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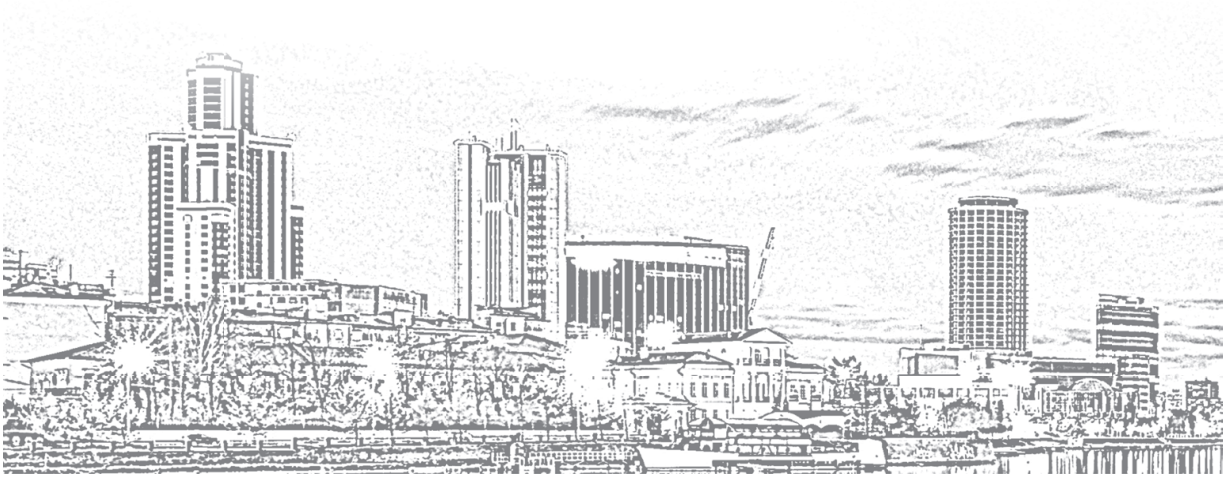

QUANTITATIVE TRENDS IN THERMAL AND SPECTRAL PROPERTIES FOR ORGANIC POLYIODIDES CONTAINING I_2

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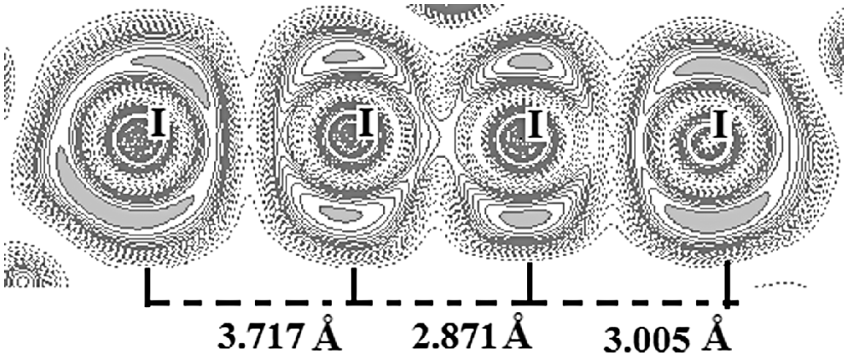
Polyiodides with bound I_2 find application as iodophors and components of dye-sensitized solar cells. Predicting of practically important properties of polyiodides is still a topic of interest, though the most popular trend is structural approach based on the analysis of geometrical parameters of noncovalent interactions. However, the usage of this approach is limited in cases when the variety of iodides from I^- to complex polyiodides is treated consistently.

A row of crystals with organic cations, including asymmetric triiodides $I^-...I_2$, pentaiodides I_5^- and polyiodides of complex structure $I_3^-...I_2...I_3^-$ was studied with the help of Raman spectroscopy and thermal analysis techniques. In all cases the decomposition start temperature was below 130 °C and valence vibration of bound I_2 in Raman spectra was located within the range 140–180 cm^{-1}. These experimental parameters were used as the criteria of bound I_2 existence in polyiodide anions.



Our experimental data were enriched with quantum-chemical calculations with periodic boundary conditions (DFT/B3LYP method, basis sets DZVP, TZP and DZP-DKH in program packages CRYSTAL14 and TOPOND). Analysis of electron localization function (ELF) [3] was made in the studied crystals, the features of ELF redistribution in the region within polyiodide anions were found. It was shown that the wavenumbers for I–I valence vibration quantitatively correlate with local ELF values in the corresponding bond critical points. Consistent usage of experimental and theoretical methods can give a clue to predicting the influence of bound I_2 on physicochemical properties of polyiodides.

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