Title:	Effect of Spacer Atoms in the Dicarboxylate Linkers on the Formation of Coordination Architectures—Molecular Rectangles vs 1D Coordination Polymers: Synthesis, Crystal Structures, Vapor/Gas Adsorption Studies, and Magnetic Properties
Authors:	Khullar, S. (/jspui/browse?type=author&value=Khullar%2C+S.) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Magnetic Properties Molecules Water Vapor Adsorption Ligands
Issue Date:	2014
Publisher:	American Chemical Society
Citation:	Crystal Growth and Design, 14(12), pp.6433-6444.
Abstract:	Using the Cu(II)-tpbn system, three new compounds-[Cu4(tpbn)2(glutarate)2(H2O)4](ClO4)4·xH2O (when x = 2, 1; x = 4, 1a), {[Cu2(tpbn)(diglyconate)(H2O)2](ClO4)2·solvent}n (when no solvent, 2; solvent = CH3OH/CH3CN, 2a), and [Cu4(tpbn)2(2,2'-thiodiacetate)2(H2O)4](ClO4)4·xH2O (when x = 0, 3; x = 4, 3a), where tpbn = N,N',N'',N'''-tetrakis(2-pyridylmethyl)-1,4-diaminobutane-have been synthesized from a one-pot self-assembly reaction in a methanol-water mixture under ambient conditions. Their formation is dependent on the spacer atom in the dicarboxylate linker: molecular rectangles (1/1a and 3/3a) are obtained with spacer atoms CH2 and S, whereas a helical one-dimensional (1D) coordination polymer (2/2a) is obtained with O as the spacer atom in the linker. These are the first molecular rectangles containing the dicarboxylates used in this study. In addition to their characterization by elemental analysis and UV-vis and IR spectroscopy, their solid-state molecular structures are determined by single-crystal X-ray diffractometry. Using electrospray mass spectrometry, their structural integrity in the solution state is confirmed. Water vapor adsorption study of 1-3 corroborates well with their solid-state structures in terms of their affinity toward water: 3 shows a stepwise adsorption with a maximum water vapor intake of 16 water molecules per molecule of 3, having a small hysteresis loop, while 1 shows a continuous adsorption with a maximum water vapor intake of 10.5 water molecules per molecule of 1, having a larger hysteresis loop, and 2 has the least affinity. Similarly, adsorption of CO2 is 3 times more by 1 than 3 at 296 K, and both show selectivity for CO2 over N2. Comparison of their magnetic behavior based on variable-temperature magnetic susceptibility measurements (2-300 K) indicates weak antiferromagnetic interactions between the Cu(II) centers in 1 and 3 and a weak ferromagnetic interaction between the Cu(II) centers in 2. This is well correlated to the Cu···Cu distances in these compounds. Each compound showed a characteristic broad isotropic electron paramagnetic resonance signal for distorted square-pyramidal Cu(II) ions at 77 K.
URI:	https://pubs.acs.org/doi/10.1021/cg501284y (https://pubs.acs.org/doi/10.1021/cg501284y) http://hdl.handle.net/123456789/2754 (http://hdl.handle.net/123456789/2754)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
need to add pdf....odt (/jspui/bitstream/123456789/2754/1/need%20to%20add%20pdf....odt)		8.12 kB	OpenDocument Text	View/Open (/jspui/bitstream/1234

Show full item record (/jspui/handle/123456789/2754?mode=full)

(/jspui/handle/123456789/2754/statistics)