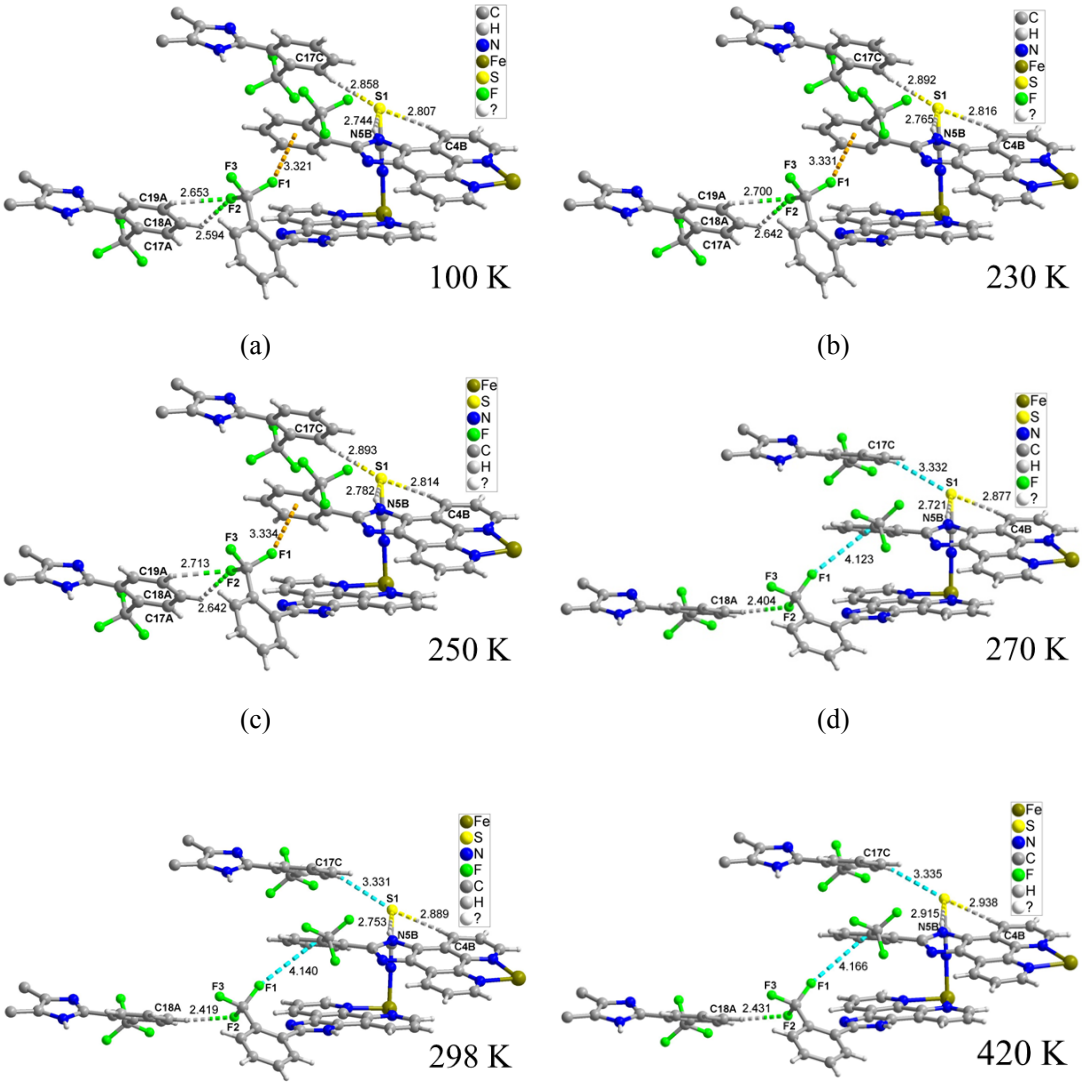
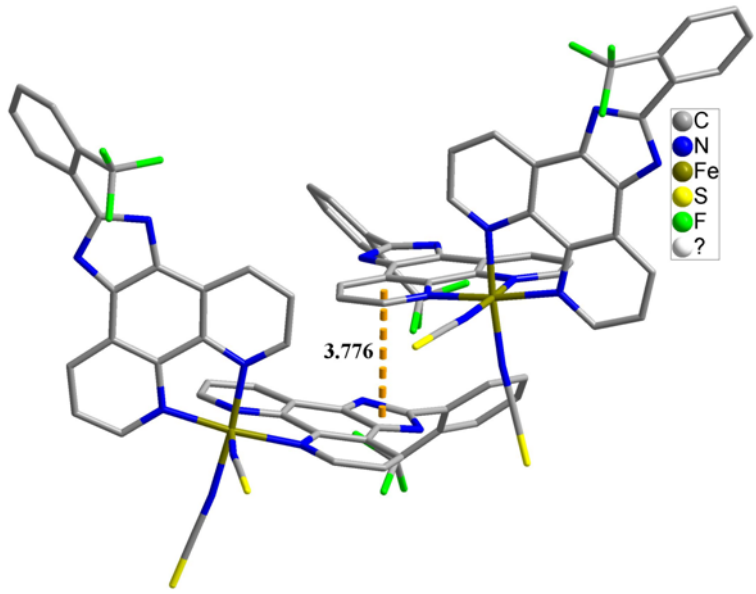
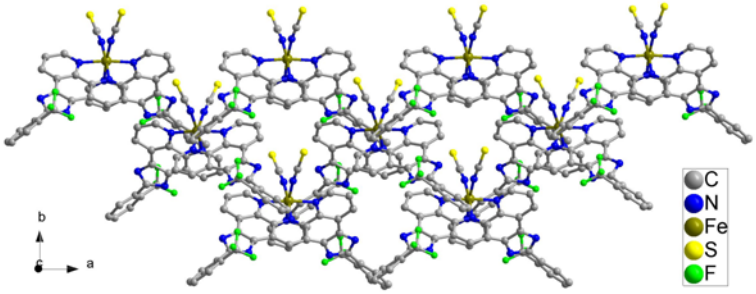


