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The generalized force constants of NF_3 and ONF_3 molecules in $X_\delta^{\ 0}$ coordinates

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Abstract

Within the framework of the approach B3LYP6-311++G(3df,3pd) the force field of NF $_3$ and ONF $_3$ molecules in coordinates $X_\delta^{\ 0}$ for the first time is obtained. Frequencies of normal vibrations were calculated. Comparison of the obtained generalized force constants with those of molecules was carried out.