

ESI

Isomorphous tetrazolate Mn^{II} and Co^{II} compounds built on 4-chain showing different magnetic behaviors

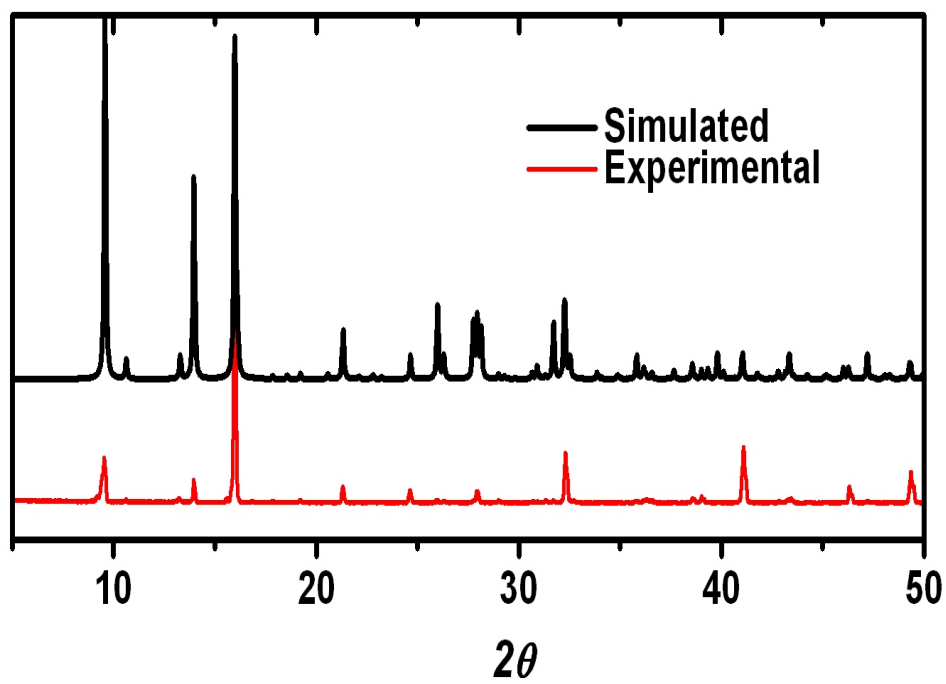
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Table S1. Selected Bond Lengths (Å) and Angles (°) for Compounds 1-2

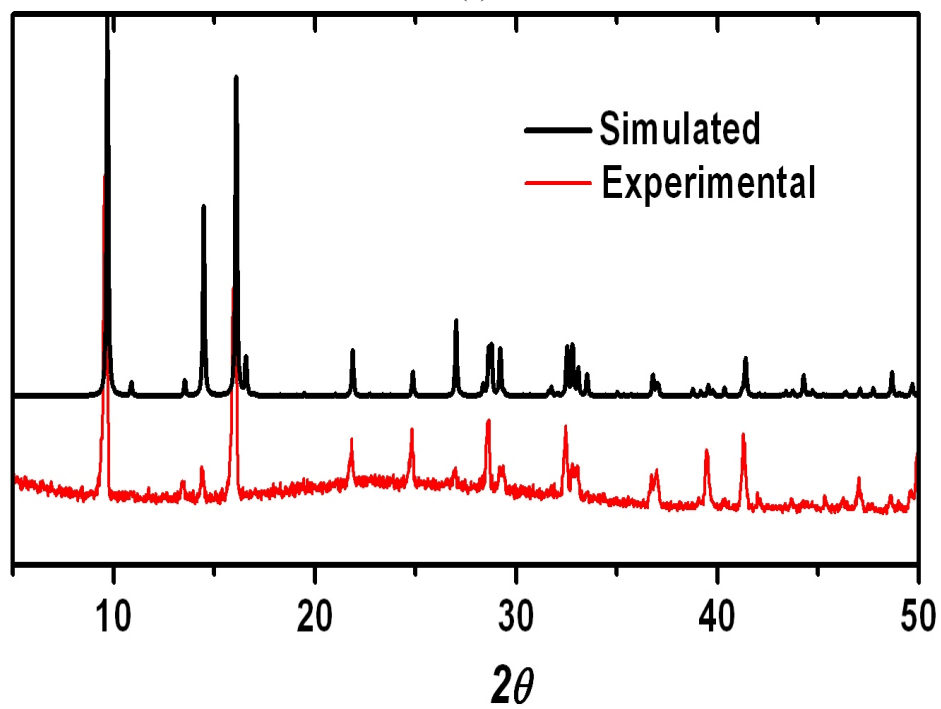
1			
Mn(1)–O(2C)	2.068(3)	Mn(1)–O(1)	2.139(3)
Mn(1)–O(4)	2.176(3)	Mn(1)–N(1B)	2.325(3)
Mn(1)–N(1)	2.325(3)	Mn(1)–N(4)	2.360(3)
Mn(2)–O(4D)	2.1558(17)	Mn(2)–O(4)	2.1558(17)
Mn(2)–O(3E)	2.206(2)	Mn(2)–O(3F)	2.206(2)
Mn(2)–N(2)	2.250(2)	Mn(2)–N(2D)	2.250(2)
O(2C)–Mn(1)–O(1)	176.94(11)	O(2C)–Mn(1)–O(4)	92.01(12)
O(1)–Mn(1)–O(4)	91.04(11)	O(2C)–Mn(1)–N(1B)	87.03(7)
O(1)–Mn(1)–N(1B)	92.99(7)	O(4)–Mn(1)–N(1B)	89.61(6)
O(2C)–Mn(1)–N(1)	87.03(7)	O(1)–Mn(1)–N(1)	92.99(7)
O(4)–Mn(1)–N(1)	89.61(6)	N(1B)–Mn(1)–N(1)	173.98(14)
O(2C)–Mn(1)–N(4)	103.75(12)	O(1)–Mn(1)–N(4)	73.19(11)
O(4)–Mn(1)–N(4)	164.24(12)	N(1B)–Mn(1)–N(4)	91.19(6)
N(1)–Mn(1)–N(4)	91.19(6)	O(4D)–Mn(2)–O(4)	180.00(12)
O(4D)–Mn(2)–O(3E)	87.73(10)	O(4)–Mn(2)–O(3E)	92.27(10)
O(4D)–Mn(2)–O(3F)	92.27(10)	O(4)–Mn(2)–O(3F)	87.73(10)
O(3E)–Mn(2)–O(3F)	180.00(11)	O(4D)–Mn(2)–N(2)	93.97(9)
O(4)–Mn(2)–N(2)	86.03(9)	O(3E)–Mn(2)–N(2)	90.68(8)
O(3F)–Mn(2)–N(2)	89.32(8)	O(4D)–Mn(2)–N(4D)	86.03(9)
O(4)–Mn(2)–N(2D)	93.97(9)	O(3E)–Mn(2)–N(2D)	89.32(8)