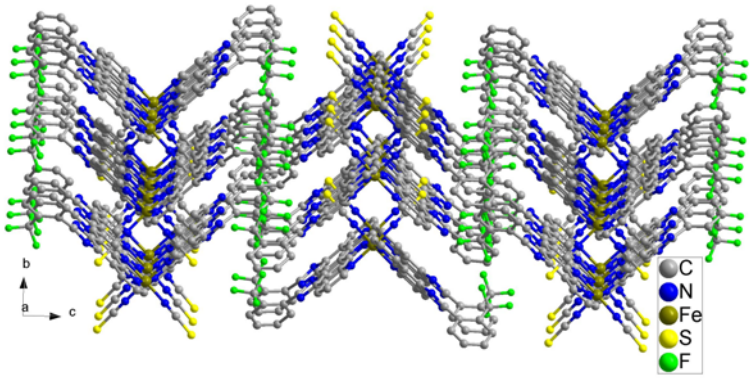
Fig. S1 H-bonds and lone pair-π interactions in **1** at (a) 100 K, (b) 230 K, (c) 250 K and (d) 270 K, (e) 298 K, (f) 420 K.



(a)



(b)



(c)

Fig. S2 (a) ***π*-*π*** stacking in LS **1**. The 3D structure of LS **1**, (b) *ab* plane, (c) *bc* plane.

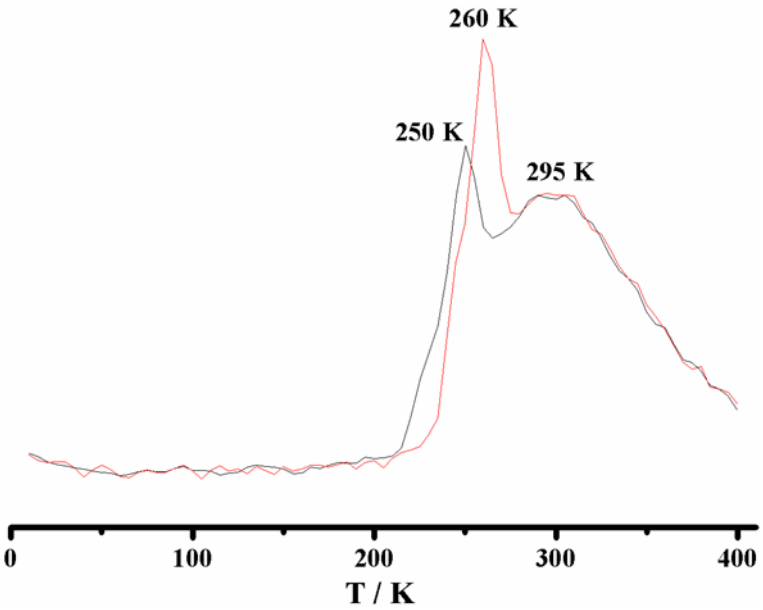


Fig. S3 $d\chi_m T/dT$ curve of **1**.

