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Title:

Construction of diverse supramolecular assemblies of dimetal subunits differing in coordinated water molecules via strong hydrogen bonding interactions: Synthesis, crystal structures and

spectroscopic properties

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Keywords:

Supramolecular Flexible ligand Hydrogen bonding Dicarboxylates

Issue

2014

Date:

Springer

Publisher:

Journal of Chemical Sciences, 126(5), pp.1515-1523.

Abstract:

Three new supramolecular assemblies (constructed through strong hydrogen bonding) of [Co2(bpta)2(adc)(H2O)4](ClO4).22H2O (1), [Cu2(bpta)2(fum)(H2O)2](ClO4)2 (2) and [Cu2(bpta)2(tdc)(H2O) (ClO4)](ClO4).3H2O (3), which are synthesised by one pot self-assembly of the metal salt, bpta ligand and the corresponding dicarboxylate under the same reaction conditions, are reported (where adc = acetylene dicarboxylate, fum = fumarate, tdc = 2.5 $thiophene dicarboxylate\ and\ bpta\ =N,N'-bis(2-pyridylmethyl)-tert-butylamine).\ These\ compounds$ have varying degrees of coordinated water molecules per dimetal subunits (four for 1, two for 2 and one for 3, respectively). Furthermore, the orientation of the coordinated water molecules in 1 and 2, with respect to the mono (carboxylato)-bridged dimetal subunit, is different (cis and trans, respectively). On the other hand, there is a coordinated perchlorate ion in 3 making the two metal centers inequivalent. Unlike 1 and 3, there are no lattice water molecules in 2. This difference in the dimetal subunit in 1-3 and the presence or absence of the lattice water molecules are the keys to forming the diverse supramolecular assemblies. In 1 and 3, the involvement of lattice water molecules in the construction of such assemblies is distinctly different. In case of 2, the formation of supramolecular assembly depends on the coordinated water molecule (trans to each other) and thus a ladder shaped supramolecular assembly is the result. The strength of hydrogen bonding observed in the networks of 1-3 is indicated in the O···O distances (2.596 Å to 3.160 Å) and the O-H...O angles 124 to 176 c. All are characterised by elemental analysis, FTIR spectroscopy and single crystal X-ray diffraction studies.

URI:

https://link.springer.com/article/10.1007%2Fs12039-014-0685-x (https://link.springer.com/article/10.1007%2Fs12039-014-0685-x)

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