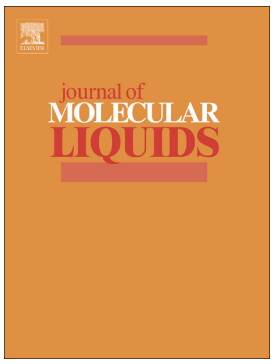

The structure of water – Acetamide hydrogen bonded complexes. Quantum chemical analysis

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The structure of water – acetamide hydrogen bonded complexes. Quantum chemical analysis.

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Abstract: The structure of acetamide dimers and hydrogen-bonded complexes of acetamide with water molecules (1-4 molecules in the complex) have been studied by quantum chemical method on the base of density functional theory (DFT) approximation using hybrid Becke, three-parameter, Lee-Yang-Parr (B3LYP) functional and gradient-corrected correlation functional of Perdew, Burke and Ernzerhof (PBE), D3 version of Grimme dispersion correction and augmented correlation-consistent polarized valence-only triple-zeta (aug-CC-pVTZ) basis set. The geometrical parameters of hydrogen bonds, binding energies, vibrational bands have been calculated and the Natural Bond Orbital (NBO), quantum theory of atoms in molecules (QTAIM) analyses have been carried out.

Keywords:

Water, Acetamide, DFT, H-bond, NBO, QTAIM

Introduction

Acetamide is on of the most simple molecules among of amides series, which might serve as a mimetic of a protein interface. The molecular structure of acetamide has been studied by X-ray and gas phase electronic diffraction methods at room temperature[1,2] and T=108 K[3,4].

The results of *ab-initio* calculations of acetamide structure, torsional potential of CH_3 groups have been presented in a number of publications[3,5,6]. A comparison of the molecular structure obtained from *ab-initio* calculations with experimental data has also been done earlier[7], and the refined crystal structure was determined.