Polyhedron
Volume 188, 15 September 2020, 114702

Seven Zn(II) and Cd(II) 1D coordination polymers based on azine donor linkers and decorated with 2-thiophenecarboxylate: Syntheses, structural parallels, Hirshfeld surface analysis, and spectroscopic and inclusion properties

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https://doi.org/10.1016/j.poly.2020.114702

Abstract

Seven mixed-ligand 1D coordination polymers [Zn2(4-bphz)(2-tpc)4]n (1), [Zn2(4-bpmhz)(2-tpc)4]n (2), [Cd(4-bphz)2(2-tpc)2]n (3), [Zn(3-bphz)(2-tpc)2]n (4), [Zn(3-bpmhz)(2-tpc)2]n (5), [Cd(4-bpmhz)(2-tpc)2]n·0.5n(4-bpmhz) (6), [Cd(3-bpmhz)(2-tpc)2]n·0.5n(H2O) (7) (where 2-tpc = 2-thiophenecarboxylate, 4-bphz = 1,2-bis(pyridin-4-ylmethylene) hydrazine, 4-bpmhz = 1,2-bis(1-(pyridin-4-yl)ethylidene)hydrazine, 3-bphz = 1,2-bis(pyridin-3-ylmethylene)hydrazine, and 3-bpmhz = 1,2-bis(1-(pyridin-3-yl)ethylidene)hydrazine) were prepared and studied using spectroscopic (FTIR, UV–Vis) and X-ray diffraction methods of analysis. Similarly, four bidentate-bridging azine ligands provide the polymers' extension, while the different mononuclear/binuclear metal nodes demonstrate the variable metals' coordination capacities that influence the crystal packing motifs and inclusion properties. The guest-free arrays 1–5 pack in parallel stacking modes, while the inclusion compounds 6 and 7 reveal criss-cross packing arrangements with large channels where guest molecules (4-bpmhz/water) serve as structure-directing templates in the formation of crystal structures. The distributions of different types of intermolecular interactions with respect to the percentage of stacking interactions in 1–7 were quantified by Hirshfeld surface and fingerprint plots analysis. The guest-exchange properties for 6 and the solid state emissive properties for 1–7 are reported.

Keywords: azomethyne ligands, coordination polymers, crystal structure, spectroscopic studies, inclusion properties, luminescence

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