Po2 - Revealing the Nature of Iodine Bond Diversity within the Triiodide Anions in Crystals

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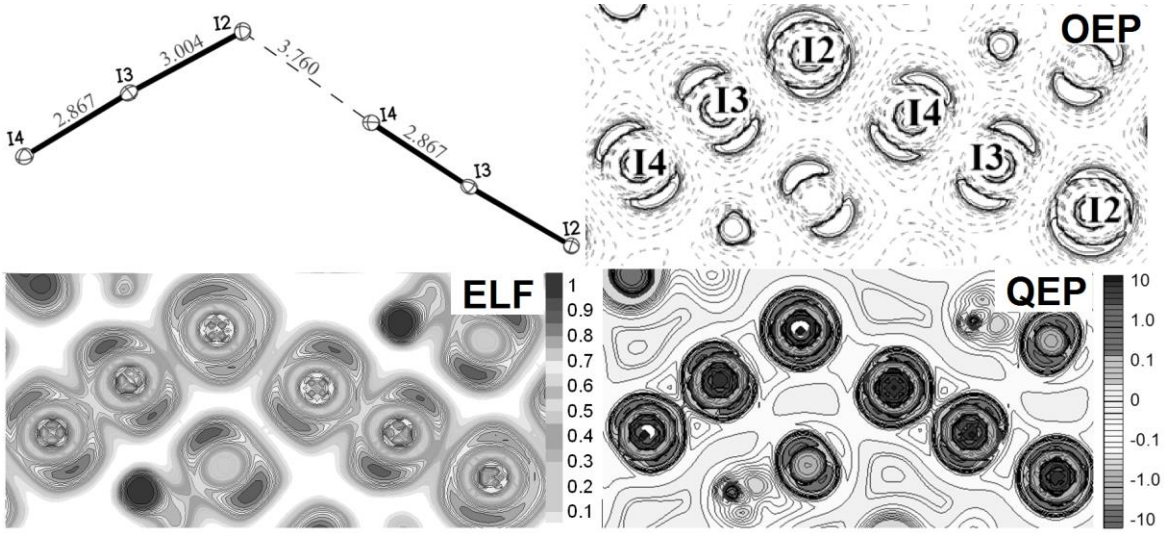
The diversity of iodine-iodine chemical bonds and non-covalent interactions in oligo- and polyiodides of organic compounds are the subjects of our interest. Challenges related with their classification are in focus our attention. Several considered polyiodides form the I…I bond in the chains of triiodide anions which are the intermediate between covalent and halogen bonds according to their lengths. Appropriate question is: what functions based on electron density features allow us to sort out the observed bonding diversity?



To answer this question we analyzed the ELF and one-electron potential (OEP). The spatial distribution of the quantum electronic pressure (QEP)[1], formed by elastic medium of electrons with included nuclei in a crystal was investigated as well. The function QEP, computed from electron density and its derivatives, shows the regions with resistance to its external compression of each elementary volume (QEP>0) and the regions with tendency to self-expanding (QEP<0). The former coincide with electron concentrations areas, while the later show the regions of electron depletion.

As Figure shown, OEP, ELF and quantum electronic pressure distributions reveal that the diiodine molecule is a part of the chain formally formed by triiodide anions[2] in one of considered crystals. Thus, the halogen binding differs from the typical bonds within a triiodide anion that commonly accepted. Thermal and spectral properties confirmed our theoretical predictions. The above functions allow to do the non-covalent interaction classification that would have been impossible if only geometrical characteristics had used. The work was supported by RFBR, grants 16-03-00057a and 14-03-00961.

References

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