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Triiodide-anion in allilurotropiniya crystal: noncovalent interaction and spectral characteristics

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Abstract

A new crystalline structure of allilurotropiniya triiodide $C_9H_{17}N_4^+I_3^-$. Was synthesized and verified by X-ray analysis. Raman spectral characteristics of mono-crystal were investigated both in unpolarized light, and with different relative orientation of the axes of the crystal polarization vector of the incident and scattered light. There have been calculated vibrational modes, active in Raman spectra using the crystalline approximation, periodic boundary conditions and localized atomic basis sets. According to quantum-topological analysis of the electron density (QTAIM) non-covalent interactions involving iodine atoms in the crystal structure are characterized in the studied crystalline structure.