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Quantum-chemical study of the molecular structure and vibrational spectra of methyl nitrate and ethyl nitrate

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Abstract

The data presented theoretical analysis of the vibrational spectra of methyl nitrate, *trans* - and *gauche* - conformations of ethyl nitrate obtained using the methods of the density functional theory *(B3LYP/6-31G(d)*). Installed most energetically favorable structure of methyl nitrate and ethyl nitrate calculated corresponding to these structures, frequencies and forms of normal vibrations. Identified spectral features conformational state of methyl-, ethyl nitrate, and the effects of the formation of intramolecular hydrogen bonds.