Electronic Supplementary Material (ESI) for *Dalton Trans.*

Spin Crossover Behaviour in One-Dimensional Fe^{II} Compounds Based on the $[M(CN)_4]^{2-}$ (M= Pd, Pt) Units

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Supporting Information

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1. X-ray crystallography and powder x-ray diffraction

Table S1. Selected bond lengths [Å] and angles [°] for complex **1**.

120 K		298 K	
Fe1-N1	1.948(3)	Fe1-N1	2.112(2)
Fe1-N3	1.928(2)	Fe1-N3	2.088(2)
Fe1-N5	1.972(3)	Fe1-N5	2.152(2)
Fe1-N6	2.032(2)	Fe1-N6	2.189(2)
Fe1-N7	1.967(2)	Fe1-N7	2.157(2)
Fe1-N8	2.020(3)	Fe1-N8	2.188(3)
Pd1-C1	1.998(3)	Pd1-C1	1.995(2)
Pd1-C2	1.992(3)	Pd1-C2	1.992(3)
Pd2-C3	1.984(3)	Pd2-C3	1.983(2)
Pd2-C4	1.995(4)	Pd2-C4	1.985(4)
C1-N1	1.150(4)	C1-N1	1.140(3)
C2-N2	1.147(4)	C2-N2	1.135(3)
C3-N3	1.145(4)	C3-N3	1.135(3)
C4-N4	1.147(5)	C4-N4	1.148(4)
Pd1-C1-N1	176.0(3)	Pd1-C1-N1	177.8(2)
Pd1-C2-N2	179.0(3)	Pd1-C2-N2	178.1(3)
Pd2-C3-N3	176.1(3)	Pd2-C3-N3	176.4(3)
Pd2-C4-N4	177.2(3)	Pd2-C4-N4	177.6(3)
N3-Fe1-N1	92.07(12)	N3-Fe1-N1	92.67(10)
N3-Fe1-N5	90.93(10)	N3-Fe1-N5	93.23(9)
N1-Fe1-N5	93.62(10)	N1-Fe1-N5	92.15(8)
N1-Fe1-N7	91.15(10)	N1-Fe1-N7	91.17(9)
N5-Fe1-N7	95.44(11)	N5-Fe1-N7	96.43(9)
N3-Fe1-N8	91.28(11)	N3-Fe1-N8	93.15(10)
N1-Fe1-N8	91.36(11)	N1-Fe1-N8	95.61(9)
N7-Fe1-N8	82.06(11)	N7-Fe1-N8	76.69(10)
N3-Fe1-N6	87.71(10)	N3-Fe1-N6	88.15(9)
N5-Fe1-N6	81.37(10)	N5-Fe1-N6	76.83(8)
N7-Fe1-N6	89.66(10)	N7-Fe1-N6	89.95(9)
N8-Fe1-N6	93.66(11)	N8-Fe1-N6	95.32(9)

Table S2. Selected bond lengths [Å] and angles [°] for complex **2**.

