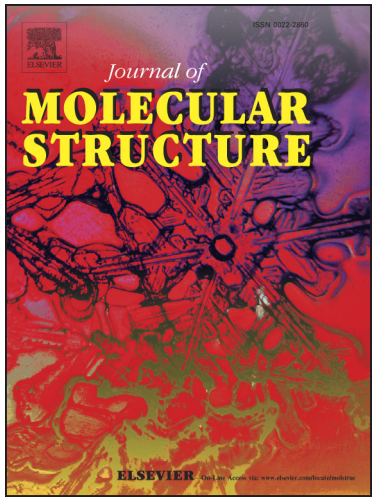

Structural characterization, thermal studies, vibrational and DFT investigation of the bis(8-hydroxyquinolinium)tetrachlorocadmate(II)

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PII: S0022-2860(14)01169-7
DOI: http://dx.doi.org/10.1016/j.molstruc.2014.11.052
Reference: MOLSTR 21130

To appear in: *Journal of Molecular Structure*

Received Date: 3 October 2014
Revised Date: 24 November 2014
Accepted Date: 24 November 2014

Please cite this article as: W. Amamou, N. Elleuch, H. Feki, N. Chniba-boudjada, F. Zouari, Structural characterization, thermal studies, vibrational and DFT investigation of the bis(8-hydroxyquinolinium)tetrachlorocadmate(II), *Journal of Molecular Structure* (2014), doi: http://dx.doi.org/10.1016/j.molstruc.2014.11.052

Structural characterization, thermal studies, vibrational and DFT investigation of the bis(8-hydroxyquinolinium)tetrachlorocadmate(II)

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Abstract

A new organic-inorganic crystal, bis(8-hydroxyquinolinium) tetrachlorocadmate(II) has been synthesized and characterized by thermal analyses (TGA and DSC), FT-IR, Raman, PXRD and fluorescence studies. The single X-ray diffraction studies have revealed that the compound crystallizes in monoclinic *C*2/*c* space group with cell parameters a=15.409(4), b=8.391(2), c=16.610(4), β=91.68(5) and Z=4. The atomic arrangement can be described as an alternation of organic and inorganic layers along the a-axis. The crystal packing is governed by the N–H···Cl, O–H···Cl and non-classical C–H···Cl hydrogen bonding interactions between the 8-hydroxyquinolinium cations and the tetrahedral $[CdCl_4]^{2-}$ anions, in which they may be effective in the stabilization of the crystal structure. Moreover, the fluorescent properties of the compound have been investigated in the solid state at room temperature.

The optimized molecular structure and the vibrational spectra were calculated by the Density Functional Theory (DFT) method using the B3LYP function with the LanL2DZ basis set. Good agreement has been found between the calculated results and the experimental data.

Keywords: Crystal structure; Thermal studies; luminescence; DFT calculations; Vibrational studies.

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