Title:	Deciphering supramolecular isomerization in coordination polymers: connected molecular squares vs. fused hexagons
Authors:	Gupta, Vijaya (/jspui/browse?type=author&value=Gupta%2C+Vijaya) Laha, Biswajit (/jspui/browse?type=author&value=Laha%2C+Biswajit) Khullar, Sadhika (/jspui/browse?type=author&value=Khullar%2C+Sadhika) Mandal, Sanjay K. (/jspui/browse?type=author&value=Mandal%2C+Sanjay+K.)
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Abstract:	The self-assembly of Mn(II), bis(tridentate) ligands and bent dicarboxylate linkers under ambient conditions has been exploited to generate a series of 1D coordination polymers in good yields. For a set of seven compounds, structural isomerization of these architectures is demonstrated through the variation of length and nature of the spacer between the tridentate capping sites of the bis(tridentate) ligands, such as tpbn (N,N′,N″,N‴-tetrakis-(2-pyridylmethyl)-1,4-diaminobutane), tphxn (N,N′,N″,N‴-tetrakis-(2-pyridylmethyl)-1,6-diaminohexane), and tpxn (N,N′,N″,N‴-tetrakis-(2-pyridylmethyl)-xylylamine) or by varying the bent dicarboxylate linker 4,4′-(dimethylsilanediyl)bis-benzoic acid (H2L1) or 4,4′-oxybis-benzoic acid (H2L2). These compounds have been structurally characterized by single-crystal and powder X-ray diffraction, FTIR, and thermogravimetric and elemental analyses. This study reveals that the supramolecular structural variation can be precisely controlled either by a judicious selection of reaction conditions or linker/ligand combinations. For example, the self-assembly of Mn(II), tpbn and H2L1 in DMF/EtOH/water affords a mixture of products (1 and 1a) while changing the solvent combination to EtOH/water results in the generation of a single isomer (1a) in a highly selective manner. On the other hand, for the Mn(II)-tphxn system, different structural isomers have been isolated by varying the dicarboxylates, H2L1 and H2L2 (2vs.5). Similarly, for the Mn(II)-H2L2 system, a variation in the spacer chain length of bis(tridentate) ligands, tpbn and tphxn resulted in the formation of different structural isomers (4vs.5).
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