120 K		298 K	
Fe1-N1	1.928(4)	Fe1-N1	2.129(4)
Fe1-N4	1.975(6)	Fe1-N3	2.102(3)
Fe1-N5	2.028(17)	Fe1-N5	2.160(4)
Fe1-N6	1.964(17)	Fe1-N6	2.210(3)
Fe1-N7	2.008(7)	Fe1-N7	2.165(4)
Fe1-N1[a]	1.928(4)	Fe1-N8	2.191(4)
Fe1-N5[a]	2.028(18)	Pt1-C1	1.993(4)
Fe1-N6[a]	1.964(17)	Pt1-C2	1.983(4)
		Pt2-C3	1.982(4)
Pt1-C1	1.980(6)	Pt2-C4	1.983(6)
Pt1-C2	1.981(13)	C1-N1	1.135(5)
Pt1-C3	1.992(10)	C2-N2	1.142(5)
C1-N1	1.164(7)	C3-N3	1.136(5)
C2-N2	1.152(17)	C4-N4	1.154(7)
C3-N3	1.142(15)	Pt1-C1-N1	178.4(4)
Pt1-C1-N1	176.2(5)	Pt1-C2-N2	178.0(5)
Pt1-C2-N2	176.9(11)	Pt2-C3-N3	177.8(4)
Pt1-C3-N3	178.2(12)	Pt2-C4-N4	178.4(5)
N1-Fe1-N1[a]	92.1(3)	N3-Fe1-N1	92.48(16)
N1-Fe1-N6	170.5(4)	N3-Fe1-N5	93.02(15)
N1-Fe1-N4	92.04(18)	N1-Fe1-N5	92.42(13)
N1[a]-Fe1-N4	92.04(18)	N1-Fe1-N7	91.39(14)
N6-Fe1-N4	95.1(4)	N5-Fe1-N7	96.81(15)
N1-Fe1-N7	91.33(19)	N3-Fe1-N8	93.38(15)
N1[a]-Fe1-N7	91.33(19)	N1-Fe1-N8	95.60(15)
N6-Fe1-N7	81.2(4)	N7-Fe1-N8	76.28(15)
N5-Fe1-N1	85.5(5)	N3-Fe1-N6	88.20(14)
N4-Fe1-N5	81.0(5)	N5-Fe1-N6	76.44(13)
N7-Fe1-N5	95.8(5)	N7-Fe1-N6	89.94(15)
N5-Fe1-N6	89.4(5)	N8-Fe1-N6	95.46(15)

Symmetry code for complex **2**: a: x, -y+1/2, z.

Table S3. Selected bond lengths [Å] and angles [°] for complex **3**.

120 K		298 K	
Fe1-N1	1.952(2)	Fe1-N1	2.141(3)
Fe1-N3	1.986(2)	Fe1-N3	2.190(2)
Fe1-N4	1.953(2)	Fe1-N4	2.185(2)
Pd1-C1	1.996(3)	Pd1-C1	1.993(3)
Pd1-C2	1.995(3)	Pd1-C2	1.987(4)
C1-N1	1.142(3)	C1-N1	1.147(4)
C2-N2	1.144(4)	C2-N2	1.147(4)
Pd1-C1-N1	174.1(2)	Pd1-C1-N1	176.5(3)
Pd2-C2-N2	178.5(3)	Pd2-C2-N2	178.8(3)
N1-Fe1-N1^{a}	89.58(13)	N1-Fe1-N1^{a}	91.24(14)
N1-Fe1-N4	91.39(9)	N1-Fe1-N4	91.36(9)
N1^{a}-Fe1-N4^{a}	91.39(9)	N1^{a}-Fe1-N4^{a}	91.36(9)
N4-Fe1-N4^{a}	87.80(13)	N4-Fe1-N4^{a}	86.96(12)
N1^{a}-Fe1-N3	88.72(9)	N1^{a}-Fe1-N3	92.50(9)
N1-Fe1-N3	96.71(9)	N1-Fe1-N3	98.04(9)
N4-Fe1-N3	94.17(9)	N4-Fe1-N3	94.16(9)
N4^{a}-Fe1-N3	80.29(9)	N4^{a}-Fe1-N3	74.76(9)
N1^{a}-Fe1-N3^{a}	96.71(9)	N1^{a}-Fe1-N3^{a}	98.04(9)
N1-Fe1-N3^{a}	88.72(9)	N1-Fe1-N3^{a}	92.50(9)
N4-Fe1-N3^{a}	80.29(9)	N4-Fe1-N3^{a}	74.76(9)
N4^{a}-Fe1-N3^{a}	94.17(9)	N4^{a}-Fe1-N3^{a}	94.16(9)

Symmetry code for complex **3**: a: -x, y, -z+1/2.

Table S4. Selected bond lengths [Å] and angles [°] for complex **4**.

