

Supporting Information

**Coordination chemistry of tetrazolate-5-carboxylate with
manganese(II): synthesis, structure and magnetism**

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Table S1. Selected bond lengths and angles for complex **1**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)					
O3-H3WB...O2#1	0.78(3)	1.98(3)	2.751(2)	169(2)					
O3-H3WA...N4#2	0.79(3)	2.02(3)	2.811(2)	177(2)					
O4-H4WB...O2#3	0.88(3)	1.91(3)	2.773(2)	166(3)					
O4-H4WA...O6#4	0.77(3)	1.91(3)	2.682(2)	173(3)					
O5-H5WB...O7	0.836(15)	1.905(17)	2.734(2)	171(2)					
O5-H5WA...O6	0.804(16)	1.980(17)	2.777(2)	171(2)					
O7-H7W...O2#1	0.821(17)	2.43(2)	3.0465(14)	132(3)					
O6-H6WA...O8#3	0.863(15)	1.879(17)	2.718(2)	164(2)					
O6-H6WB...N3#5	0.809(16)	2.097(19)	2.851(2)	155(3)					
O8-H8W...O1#4	0.77(2)	2.00(2)	2.7578(17)	168(3)					
Symmetry codes:									
#1	x+1, y, z	#2	-x,-y+1,-z+1	#3	x+1/2,y+1/2,z	#4	-x,y,-z+1/2	#5	x+1/2,-y+3/2,z-1/2

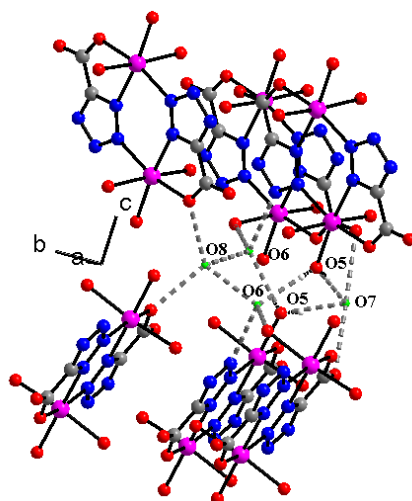


Figure S1. The interlayer hydrogen bonds through free water molecules in **1**.

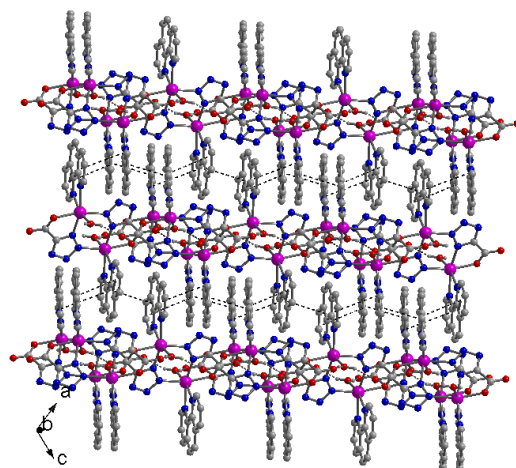


Figure S2. The 3D supramolecular structure assembled via hydrogen bond and π - π interactions of **3**.

Table S2. Hydrogen bonds parameters for complex **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O3-H3B...O4#1	0.825(19)	2.00(2)	2.816(5)	168(4)
O3-H3A...N3#2	0.849(19)	1.93(2)	2.778(16)	173(4)
O3-H3A...O2'#2	0.849(19)	2.02(3)	2.838(18)	162(5)
O4-H4B...N2#3	0.829(19)	1.81(2)	2.619(8)	166(5)
O4-H4B...O1'#3	0.829(19)	2.12(2)	2.945(10)	171(5)
O4-H4A...N4#4	0.849(19)	1.82(3)	2.634(6)	161(5)
O4-H4A...O2'#4	0.849(19)	2.14(3)	2.954(11)	160(6)

Symmetry codes: #1 $x-1,y,z$ #2 $x,-y+1/2,z+1/2$ #3 $-x+1,-y,-z$
#4 $-x+1,-y+1,-z$

Table S3. Hydrogen bonds parameters for complex **6**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O4-H4W2...N4#1	0.85(2)	1.88(3)	2.712(7)	168(6)
O4-H4W2...O2'#1	0.85(2)	2.23(3)	3.06(3)	165(5)
O4-H4W2...N4'#1	0.85(2)	2.51(5)	3.046(13)	122(5)
O4-H4W1...N2#2	0.85(2)	1.96(2)	2.809(9)	176(8)
O4-H4W1...O1'#2	0.85(2)	2.23(4)	3.054(19)	163(7)
O3-H3W2...N5#3	0.95(6)	1.81(6)	2.757(6)	173(5)
O3-H3W1...N3#3	0.81(6)	2.09(7)	2.868(17)	163(6)
O3-H3W1...O2'#3	0.81(6)	2.16(7)	2.96(3)	174(7)

