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Construction of one dimensional Co(II) and Zn (II) coordination polymers based on expanded N,N'-donor ligands

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Abstract

Four new 1-D coordination polymers [Zn(acac)₂(L1)]_n (**1**), [Co(acac)₂(L1)]_n (**2**), [Co(acac)₂(L2)]_n (**3**) and [Co(acac)₂(L3)]_n (**4**) were afforded by the complexation reaction of appropriate zinc and cobalt metal salts, acetylacetone co-ligand as well as three linear electron rich and bi-functional N,N'-bipyridyl-base ligands of N,N'-bis(pyridin-4-ylmethylene)naphthalene-1,5-diamine (L1), N,N'-bis(pyridin-4-ylmethylene) phenylene-1,4-diamine (L2) and N,N'-bis(pyridin-4-ylmethylene)hydrazine (L3). The structures of these compounds were characterized by FT-IR spectroscopy, elemental analysis, X-ray powder and single crystal X-ray diffractions. X-ray crystallography analyses revealed that these compounds have 1-D linear chain structures containing {N₂O₄} metal coordination environment in which the N-donor L_x (x=1–3) bridges occupy *trans* positions. The acetylacetone (acac) ancillary ligands control the coordination number of the metal cation and adopt chelating binding mode on octahedral metal center. Furthermore, 1-D chains are held together with their neighboring ones by C–H···O, C–H···π and π–π stacking intermolecular interactions to stabilize 2-D supramolecular networks. The two former cases **1** and **2**, containing same L1 spacer ligand generate isomorphous structures. Theoretical calculations invoking electronic properties, frontier molecular orbital description and the strength of interactions between metal ion and coordinated atoms via second order perturbation energies were carried out using natural bond orbital analysis (NBO). Finally, thermal stability of compound **2–4** was examined by thermogravimetric (TGA) analysis.

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