120 K		298 K	
Fe1-N1	1.951(4)	Fe1-N1	2.139(2)
Fe1-N3	1.994(4)	Fe1-N3	2.186(2)
Fe1-N4	1.962(4)	Fe1-N4	2.182(2)
Pt1-C1	1.993(5)	Pt1-C1	1.990(3)
Pt1-C2	2.002(5)	Pt1-C2	1.982(3)
C1-N1	1.162(6)	C1-N1	1.140(3)
C2-N2	1.144(7)	C2-N2	1.146(4)
Pt1-C1-N1	174.4(4)	Pt1-C1-N1	177.7(2)
Pt2-C2-N2	178.4(5)	Pt2-C2-N2	178.4(3)
N1-Fe1-N1^{a}	90.3(2)	N1-Fe1-N1^{a}	91.26(13)
N1-Fe1-N4	91.13(15)	N1-Fe1-N4	91.53(9)
N1^{a} -Fe1-N4^{a}	91.13(15)	N1^{a}-Fe1-N4^{a}	91.53(9)
N4-Fe1-N4^{a}	87.7(2)	N4-Fe1-N4^{a}	86.67(12)
N1^{a}-Fe1-N3	88.87(15)	N1-Fe1-N3^{a}	92.63(8)
N1-Fe1-N3	96.64(16)	N1-Fe1-N3	97.59(8)
N4-Fe1-N3	94.13(16)	N4-Fe1-N3	94.31(8)
N4^{a}-Fe1-N3	80.20(16)	N4^{a}-Fe1-N3	74.90(8)
N1^{a}-Fe1-N3^{a}	96.64(16)	N1^{a}-Fe1-N3^{a}	97.59(8)
N1-Fe1-N3^{a}	88.87(15)	N1^{a}-Fe1-N3	92.63(8)
N4-Fe1-N3^{a}	80.20(16)	N4^{a}-Fe1-N3	74.90(8)
N4^{a}-Fe1-N3^{a}	94.13(16)	N4^{a}-Fe1-N3^{a}	94.31(8)

Symmetry code for complex **4**: a: -x, y, -z+1/2.

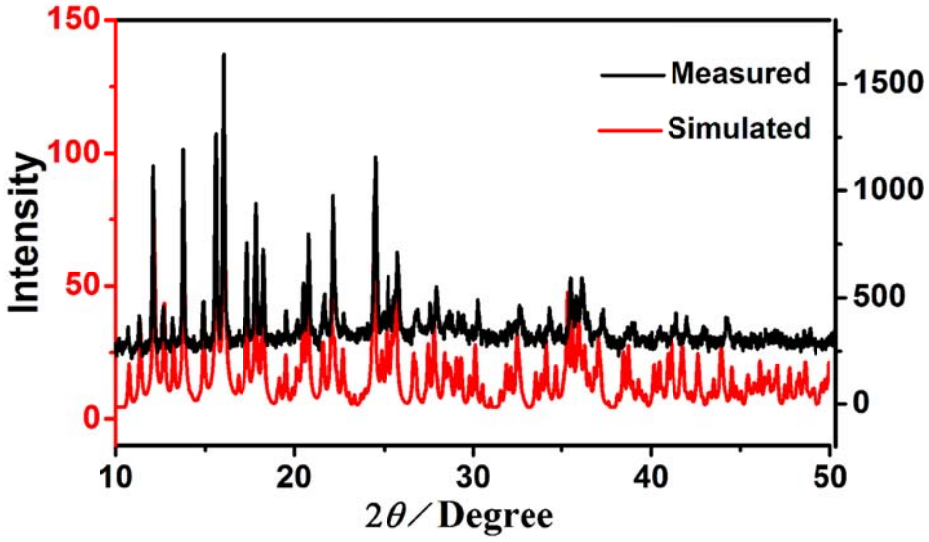

Figure S1. The powder X-ray diffraction patterns of complex **1** in black and its simulation in red at 298 K.

