Supplementary Material (ESI) for Dalton Transactions

Supporting Information

The First Solid Composed of $\{As_4V_{16}O_{42}(H_2O)\}$ Clusters

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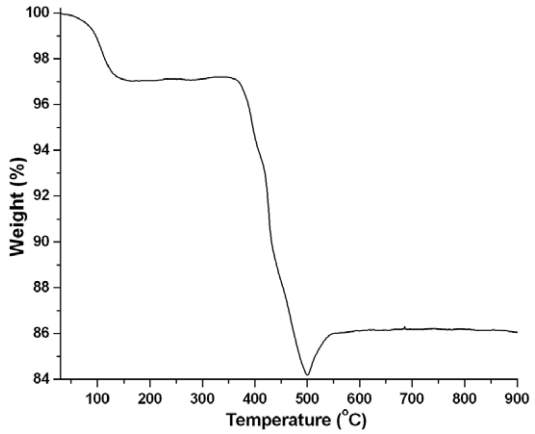
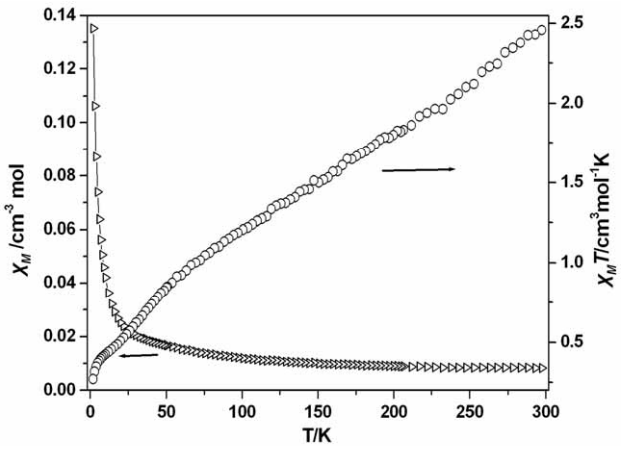
Figure S1. TG curve of **1**.



TGA of **1** shows two major steps of weight losses (Figure S1). The first weight loss of **1** corresponds to the removal of lattice water molecules at relatively lower temperature (below ~ 150 ºC). The remainder stages of **1** (in the range 400-500ºC) are attributed to the loss of the organic ligands and the sublimation of part As_2O_3 molecules. A weight gain was shown between 500 and 550 ºC, which is consistent with the oxidation of V atoms form V^{4+} to V^{5+} and some of the As atoms from As^{3+} to As^{5+}.

Figure S2. Temperature dependence of χ_m (Δ) and $\chi_m T$ (O) values for **1**.



The variable temperature magnetic susceptibility of **1** was measured between 2 and 300 K. As shown in Figure S2, the $\chi_M T$ value at 300 K is 2.45 cm^3 K mol^{-1} (4.43 μ_B), much smaller than that expected value 6.00 cm^3 K mol^{-1} (μ_{eff} = 6.93 μ_B) for the sixteen uncoupled S = 1/2 spins of V^{4+} atoms with g = 2. The $\chi_M T$ value decreases nearly linearly with decreasing temperature from 2.45 cm^3 Kmol^{-1} at 300 K to 0.41 cm^3 Kmol^{-1} at 8 K, and then decreases rapidly from 8 K and reaches

a minimum value of 0.27 $cm^3 Kmol^{-1}$ at 2 K. The temperature-dependences of $\chi_M T$ demonstrate the presence of strong antiferromagnetic coupling interactions, which is a common feature for most polyoxovanadates.(A. Müller, F. Peters, M. T. Pope, D. Gatteschi, *Chem. Rev*. **1998**, 98, 239). Unfortunately, it is too difficult to fit the experimental magnetic data of these extended heteropolymetallic spin system using a suitable theoretical model.(O. Kahn, *Molecular Magnetism*, VCH, Weinheim, Germany, **1993)**