Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information

Coordination compounds of bis(5-tetrazolyl)amine with manganese(II), zinc(II) and Cadium(II): synthesis, structure and magnetic properties

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Table S1 Hydrogen bond lengths (Å) and angles (°) for the complexes 1-3

	D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry codes[a]
1	O3-H3WB···O3	0.79(3)	2.22(3)	2.885(3)	141(3)	-x+y, -x+1, z
	O3-H3WA···N4	0.84(3)	1.90(3)	2.717(3)	165(3)	y, -x+y+1, -z+1
	N5-H5N···N8	0.799(15)	2.126(15)	2.914(3)	169(2)	-y+2, x-y+1, z
	O2-H2WB···N7	0.72(3)	2.14(3)	2.796(3)	153(3)	x-y+1,-y+2,-z+1/2
	O2-H2WA···N3	0.83(3)	1.97(3)	2.788(3)	174(3)	-x+1,-x+y+1,-z+1/2
2	O3-H3WB···O3	0.76(4)	2.36(4)	2.896(4)	128(4)	-x+y, -x+1, z
	O3-H3WA···N4	0.82(4)	1.98(4)	2.766(4)	160(4)	y, -x+y+1, -z+1
	N5-H5N···N8	0.831(18)	2.163(19)	2.988(3)	172(3)	-y+2, x-y+1, z
	O2-H2WB···N7	0.83(4)	1.94(4)	2.768(3)	171(3)	x-y+1,-y+2,-z+1/2
	O2-H2WA···N3	0.74(4)	2.07(4)	2.786(3)	163(4)	-x+1,-x+y+1,-z+1/2
3	O3-H3WB···O3	0.73(4)	2.33(3)	2.926(3)	140(3)	-x+y, -x+1, z
	O3-H3WA···N4	0.80(3)	1.95(3)	2.730(2)	163(3)	y, -x+y+1, -z+1
	N5-H5N···N8	0.83(2)	2.11(2)	2.9186(19)	165(2)	-y+2, x-y+1, z
	O2-H2WB···N7	0.84(3)	1.97(3)	2.7993(19)	169(2)	x-y+1,-y+2,-z+1/2
	O2-H2WA···N3	0.83(3)	2.02(3)	2.819(2)	162(3)	-x+1,-x+y+1,-z+1/2

Table S2 Hydrogen bond lengths (Å) and angles (°) for the complex 4

D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry codes[a]
N5-H5...N7	0.84(2)	1.97(2)	2.8126(19)	172.2(19)	x+1/2, -y+3/2, -z
N14-H14...N12	0.75(2)	2.33(2)	3.080(2)	178(2)	x+1/2, -y+1/2, -z+1
O1-H1WB...N13	0.73(3)	2.12(3)	2.845(2)	172(3)	-x+1/2, y+1/2, -z+1
O1-H1WA...N11	0.88(3)	1.91(3)	2.762(2)	163(3)	-x, -y+1, z
O2-H2WB...O7	0.88(3)	1.91(3)	2.7726(18)	169(3)	
O2-H2WA...O5	0.86(3)	2.23(3)	3.084(2)	171(3)	-x, -y+1, z
O3-H3WB...N13	0.78(3)	2.19(3)	2.934(2)	159(3)	-x+1/2, y+1/2, -z
O3-H3WA...N18	0.96(3)	1.78(3)	2.7253(19)	170(3)	-x+1, -y+1, z-1
O4-H4WB...O8	0.86(2)	1.94(2)	2.7989(19)	174(2)	x-1, y, z
O4-H4WA...O3	0.78(3)	2.17(3)	2.946(2)	177(3)	-x, -y+1, z+1
O5-H5WA...N3	0.91(2)	1.79(2)	2.6947(19)	168(2)	
O5-H5WB...N4	0.80(3)	2.25(3)	3.035(2)	166(3)	-x+1, -y+1, z
O6-H6WB...N4	0.91(3)	2.12(3)	2.987(2)	159(3)	-x+1, -y+1, z+1
O6-H6WA...N8	0.82(3)	2.02(3)	2.834(2)	175(3)	-x+1/2, y-1/2, -z+1
O7-H7WB...N17	0.79(2)	2.21(2)	2.9894(18)	169(2)	-x+1, -y+1, z-1
O8-H8WA...N2	0.78(2)	2.23(2)	2.9998(19)	173(3)	**-x+1, -y+1, z**

