

# CHALCOGENAZINOQUINOLINIUM MONOIODIDES: PHASE TRANSITION, SPECTRAL PROPERTIES AND NON-COVALENT BONDING

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## Abstract:

The study of phase transitions in organic crystals as a step to tunable modification of their physicochemical properties is in the center of modern crystal engineering approaches. Organic crystals with polyiodide anions and S,N-containing heterocycles, such as the substituted thiazolo(azino)quinolinium salts [1-3] open possibility for the design of wide row of nonlinear optical and semiconductor materials and serve as components of dye-sensitized solar cell devices. Variety of crystal structures, available for material engineering is due to their ability to form different types of non-covalent interactions with iodine participation. The methodology of the present work includes consistent analysis of X-Ray diffraction and Raman spectroscopy data accompanied by the results of periodic quantum-chemical calculations in order to reveal the changes in crystal packing, non-covalent interactions feature and spectral properties as a result of undergoing phase transition under non-ambient conditions. In the center of the present work is the case of two newly obtained crystal structures of substituted thia- and oxazinoquinolinium iodides with the typical I...I halogen bonds. Substituted thiazinoquinolinium monoiodide undergoes low-temperature phase transition with decrease of symmetry from P21/c to P-1 registered by X-Ray diffraction and Raman spectroscopy. The interpretation of the observed changes in the Raman spectra is made on the basis of theoretic spectra in low wavenumber region. The work was supported by Ministry of Education and Science of the Russian Federation FENU-2020-0019.

1. Bartashevich E.V.; Yushina I.D.; Stash A.I.; Tsirelson V.G. *Crystal Growth & Design*, 2014, 14 (11), P. 5674-5684

2. Yushina I.D.; Kolesov B.A.; Bartashevich E.V. *New Journal of Chemistry*, 2015, 39 (8), P. 6163-6170

3. Yushina I.D., Tarasova N.M., Kim D.G., Sharutin V.V., Bartashevich E.V. *Crystals*, 2019, 9, P. 506.

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