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Computation of vibrational spectra of furoxane and dimethylfuroxane molecules in coordinates X_{δ}^{0} with an estimation of a force fields in frameworks DFT

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Abstract

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