Poster Presentation

Comparative study of halogenocadmate (II) hybrids incorporating (DABCOH2)2+ cations

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Two compounds (DABCOH2)[CdCl4]·H2O (1) [*] and (DABCOH2)[CdI4] (2) were synthesized by reaction of cadmium iodide (CdI2) and 1,4-Diazabicyclo[2.2.2]octane (DABCO) in an aqueous solution of (HX) acid (1: X = Cl, 2: X = I) . The first compound (1) crystallizes in the orthorhombic system with a = 8.528(5) Å, b = 11.653(2) Å, c = 13.114(6) Å, V = 1303.2(10) Å3, Z = 4, space group P212121 and the second one (2) cystallizes in the monoclinic system with a = 10.437(2) Å, b = 7.245(3) Å, c = 20.645(4) Å, β = 91.46(5)°, V = 1561.2(8) Å3, Z = 4, space group P21/c. A full comparative study between these halogenocadmate (II) hybrids has been performed. The structures of both compounds are self-assembled into alternating organic and inorganic layers. The anionic layer consists of isolated [CdX4]2- anions (1: X = Cl, 2: X = I). The organic part is made up of (DABCOH2)2+ cations linked to the anionic layer via N-H···X hydrogen bonds. This organic-inorganic alternation is organized according to the (002) planes for hydrated compound and (102) planes for anhydrous one (Fig. 1). In the comparative part, the role of the water molecule on the structural arrangement has been analysed. The temperature dependence of the emission spectra has been investigated in detail, especially for (DABCOH2)[CdCl4]·H2O. This study shows the existence of the localization phenomenon in this material. [*] Ben Rhaiem, T. & Boughzala, H. (2014). Acta Cryst. E70, m178-m178.



The structure of the compound (1), projected along the b axis.

The structure of the compound (2), projected along the b axis.

Keywords: Organic-inorganic hybrid material, Chlorocadmate (II), Photoluminescence.