Isolated versus Condensed Anion Structure VII: X-ray Structure Analysis of 1,3-Propanediammonium Dibromodichlorocadmate(II), $[H_3N(CH_2)_3NH_3]CdBr_2Cl_2$, and Estimation of Stability of Five-coordinated Halide Anions, MX_5^{3-} (M = Cd, Zn; X = Cl, Br) by Means of *Ab-initio* MO Calculations

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The coordination capability of Cl and Br in halogenocadmate(II) complexes is estimated by a solution of the structure of 1,3-propanediammonium dibromodichlorocadmate(II). The compound crystallizes as a layered anion structure with Cl bridges and Br terminals at 293 K: Imma, a = 741.56(7), b = 1869.5(5), and c = 771.55(8) pm, Z = 4. In order to explain the stronger tendency of halogenocadmate(II) complexes to form layered structures as compared to halogenozincate(II), *ab-initio* calculations were performed. The stability of MX_5^{3-} (M = Cd, Zn; X = Cl, Br) is compared. Isolated ZnX_5^{3-} and $CdBr_5^{3-}$ ions are not stable. On the other hand a trigonal bipyramid $CdCl_5^{3-}$ ion is considered to be subtly stable in the crystal mainly due to Coulomb attractive interactions between the positively charged metal cation Cd^{2+} in a $CdCl_3^-$ fragment and two Cl^- ions.

Key words: Crystal Structure; Halogenocadmate(II); *Ab-initio* MO Calculations.