Title:	Steric effect of a capping ligand on the formation of supramolecular coordination networks of Ni(II): Solid-state entrapment of cyclic water dimer
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Abstract:	Supramolecular dimer of water is the simplest of the small water clusters [(H2O)n, n = 2–10]. During the course of our work on supramolecular coordination networks of three-component systems (divalent metal ion, tridentate capping ligand, and ditopic carboxylate linker), a cyclic water dimer is found to be entrapped in the network of [Ni2(6-Mebpta)2(adc)2]·2H2O (1) (6-Mebpta = 2-methyl-N-((6-methylpyridin-2-yl)methyl)-N-(pyridin-2-ylmethyl)propan-2-amine and adc = acetylenedicarboxylate). Based on the single-crystal structure of 1, the water dimer plays an important role in connecting the bis(adc) bridged dinickel synthons to form a one-dimensional (1D) supramolecular network. To emphasize the role of 6-Mebpta in the judicious choice of components for 1, one simple modification to it by having another methyl group in the second pendant pyridyl group to make 6,6′-Me2bpta (2-methyl-N,N-bis((6-methylpyridin-2-yl)methyl)propan-2-amine) did not allow the formation of any water cluster in [Ni(6,6′-Me2bpta)(adc)(H2O)]·H2O (2), where a different coordination environment around Ni(II) is also observed. Further quantification of the difference in supramolecular interactions observed in 1 and 2 has been assessed by Hirshfeld surface analysis. Both 1 and 2 are obtained in good yields at room temperature (methanol as solvent) and are further characterized by elemental analysis, Fourier transform infrared (FTIR) and Raman spectroscopy, powder X-ray diffraction, and thermogravimetric analysis.
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