Table S3 Hydrogen bond lengths (Å) and angles (°) for the complexes 5 and 6

	D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry codes[b]
5	N5-H5A...N2	0.86	1.99	2.842(8)	170.6	x+1/2, -y+3/2, -z
	N14-H14A...N17	0.86	2.04	2.897(8)	176.7	x-1/2, -y+3/2, -z-1
	N19-H19A...N8	0.89	2.32	3.071(7)	141.4	-x+3/2, y-1/2, z-1
	N20-H20C...N13	0.89	2.29	3.037(7)	141.7	x+1/2, -y+3/2, -z
	O1-H1W...N7	0.85(2)	2.17(7)	2.913(8)	145(12)	
	O2-H2W...N12	0.85(2)	2.23(11)	2.908(8)	137(14)	
6	N4-H4...N8	0.95(6)	1.86(6)	2.802(5)	171(5)	-x+3, y-1/2, -z+1/2
	N5-H5...O2	0.85(5)	1.90(5)	2.735(5)	169(5)	
	O1-H1B...N9	0.833(19)	2.05(2)	2.882(5)	172(5)	x-1, y, z
	O1-H1A...N3	0.848(19)	2.13(2)	2.974(5)	175(6)	x, -y+3/2, z+1/2
	O2-H2B...N7	0.819(19)	2.15(3)	2.828(5)	140(4)	-x+3, y-1/2, -z+1/2
	O2-H2A...N7	0.86(2)	2.244(19)	2.957(5)	141(4)	-x+3, -y+2, -z+1

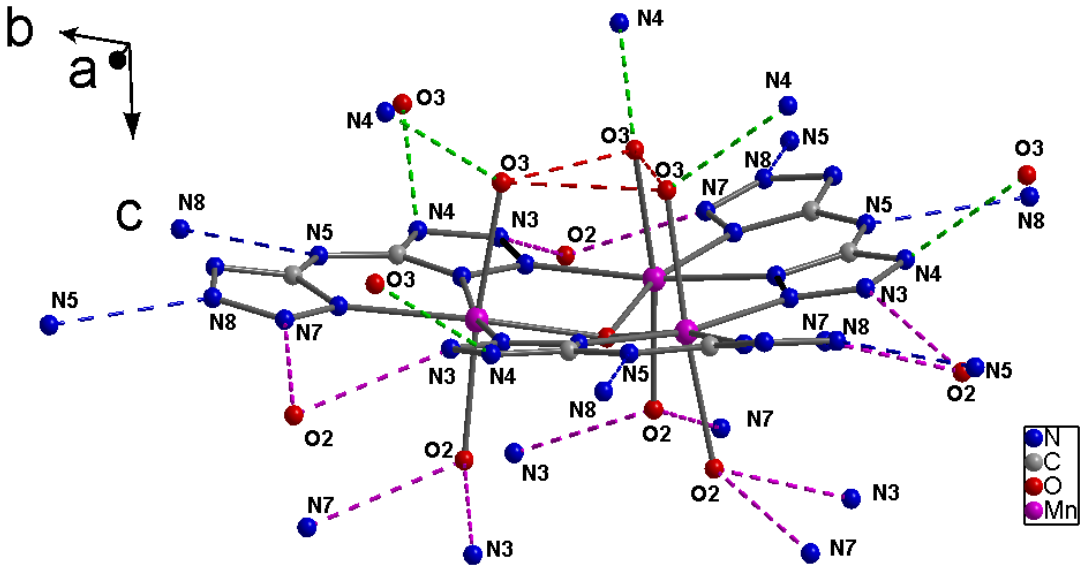

Fig. S1. The hudrogen bonding pattern of a triangular motif in **1**. Different colors are used for the four types of hydrogen bonds (dashed lones): red, O3-H···O3 within the motif; blue, intralayer N5-H···N8; green, intralayer O3-H···N4; .purple, interlayer O2-H···N3 and O2-H···N7. See Table S1.

