

ASYMMETRICAL TRIIODIDE ANION AS A PARTICIPANT OF THE HALOGEN BONDING IN CRYSTALS

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Objective view of chemical bond and noncovalent interactions features on the electronic level allows us to predict physico-chemical, thermal and thermodynamic properties of substances and to develop functional materials. Crystals of organic polyiodides are representatives of compounds with useful conductive and nonlinear optical properties. Polyiodide anion fragments in these crystals interact with each other *via* halogen bonds that usually act as structure-forming interactions defining overall crystal packing and practically important properties [1].

Symmetric and asymmetric triiodide-anions inside the crystal structures of polyiodides with organic cation have been chosen as the objects of the present study. Crystal structure optimization and wave functions have been obtained using the CRYSTAL14 [2]. We have explored the distribution of the anisotropy of the outer electron shells of iodine atoms as a part of triiodide-anion using a row of functions, including the Laplacian of electron density, the one-electron potential, the position uncertainty curvature [3] and the electronic pressure [4], calculated using TOPOND14 [5] and WinXPRO [6].

Analysis of the obtained data showed that the outer part of the valence shell of the central atom in triiodide anion is considerably flattened in comparison to terminal iodine atoms. Anisotropy of the properties of the valence shells is also manifested in the direction of the σ -hole and orthogonal to her.

References

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