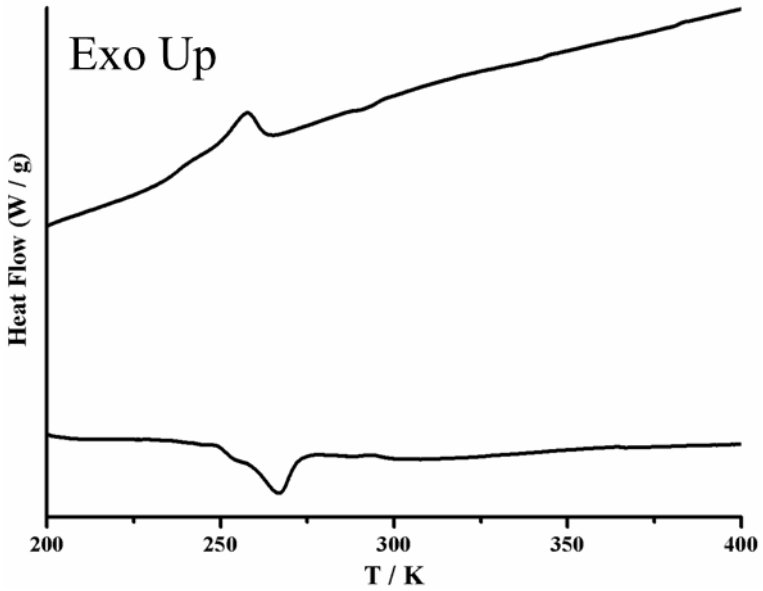


Fig. S4 The differential scanning calorimetry (DSC) curve of **1**.

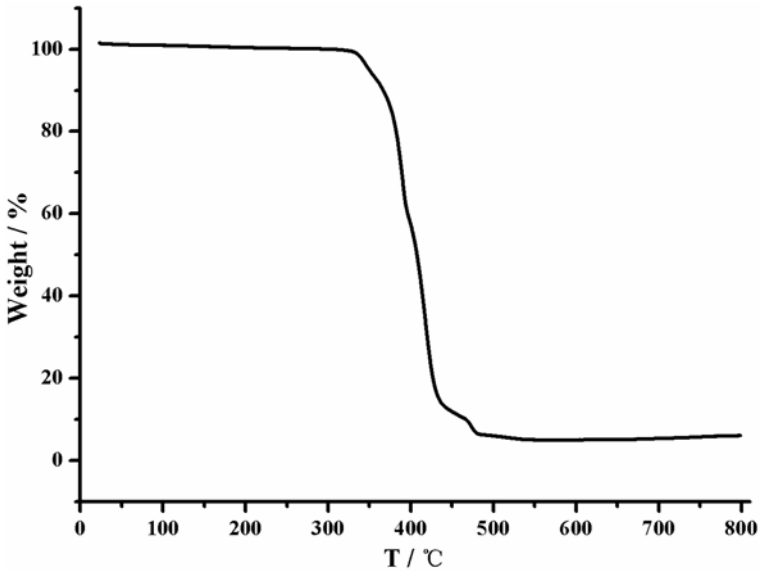


Fig. S5 The thermogravimetric analysis (TGA) curve of **1**.

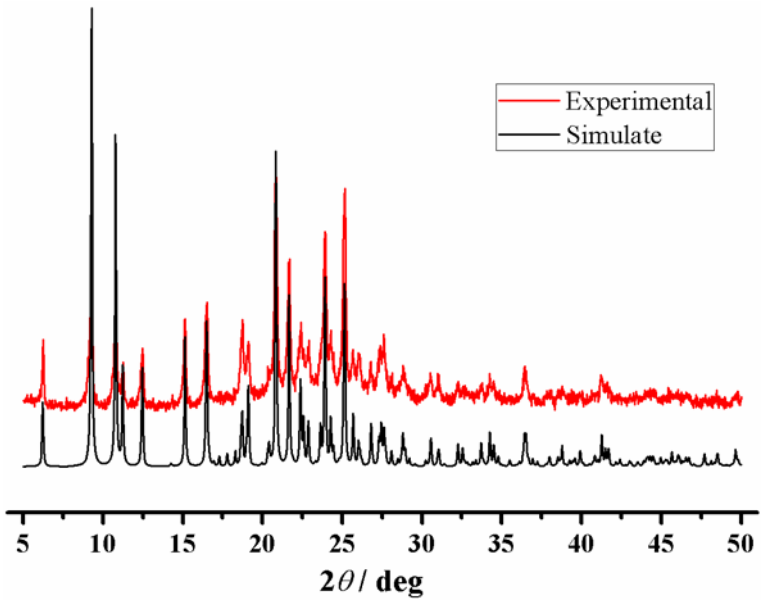


Fig. S6 The XRPD of **1**.