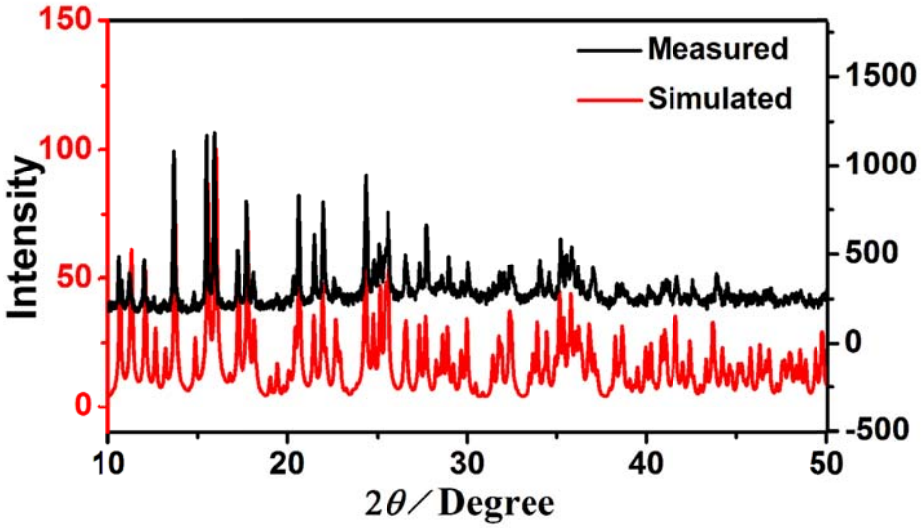

Figure S2. The powder X-ray diffraction patterns of complex **2** in black and its simulation in red at 298 K.

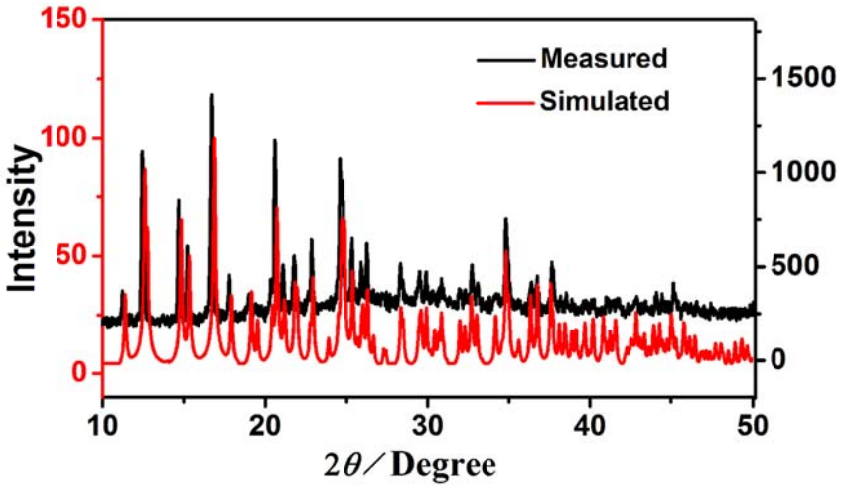

Figure S3. The powder X-ray diffraction patterns of complex **3** in black and its simulation in red at 298 K.

