

MS36-P01 | FOUR-COMPONENT ISOMORPHISM IN THE CRYSTAL STRUCTURE OF [HL][Cd(HL)(NCS)₂XY]·H₂O, WHERE L = 2-ACETYLPIRIDINE-AMINO GUANIDINE, X = Cl⁻/Br⁻, AND Y = Br⁻/SCN⁻

Rodic, Marko (Faculty of Sciences, University of Novi Sad, Novi Sad); Radanovic, Mirjana (Faculty of Sciences, University of Novi Sad, Novi Sad); Vojinovic-Ješić, Ljiljana (Faculty of Sciences, University of Novi Sad, Novi Sad); Leovac, Vukadin (Faculty of Sciences, University of Novi Sad, Novi Sad)

This study emerged from our ongoing research on transition metal complexes with Schiff base ligands, as this class of compounds has shown wide spectra of biological activities, catalytic behavior, magnetism, and optoelectronic properties, depending on the choice of the particular transition metal, and Schiff base ligand.

The title compound was obtained in the form of white rod-like single crystals, by reaction of warm aqueous solutions of CdBr₂ and the chloride salt of 2-acetylpyridine-aminoguanidine (L·2HCl), in molar ratio 1:1, in the presence of double excess of LiOAc and NH₄NCS.

Single crystal X-ray analysis revealed that crystal structure consists of organic cation HL⁺, Cd(II)-containing complex anion of the formula [Cd(HL)(NCS)₂XY]⁻, as well as one water molecule. Coordination environment of Cd(II) in the complex anion is distorted octahedral, with two axial sites occupied with NCS⁻ ions, two equatorial sites occupied by bidentately coordinated organic ligand in monocationic form (HL⁺), while the remaining two equatorial sites (X, and Y) are occupied by Cl⁻/Br⁻ and Br⁻/SCN⁻ ions, respectively. This means that the crystal structure contains four different anions: [Cd(HL)(NCS)₂Br₂]⁻ (ca. 3%), [Cd(HL)(NCS)₂ClBr]⁻ (ca. 35%), [Cd(HL)(NCS)₂Br(SCN)]⁻ (ca. 61%), and [Cd(HL)(NCS)₂Cl(SCN)]⁻ (ca. 1%).

The geometrical details of the crystal structure will be reported, as well as Hirshfeld surface analysis of the individual building-blocks with the aim of better understanding the nature of the isomorphism.