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Title: Hierarchical importance of coordination and hydrogen bonds in the formation of homochiral 2D

coordination polymers and 2D supramolecular assemblies

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Homochiral 2D

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Abstract:

In exploring the chemistry of reduced Schiff base derivatives of amino acids with Cu(ii) ions, a series of homochiral two-dimensional (2D) coordination polymers (CPs) with a unique loop-like structure comprised of five Cu(ii) centers, {[Cu2(Hsersal)2(H2O)]·2.5H 2O}n, (1), {[Cu2(Hser-5OMe-sal) 2(H2O)]·DMF}n (2), [Cu 2(Hser-5NO2-sal)2(H2O)]n (3), {[Cu2(Hser-5Cl-sal)2(H2O)]·2H 2O}n (4), {[Cu2(Hser-3Cl-sal) 2(H2O)]·3H2O}n (5) and {[Cu2(Hser-o-Van)2(H2O)]·3H 2O}n (6) [where H3sersal = N-(2-hydroxybenzyl)- serine, H3ser-5OMe-sal = N-(2-hydroxy-5methoxybenzyl)-serine, H 3ser-5NO2-sal = N-(2-hydroxy-5-nitrobenzyl)-serine, H 3ser-5-Cl-sal = N-(2-hydroxy-5-chlorobenzyl)-serine, H 3ser-3-Cl-sal = N-(2-hydroxy-3-chlorobenzyl)-serine, H 3ser-o-van = N-(2-hydroxy-3-methoxybenzyl)-serine], have been isolated in good yields from the reaction of a methanolic solution of CuSO 4·5H2O and potassium salt of the respective ligands (in a 1:1 ratio) either at room temperature or under reflux. In these CPs, the two Cu(ii) centers have different coordination environments with one coordinated to a water molecule. Using a bifunctional linker, such as 4,4'- bipyridine, four of these 2D CPs are converted in methanol under reflux to the corresponding 2D supramolecular coordination complexes (SCCs) constructed through very strong hydrogen bonding interactions, [Cu2(4,4'- bpy)(Hsersal)2]·2H2O (7), [Cu2(4, 4'-bpy)(Hser-5-OMesal)2]·6H2O (8), [Cu 2(4,4'-bpy)(Hser-5-NO2-sal)2]·H2O (9) and [Cu2(4,4'-bpy)(Hser-5-Cl-sal) 2]·4H2O·DMF (10). This chemical conversion of a CP to an SCC is unknown in the literature and indicates the hierarchical importance of coordination and hydrogen bonds in their formation. The complexes are structurally characterized by elemental analysis, UV-Vis spectroscopy, circular dichroism, IR and Raman spectroscopy, ESI mass spectrometry, single crystal and powder X-ray diffraction, polarimetry and thermogravimetric analysis. A magneto-structural correlation for the change from 1 to 7 is established through variable temperature magnetic susceptibility measurements (2-390 K) indicating strong antiferromagnetic coupling (2J = -278 cm -1) in 1 and no interaction in 7 between the Cu(ii) centers. As an example, water adsorption studies of 1 and 7 were carried out to demonstrate the porous nature of the SCCs compared to the CPs.

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