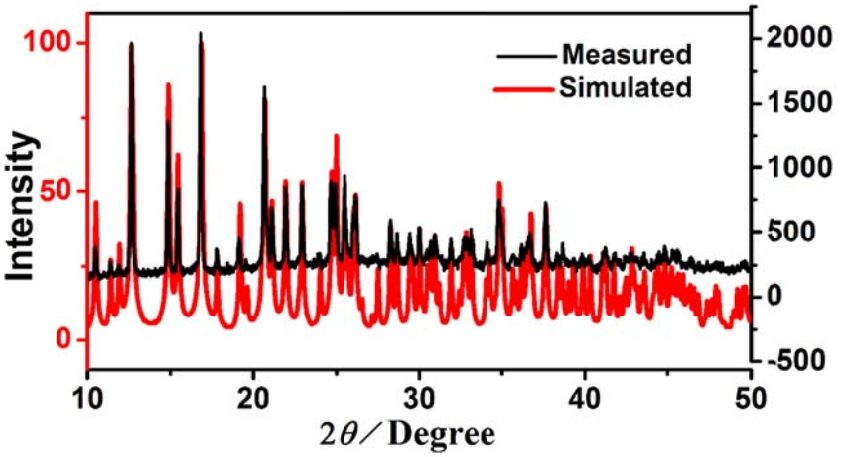

Figure S4. The powder X-ray diffraction patterns of complex **4** in black and its simulation in red at 298 K.

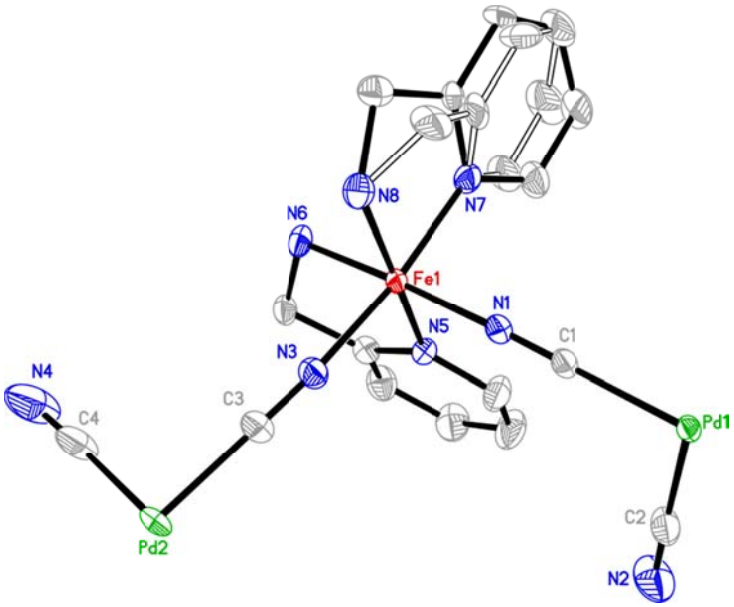

Figure S5. The asymmetry unit of complex **1** at 120 K (showing 50% probability ellipsoids).

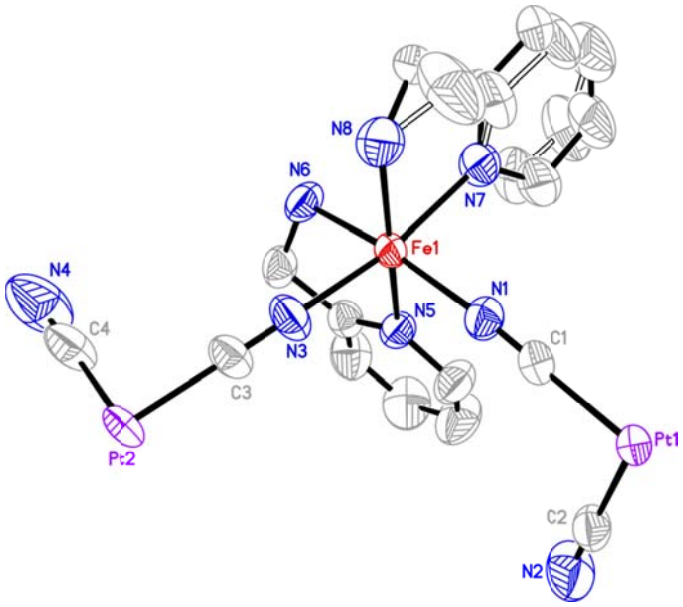

Figure S6. The asymmetry unit of complex **2** at 298 K (showing 50% probability ellipsoids).