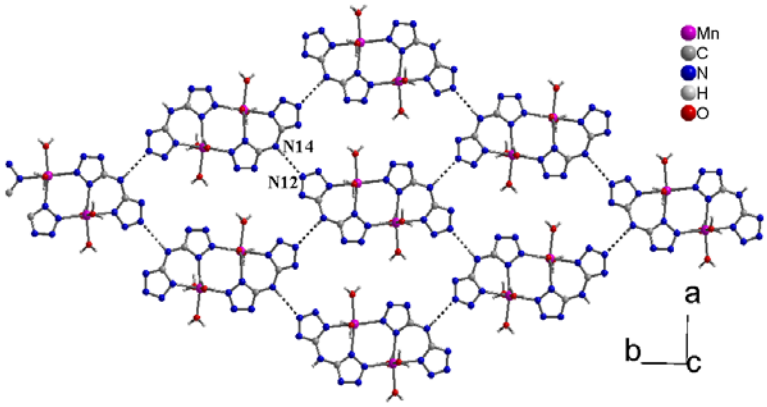

Fig. S2. The self-assembly of the binuclear motifs in **4** via N-H···N hydrogen bonds along the ab plane.

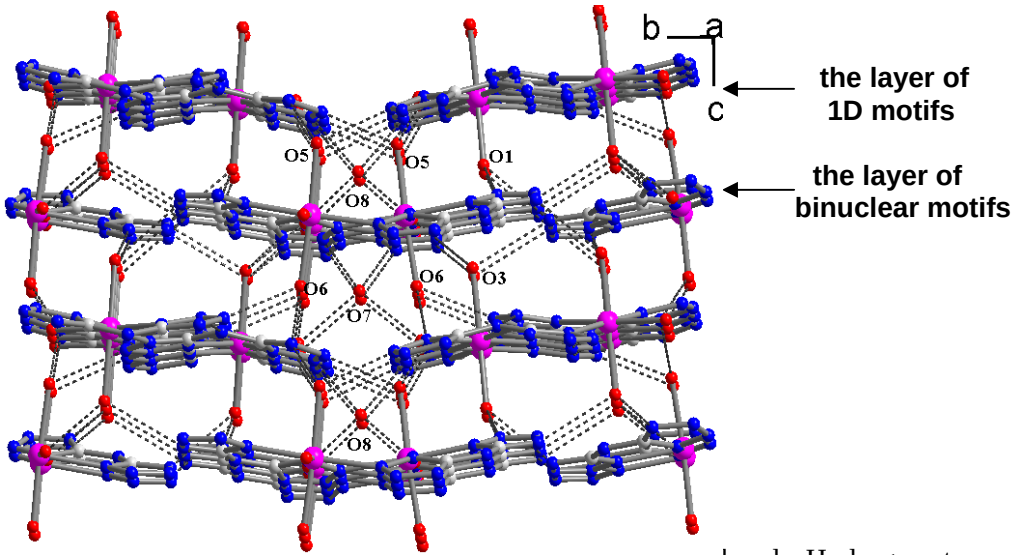

Fig. S3 The packing of the binuclear and 1D motifs in **4** through hydrogen bonds. Hydrogen atoms are omitted for clarity.

