Categorizing of organic polyiodides according to theoretical and experimental Raman data

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Polyiodides I_n^{x-} are widely used in electronic devices, water disinfection and crystal engineering. Conducting, optical and bacteriostatic properties depend on the features of polyiodide-anions spacial organization and are closely connected with the processes of iodine adsorption, storage and release from the crystalline state. Raman spectroscopy is one of the most informative tools to analyze properties of I–I bonds and intermolecular interactions. Analysis of experimental and theoretic Raman spectra of oriented single crystal in this work is used to localize chains and layers of polyiodide-anions in bulk crystal as a preliminary step for further anisotropic measurements.

In this work we demonstrate the possibilities of experimental and theoretic Raman spectra in the understanding of intermolecular interactions with iodine participation, localization of polyiodide chains and layers in bulk crystals, identification of polyiodide subunits in anions of complex structure, observation of iodine loss processes [1].

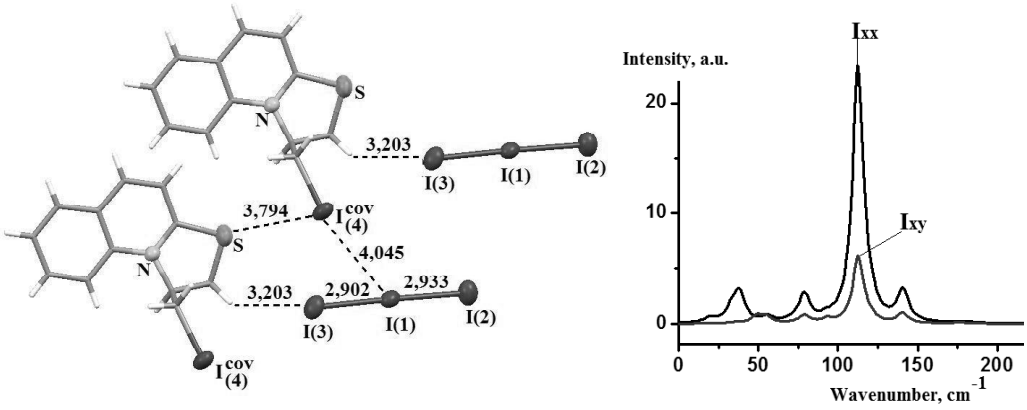

Figure 1. Fragment of crystal structure (left) and theoretic polarized spectra of thiazoloquinolinium triiodide I_3^- (right); agreement with experiment in the triiodide stretching vibration value is 3 cm^{-1}

Good agreement of obtained theoretical spectra in crystalline state (3D periodic Kohn-Sham calculations in Crystal14) allowed us to use these data to solve a row of cases concerning interpretation of nontypical experimental spectra [2], spectral properties of unstable under laser explosion polyiodides, comparison of theoretic spectra in specific directions with experimental polarized spectra, analyzing theoretic polarizability tensors. This work has been supported by the Ministry of Education and Science of the Russian Federation GZ 729.

References:

[1] Yushina I.D. *et al.* (2015) *New Journal of Chemistry* **39**, 6163.

[2] Bartashevich E.V. *et al.* (2016) *Acta Crystallographica C* **72**, 341.