Electronic Supplementary Material (ESI) for Dalton Transactions
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Electronic Supporting Information (ESI)

Three-dimensional networks based on trinuclear motifs with tricomponent azide-carboxylate-tetrazolate cobridges: synthesis, structure and magnetic properties

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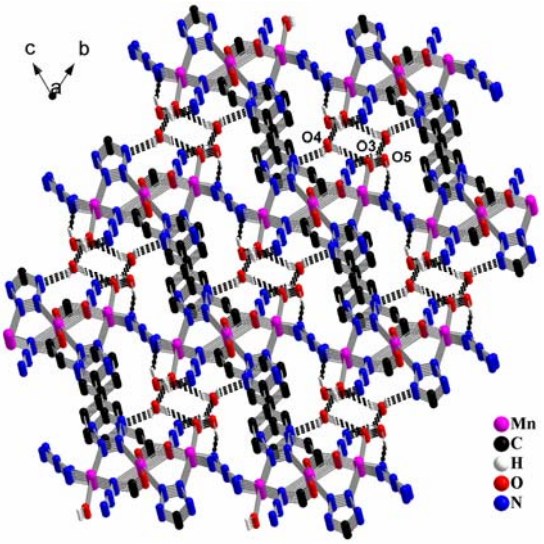

Fig. S1. 3D structure of **1** with O-H···O and O-H···N hydrogen bonds between coordinated aqua water molecules, lattice water molecules, azide groups and tetrazolate groups. Relevant hydrogen bonding parameters: O5-H5···N1 = 149.6(2)°, H5···N1 = 2.077(3) Å, O5···N1 = 2.943(3) Å; O5-H5···N11 = 147.4(2)°, H5···N11 = 2.293(3) Å, O5···N11 = 3.055(4) Å; O3-H3···O5 = 170.6(1)°, H3···O5 = 1.930(2) Å, O5···O3 = 2.795(3) Å; O3-H3···O4 = 148.1(1)°, H3···O4 = 2.034(2) Å, O4···O3 = 2.823(2) Å; O4-H4···O3 = 168.9(1)°, H4···O3 = 2.248(2) Å, O4···O3 = 3.007(2) Å; O4-H4···N7 = 147.7(1)°, H4···N7 = 2.264(2) Å, O4···N7 = 2.977(2) Å.

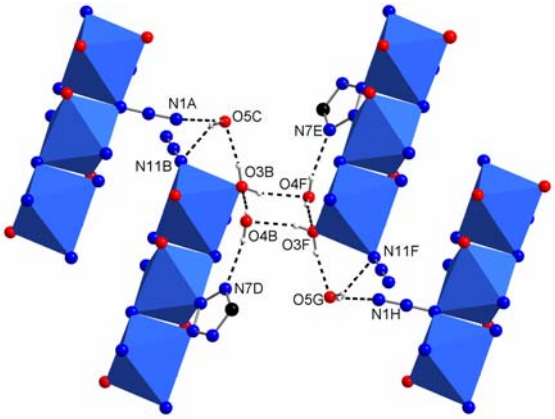

Fig. S2. The hexanuclear water cluster in **1**. Relevant hydrogen bonding parameters: O5C-H5B···N1A = 149.6(2)°, H5B···N1A = 2.077(3) Å, O5C···N1A = 2.943(3) Å; O5C-H5C···N11B = 147.4(2)°, H5C···N11B = 2.293(3) Å, O5C···N11B = 3.055(4) Å; O3B-H3C···O5C = 170.6(1)°, H3C···O5C = 1.930(2) Å, O5C···O3B = 2.795(3) Å; O3B-H3B···O4F = 148.1(1)°, H3B···O4F = 2.034(2) Å, O4F···O3B = 2.823(2) Å; O4B-H4B···O3B = 168.9(1)°, H4B···O3B = 2.248(2) Å, O4B···O3B = 3.007(2) Å; O4B-H4A···N7D = 147.7(1)°, H4A···N7D = 2.264(2) Å, O4B···N7D = 2.977(2) Å. (symmetry codes: A -x, 1-y, -z; B 1-x, 1-y, -z; C -x, -y, 1-z; D x, y, -1+z; E 1-x, -y, 1-z; F x, -1+y, z; G 1+x, y, -1+z; H 1+x, -1+y, z).