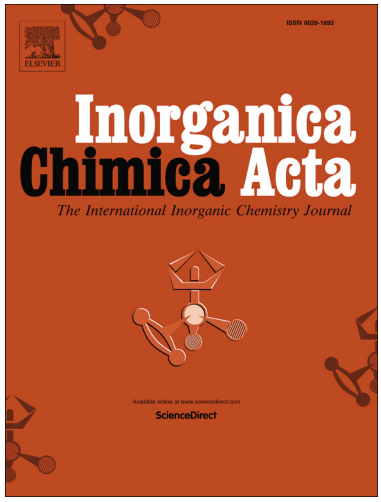

Research paper

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

Mansoureh Zahedi, Behrouz Shaabani, Muhittin Aygün, Canan Kazak

PII: S0020-1693(17)30782-X
DOI: http://dx.doi.org/10.1016/j.ica.2017.09.023
Reference: ICA 17879

To appear in: *Inorganica Chimica Acta*

Received Date: 17 May 2017
Revised Date: 17 August 2017
Accepted Date: 8 September 2017

Please cite this article as: M. Zahedi, B. Shaabani, M. Aygün, C. Kazak, Construction of one dimensional Co(II) and Zn (II) coordination polymers based on expanded N,N'-donor ligands, *Inorganica Chimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.ica.2017.09.023

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

Mansoureh Zahedi[a], **Behrouz Shaabani***[, a], **Muhittin Aygün**[b] **and Canan Kazak**[c]

[a]*Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz , Iran*

**Email:* shaabani.b@gmail.com (*shaabani@tabrizu.ac.ir)*

[b]*Department of Physic, Faculty of Arts & Sciences Dokuz Eylul University, Izmir, Turkey*

[c]*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, Samsun , Turkey*

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 a containing $\{N_2O_4\}$ metal coordination environment in which the *N*-donor Lx (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.