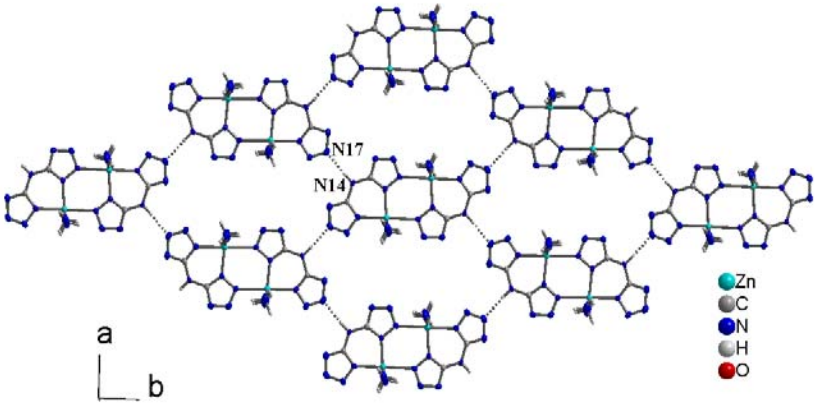

Fig. S4. The self-assembly of the binuclear motifs in **5** via N-H···N hydrogen bonds along the ab plane.

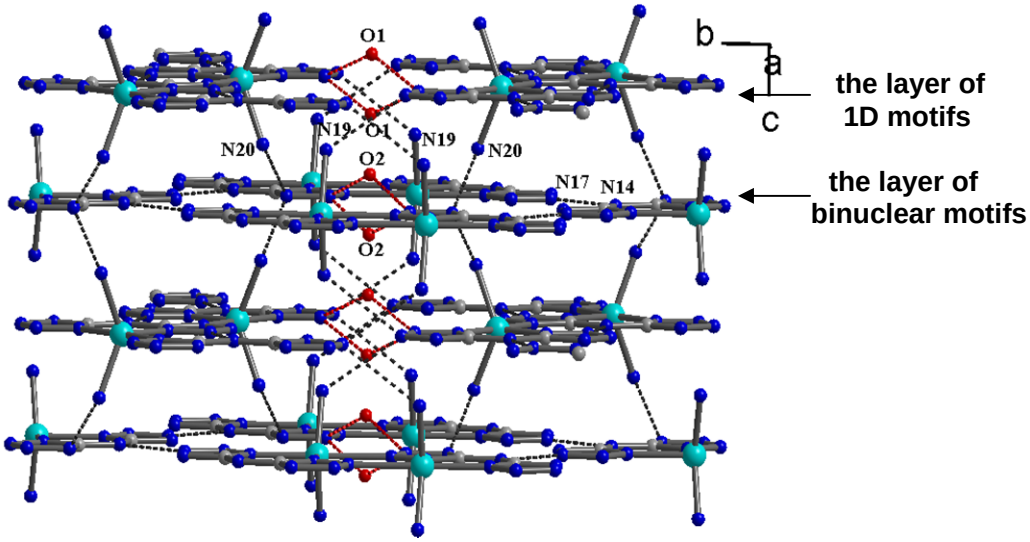

Fig. S5 The packing of the binuclear and 1D motifs in **5** through hydrogen bonds. Hydrogen atoms are omitted for clarity.

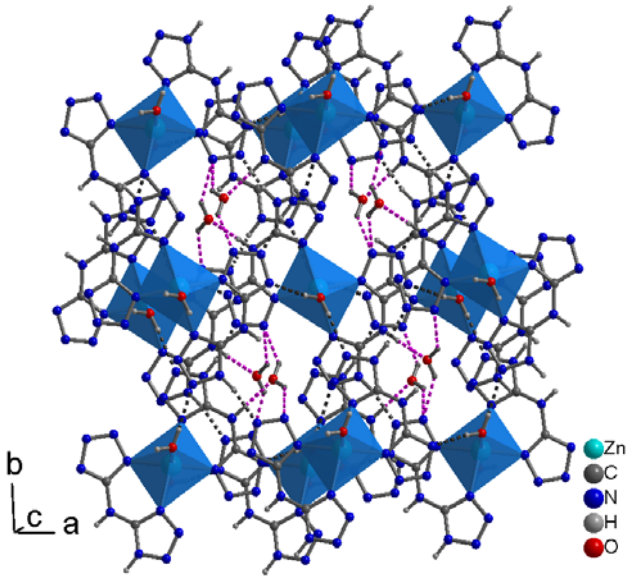

Fig. S6. A view showing the hydrogen bonds of the lattic water molecules in **6**.