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Computation of vibration spectra of 4-nitro-benzofuroxan in coordinates X_{δ}^{0}

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Abstract

Within the framework of approach B3LYP 6-311++G(3df,3pd) the force field of 4-nitro-benzofuroxan molecule in coordinates X_{δ}^{0} for the first time is received. Frequencies of normal vibrations were calculated. Generalized force constants of molecule was carried out.