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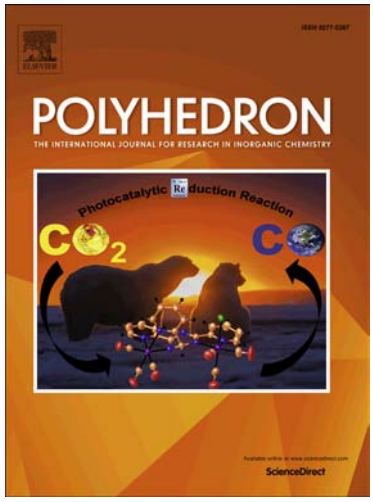

Metal-Directed Assembly of Two One-Dimensional Coordination Polymers: Structural, Theoretical, Fluorescent and Non-linear Optical Studies

Huajian Zhao, Ding Jia, Suci Meng, Jianghua Li, Chi Zhang

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Metal-Directed Assembly of Two One-Dimensional Coordination Polymers: Structural, Theoretical, Fluorescent and Non-linear Optical Studies

Huajian Zhao,[a] Ding Jia,[b] Suci Meng,[b] Jianghua Li,[b] Chi Zhang*[a,b]

[a] Molecular Materials Research Center, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China

[b] China-Australia Joint Research Center for Functional Molecular Materials, Scientific Research Academy, Jiangsu University, Zhenjiang 212013, P. R. China

Highlights

- Two 1-D Zn(II)/Cd(II) coordination polymers were synthesized.
- The absorption spectra of 4,4′-azpy and **1** were calculated.
- The fluorescence and non-linear optical properties of CPs **1** and **2** have been investigated.

Abstract

The reaction of Zn(II)/Cd(II) salts with azo-containing bipyridyl ligands afforded two coordination polymers (CPs), $[Zn(\mu_2\text{-}4,4'\text{-azpy})(NO_2)_2]_n$ (**1**) and $[Cd_2(\mu_2\text{-}4,4'\text{-azpy})_3(NO_2)_4]_n$ (**2**) (4,4′-azpy = 4,4′-azopyridine). The identities of the CPs **1** and **2** have been unambiguously established by single-crystal X-ray diffraction, and further characterized by elemental analysis, powder X-ray diffraction, thermogravimetric analyses, electrospray ionization-mass spectrometry (ESI-MS), fluorescence analysis, Fourier-transform infrared and ultraviolet/visible spectroscopies. CP **1** exhibits one-dimensional (1-D) zigzag chains containing an octahedral $[ZnO_4N_2]$ unit bridged by N-donor ligands in the crystal lattice. CP **2** presents a 1-D ladder chain constructed by T-shape units of $[Cd(NO_2)_2(\mu_2\text{-}4,4'\text{-azpy})_3]$ and further forms a 1-D → three-dimensional (3-D) interpenetrated structure. In addition, density functional theory and time-dependent density functional theory calculations at the B3LYP/LanL2DZf+6-31G* level were performed on 4,4′-azpy and CP **1** to rationalize their experimental absorption spectra. The fluorescent properties of the free 4,4′-azpy

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