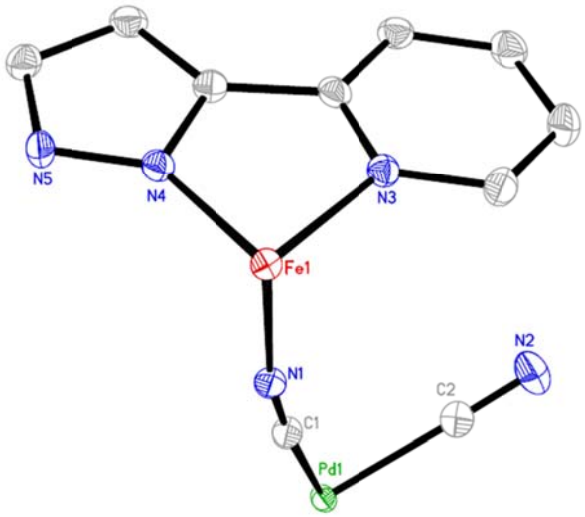

Figure S7. The asymmetry unit of complex **3** at 120 K (showing 50% probability displacement ellipsoids).

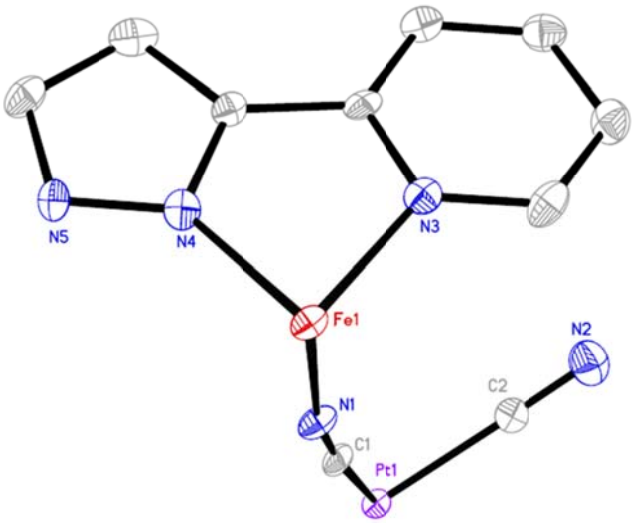

Figure S8. The asymmetry unit of complex **4** at 120 K (showing 50% probability ellipsoids).

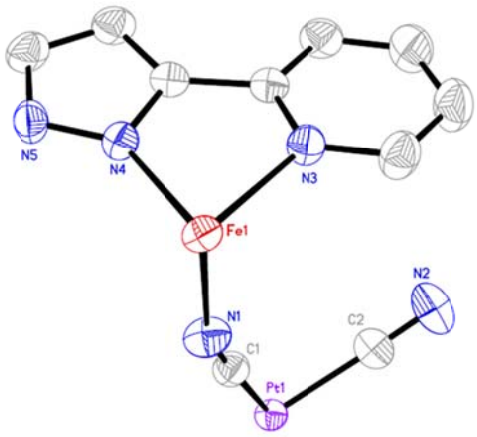

Figure S9. The asymmetry unit of complex **4** at 298 K (showing 50% probability displacement ellipsoids).

