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Matrix-isolation FT-IR and theoretical investigation of the competitive intramolecular hydrogen bonding in 5-methyl-3-nitro-2-hydroxyacetophenone.

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Streszczenie

The paper presents the conformational, vibrational and hydrogen bond characteristics of 5-methyl-3-nitro-2-hydroxyacetophenone studied with the combined matrix-isolation FT-IR spectroscopic and theoretical (DFT/B3LYP/6-31++G**) technique. Theoretical calculations predict three stable conformations of the studied compound. Only two of these conformations could be identified experimentally using the matrix-isolation FT-IR technique. The conformation with the intramolecular hydrogen bond OH···ON has been found to be more stable than the conformation with the OH···OC type of hydrogen bond by 7.28 kJ/mol. The complete assignment of the experimental spectra could be performed based on the theoretical calculations including the normal coordinate analysis and isotopic substitution.

Słowa kluczowe

Ortho-hydroxyacetophenone, Intramolecular H-bonding, Matrix-isolation FT-IR spectroscopy, DFT calculations

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