isolated versus condensed anion structure VII: X-ray structure analysis of 1,3-propanediammonium dibromodichlorocadmate(II), [H₃N(CH₂)₃NH₃]CdBr₂Cl₂, and estimation of stability of five-coordinated halide anions, MX₅³⁻ (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 MX₅³⁻ (M = Cd, Zn; X = Cl, Br) is compared. Isolated ZnX₅³⁻ and CdBr₅³⁻ ions are not stable. On the other hand a trigonal bipyramid CdCl₅³⁻ ion is considered to be subtly stable in the crystal mainly due to Coulomb attractive interactions between the positively charged metal cation Cd²⁺ in a CdCl₅⁻ fragment and two Cl⁻ ions.

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