Polyiodides of amino acids

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The study of polyiodides is of great interest from scientific and practical points of view [1,2]. The incorporation of iodine (I_2) molecules and triiodide (I_3^-) anions into the structure of halogenobismuthate salts allows to significantly narrow the bandgap [3,4]. Recently, we started searching for new amino acid salts with halogenobismuthate anions as materials for solar energy conversion. Amino acid salts containing polyiodide anions and an iodine molecule can serve as starting materials and are also interesting in their own right. In this regard, we also began to search for new amino acid salts containing polyiodide anions and an iodine molecule. Previously, two such salts were known: (L-AlaH···L-Ala)(I_3) [5] and (GlyH)(I_3) [6]. We also managed to obtain a simple salt of L-alanine: (L-AlaH)(I_3).H_2O, as well as a glycine salt with a dimeric cation $(GlyH\cdots Gly)_3(I_3)_3(I_2)$. In addition, we obtained polyiodide salts of sarcosine (Sar), dimethylglycine (DMG), betaine (Bet), L-proline (L-Pro), L-cystine (L-Csn), L-lysine (L-Lys), L-arginine (L-Arg), L-histidine (L-His), etc. with various compositions and structures. A dimeric cation of the type ($A^+\cdots A^+$) was found in the structure of (BetH)(I_3). Salts with dimeric cation of the ($A^+\cdots A$) type were found for sarcosine (two polymorphs), dimethylglycine and L-proline. A salt with trimeric cation (($A^+\cdots A\cdots A^+$) was found in the structure of $(BetH)_6(Bet)_3(I_3)_6(I_2)$. A peculiar tetrameric cation [L-ProH···(L-Pro-H-L-Pro)···L-ProH] was found in the structure of $(L\text{-}ProH)_3(L\text{-}Pro)(I_3)_3$ with very short O···O distance (2.427(4) Å) in pseudo symmetric (L-Pro-H-L-Pro) dimer. Salts with doubly charged cations were obtained for L-cystine, L-lysine, L-arginine and L-histidine. Additionally, a salt with ($A^{2+}\cdots A^+$) dimeric cation was found in the structure of $(L\text{-}HisH_2\cdots L\text{-}HisH)_3(I_3)_6(I_4)(I_5)$ with short O···O distances. Single crystals were grown by slow evaporation from aqueous and ethanolic solutions. Crystal structures of obtained salts were determined by X-Ray diffraction and characterized by IR and Raman spectroscopy. Bandgaps (E_g) of the salts were established through the diffuse reflectance method and determined from electronic structures calculated based on crystal structures.

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