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Title:	Structural and luminescent properties of a new 1D Cadmium(II) coordination polymer: A combined effort with experiment & theory
Authors:	Joshi, Mayank (/jspui/browse?type=author&value=Joshi%2C+Mayank) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Cd(II) X-ray structure 1D coordination polymer Supramolecular architecture Spectroscopic study DFT study
Issue Date:	2018
Publisher:	Elsevier B.V.
Citation:	Journal of Molecular Structure, 1167, pp. 187-193
Abstract:	In this work, we have developed a new one-dimensional cadmium(II) coordination polymer, [Cd(phen)(NO ₃) ₂ (H ₂ O)] _n (1) (phen = 1,10-phenanthroline) and structurally characterized by different spectroscopic techniques including single crystal X-ray diffraction analysis. Single crystal X-ray structural analysis of 1 indicates that Cd(II) ion in the coordination polymer crystallizes in a monoclinic system with P2 ₁ space group and adopts a distorted pentagonal bipyramidal coordination geometry. This will be the first citation of a 1D Cd(II) polymer till date where nitrate ions exhibit diverse coordination motifs. Solid state emission suggests good luminescence behavior of the polymer. Spectroscopic studies reveal that the polymer is unstable in polar solvents and dominates in monomeric form. Molar conductivity and electrospray ionization mass spectral analysis in methanolic solution confirm the instability of the polymer at room temperature and authenticates the decomposition of the polymer into monomer in solution. In addition, all the structural parameters and spectroscopic behaviors have been well corroborated with the theoretical findings.
Description:	Only IISERM authors are available in the record.
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