O(3F)–Mn(2)–N(2D)	90.68(8)	N(2)–Mn(2)–N(2D)	180.0
2			
Co(1)–O(2C)	2.008(4)	Co(1)–O(1)	2.063(4)
Co(1)–O(4)	2.127(4)	Co(1)–N(4)	2.196(5)
Co(1)–N(1)	2.197(3)	Co(1)–N(1B)	2.197(3)
Co(2)–O(4)	2.074(3)	Co(2)–O(4D)	2.074(3)
Co(2)–N(2D)	2.101(3)	Co(2)–O(3E)	2.127(3)
Co(2)–O(3C)	2.127(3)		
O(2C)–Co(1)–O(1)	178.56(17)	O(2C)–Co(1)–O(4)	92.50(18)
O(1)–Co(1)–O(4)	88.94(18)	O(2C)–Co(1)–N(4)	101.81(18)
O(1)–Co(1)–N(4)	76.75(17)	O(4)–Co(1)–N(4)	165.69(19)
O(2C)–Co(1)–N(1)	87.35(10)	O(1)–Co(1)–N(1)	92.72(10)
O(4)–Co(1)–N(1)	87.33(8)	N(4)–Co(1)–N(1)	93.27(8)
O(2C)–Co(1)–N(1B)	87.35(10)	O(1)–Co(1)–N(1B)	92.72(10)
O(4)–Co(1)–N(1B)	87.33(8)	N(4)–Co(1)–N(1B)	93.27(8)
N(1)–Co(1)–N(1B)	172.31(18)	O(4)–Co(2)–O(4D)	180.000(1)
O(4)–Co(2)–N(2D)	94.68(13)	O(4D)–Co(2)–N(2D)	85.32(13)
O(4)–Co(2)–N(2)	85.32(13)	O(4D)–Co(2)–N(2)	94.68(13)
N(2D)–Co(2)–N(2)	180.0	O(4)–Co(2)–O(3E)	88.51(16)
O(4D)–Co(2)–O(3E)	91.49(16)	N(2D)–Co(2)–O(3E)	90.06(12)
N(2)–Co(2)–O(3E)	89.94(12)	O(4)–Co(2)–O(3E)	91.49(16)
O(4D)–Co(2)–O(3E)	88.51(16)	N(2D)–Co(2)–O(3E)	89.94(12)
N(2)–Co(2)–O(3E)	90.06(12)	O(3E)–Co(2)–O(3C)	180.000(1)

Symmetry codes: for **1** A x, -y-1/2, z; B x, -y+1/2, z; C x+1/2, y, -z+3/2; D -x+1, -y, -z+1; E x+1/2, -y+1/2, -z+3/2; F -x+1/2, y-1/2, z-1/2; for **2** A x, -y+5/2, z; B x, -y+3/2, z; C x+1/2, y, -z+1/2; D -x+1, -y+2, -z+1; E -x+1/2, -y+2, z+1/2.

