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Title:	Supramolecular assemblies of dimanganese subunits and water clusters organized by strong hydrogen bonding interactions: Single crystal to single crystal transformation by thermal De-/rehydration processes.
Authors:	Khullar, S. (/jspui/browse?type=author&value=Khullar%2C+S.) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Ambient conditions Bound water molecules Equimolar amount
Issue Date:	2012
Publisher:	American Chemical Society.
Citation:	Crystal Growth and Design, 12 (11), pp. 5329-5337.
Abstract:	New three-dimensional (3D) supramolecular assemblies held together by strong hydrogen bonding interactions between two-dimensional (2D) layers of the $[\text{Mn}_2(\text{adc})_2(\text{bpta})_2(\text{H}_2\text{O})_2]$ subunit (where adc = acetylene dicarboxylate and bpta = N,N-bis-(2- pyridylmethyl)-tert-butylamine) containing a pore ($8.225 \text{ \AA} \times 4.048 \text{ \AA}$) and a cluster of water molecules (five at 296 K and six at 120 K) are reported. The water cluster arrangement in the channel is found to be different at these two temperatures. In the two-dimensional layers, there exists strong intermolecular hydrogen bonding interactions ($\text{O} \cdots \text{H}-\text{O}$) between the uncoordinated oxygen atoms of the adc and hydrogen atoms of the bound water molecules. $[\text{Mn}_2(\text{adc})_2(\text{bpta})_2(\text{H}_2\text{O})_2] \cdot 5\text{H}_2\text{O}$ ($1 \cdot 5\text{H}_2\text{O}$) is prepared by mixing equimolar amounts of bpta and $\text{Mn}(\text{ClO}_4) \cdot 2 \cdot 6\text{H}_2\text{O}$ in methanol at room temperature followed by the addition of 1 equiv of disodium acetylene dicarboxylate in 55% yield. Direct layering of the starting materials results in the formation of a similar 3D supramolecular assembly, $1 \cdot 4\text{H}_2\text{O} \cdot \text{CH}_3\text{OH}$. When a single crystal of $1 \cdot 5\text{H}_2\text{O}$ is slowly heated to 350 K, it undergoes a solid-state structural transformation to the 2D framework 1, where the cluster of five water molecules in the channel of the former is completely removed, showing remarkable stability. Upon rehydration of 1 under ambient conditions over a few weeks, the 3D supramolecular assembly $1 \cdot 4\text{H}_2\text{O}$, where strong hydrogen bonding as well as $\text{C}-\text{H} \cdots \text{O}$ interactions exist, was obtained. The solid-state structural transformation between 3D, 2D, and 3D during the dehydration and rehydration processes in $1 \cdot 5\text{H}_2\text{O}$, 1, and $1 \cdot 4\text{H}_2\text{O}$, respectively, was verified by single crystal and powder XRD measurements. These compounds were also characterized by elemental analysis, IR, and Raman spectroscopy and thermogravimetric and differential scanning calorimetry analyses.
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