

N-propyl nitrate vibrational spectrum analysis using DFT B3LYP quantum-chemical method

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Abstract

© Published under licence by IOP Publishing Ltd. Calculation of a molecular structure, conformation and related vibrational spectra of the n-propyl nitrate C₃H₇NO₃ was carried out by means of density functional theory (DFT) by employing the Gaussian 03 package. The molecular geometries were fully optimized by using the Becke's three-parameter hybrid exchange functional combined with the Lee-Yang-Parr correlation functional (B3LYP) and using the 6-31G(d) basis set. By scanning the dihedral angles around C-O and C-C bonds, five energetically most favorable conformers of n-propyl nitrate - TG, TT, GT, GG and GG forms were found. Vibrational spectra of the most energetically favorable conformers were calculated. The comparative analysis of calculated and experimental spectra is carried out, the spectral features of the conformational state of n-propyl nitrate and the spectral effects of formation of intramolecular hydrogen bonds are established.

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