2. Magnetic Property

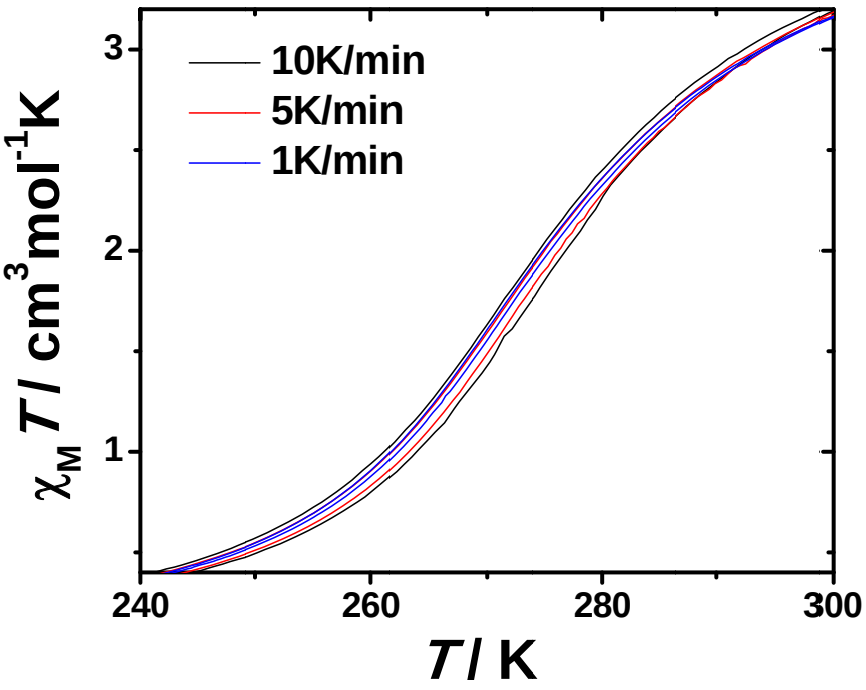

Figure S10 Temperature dependent $\chi_M T$ plots for complex **1** at scan rate of 1, 5, and 10 K/min.

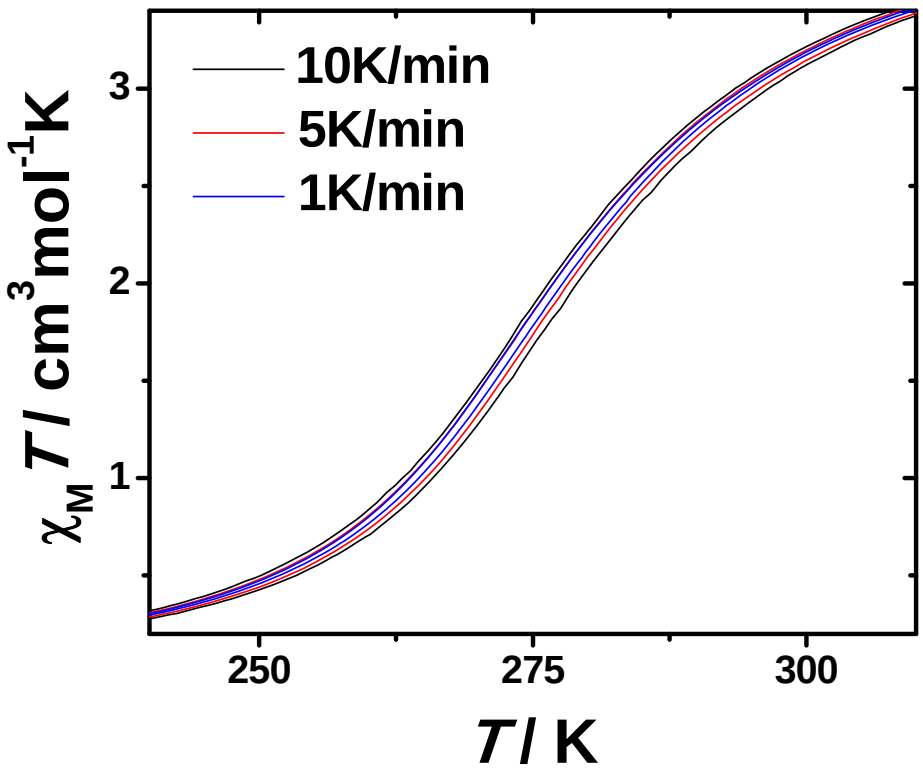

Figure S11 Temperature dependent $\chi_M T$ plots for complex **2** at scan rate of 1, 5, and 10 K/min.