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Thiazoloquinolinium iodides according to Raman spectroscopy data

I.D. Yushina[1], E.V. Bartashevich[2], D.G. Pikhulya[3,4]

[1]SEC "Nanotechnology" South Ural State University, 454080, Lenin Avenue, 76, Chelyabinsk, Russia
iushinaid@susu.ac.ru
[2]Organic chemistry Department, Chemical faculty, South Ural State University
[3]Nonlinear optics laboratory, Institute of Electrophysics UD RAS
[4]Optics and Spectroscopy Department, Physical faculty, South Ural State University

Polyiodides I_n^{x-} are widely used in nanostructured materials and their intra- and intermolecular interactions with anion participation are of practical and fundamental interest. Raman spectroscopy is one of the most informative methods in order to obtain data concerning I–I bond properties and features of I…I noncovalent interactions including halogen bonds [1].

The goal of this work is to reveal the changes in experimental wavenumbers of anion vibrations that occur during surface aging in single crystals of thiazoloquinolinium iodides. Experimental spectra were exited by a laser beam with wavelength equal to 632.8 nm and registered by NT-MDT Ntegra Spectra equipment. The results of experimental study can be seen in Table. Theoretical spectrum was obtained in solid state approach using 3D periodic Kohn-Sham calculations in Crystal14 program package.

Table 1. Experimental wavenumbers of anion vibrations in crystals of thiazoloquinolinium iodides (the most intense bands are shown in bold)

I_3^-	$I_3^-…I_2…I_3^-$	Aged surface of $I_3^-…I_2…I_3^-$
113 υ_{sym} I_3^-, 137 υ_{asym} I_3^-	108, 122, **165** υ I_2	**113** υ_{sym} I_3^-, 138 υ_{asym} I_3^-

Aging of single crystal surface is observed for $I_3^-…I_2…I_3^-$ polyiodide, it is expressed in the change of color from almost black to brownish and in the absence of metal glow. Experimental Raman spectra show that aging of surface of $I_3^-…I_2…I_3^-$ polyiodide is accompanied by the disappearance of band corresponding to a bound molecular iodine vibration near 165 cm^{-1}. Observed bands for υ_{sym} I_3^- and υ_{asym} I_3^- are close to those for crystalline triiodide [2].

Theoretic Raman spectra were obtained for thiazoloquinolinium triiodide. Results of quantum-chemical calculations are in good agreement with experiment: 1 cm^{-1} for symmetric vibration and 3 cm^{-1} for asymmetric one.

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