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Quantum chemical study of the molecular structure and vibrational spectra of methyl nitrite

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Abstract

The vibration spectra and structure of the *cis* and *trans* conformers of methyl nitrite have been studied by *ab initio* MO method and methods of density functional theory *(B3LYP, MP2, MP3, G2)* using *6-31G(d)* and *6-311++G(df,p)* basis sets. The most suitable quantum chemical method is determined by statistical analysis of experimental and calculated vibration spectra. Spectral characteristics of the intermolecular hydrogen bonds formation of the *cis* and *trans* conformers of methyl nitrite have been established.