Symmetry codes: #1. $-x+1/2, -y+3/2, -z+1$ #2. $-x+1/2, -y+1/2, -z+1$

#3. $x, -y+1, z+1/2$

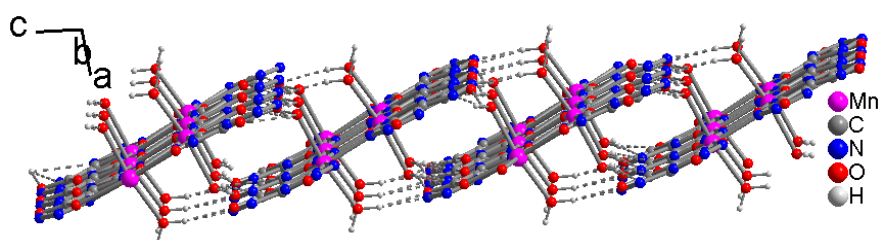


Figure S3. The 2D supramolecular layer assembled via hydrogen bonds in **2**.

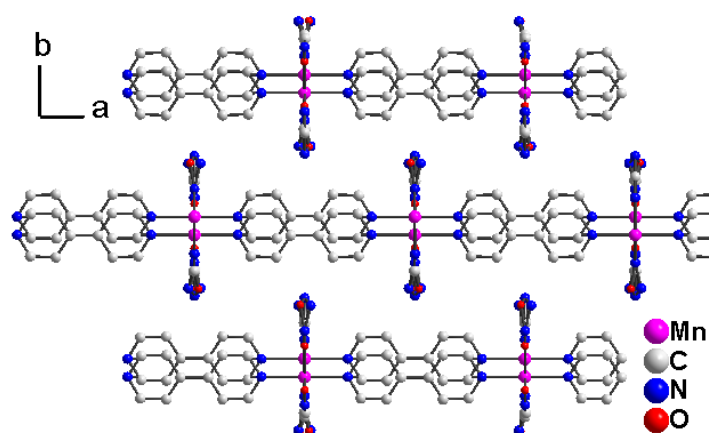


Figure S4. The packed view of extended 2D layers along the *ac* plane of **5**.

Table S4. Selected bond lengths and angles of **4**.

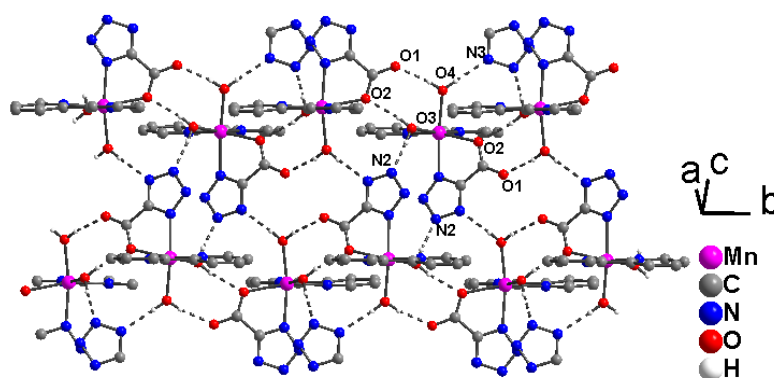
Mn1-O4	2.134(2)	Mn1-N4	2.240(2)
Mn1-O3	2.167(2)	Mn1-N5	2.259(2)
Mn1-O2	2.2372(19)	Mn1-N6	2.265(2)
O4-Mn1-O3	82.80(10)	O2-Mn1-N5	89.32(8)
O4-Mn1-O2	94.93(8)	N4-Mn1-N5	100.82(9)

O3-Mn1-O2	104.74(8)	O4-Mn1-N6	98.53(10)
O4-Mn1-N4	163.22(9)	O3-Mn1-N6	95.16(9)
O3-Mn1-N4	87.74(8)	O2-Mn1-N6	157.21(8)
O2-Mn1-N4	74.08(7)	N4-Mn1-N6	96.09(8)
O4-Mn1-N5	91.51(10)	N5-Mn1-N6	72.09(9)
O3-Mn1-N5	165.19(9)		

Table S5. Hydrogen bonds parameters for complex **4**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O3-H3W2...O2#1	0.843(17)	1.920(18)	2.755(3)	170(3)
O4-H4W1...O1#1	0.842(17)	1.897(17)	2.729(3)	169(3)
O3-H3W1...N2#2	0.848(17)	1.904(18)	2.750(3)	176(3)
O4-H4W2...N3#3	0.814(17)	1.959(17)	2.772(3)	176(3)

Symmetry codes: #1 $-x+1/2, y+1/2, -z+1/2$ #2 $-x+1, -y+1, -z+1$ #3 $x-1/2, -y+1/2, z-1/2$

**Figure S5.** The 2D hydrogen bonding layer in **4**.