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# Computation of vibrational spectra of 4-methylfuroxane and 3-methylfuroxane molecules in coordinates $X_\delta^0$ 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 field of 4-methylfuroxane and 3-methylfuroxane molecules in coordinates $X_\delta^0$ for the first time is received. Frequencies of normal vibrations were calculated. Comparison of the received generalized force constants with those of molecule was carried out.

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