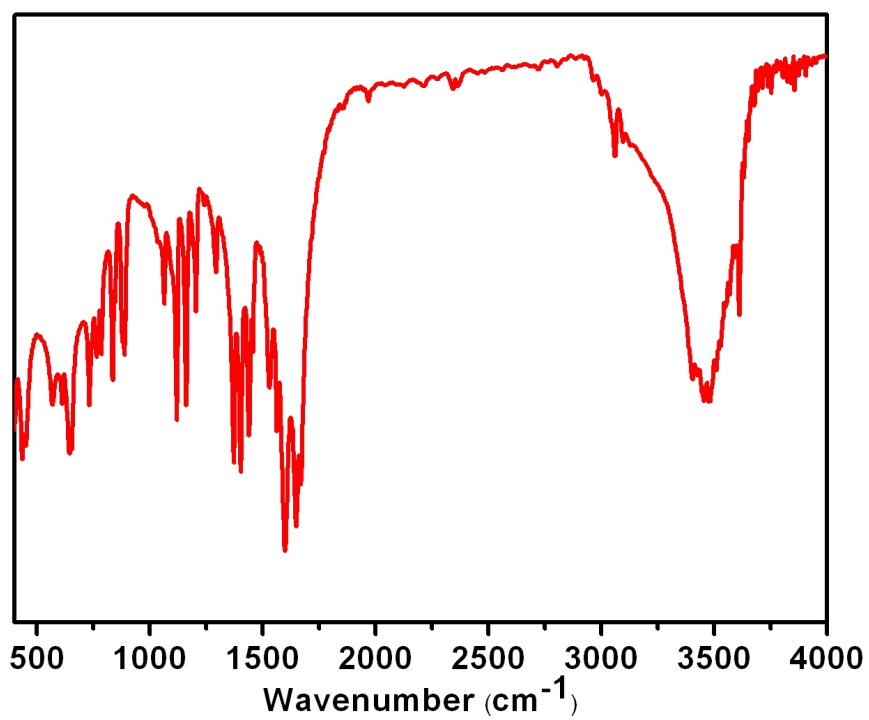


(a)

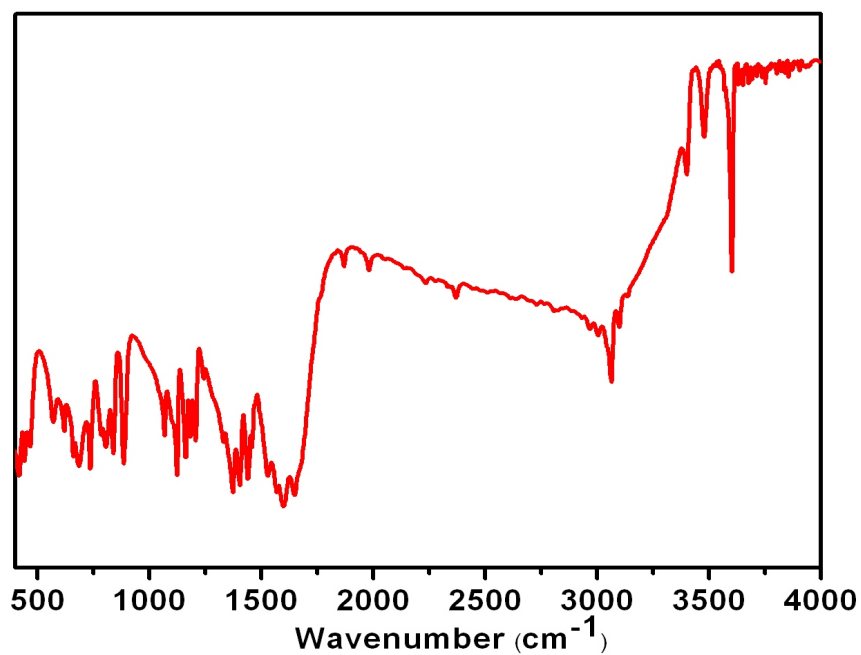


(b)

Fig. S1 XRPD patterns for **1** (a) and **2** (b).



(a)



(b)

Fig. S2 FT-IR spectra of **1** (a) and **2** (b).