Accepted Manuscript

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

M.A. Krestyaninov, E.G. Odintsova, A.M. Kolker, M.G. Kiselev

PII: S0167-7322(17)36137-8

DOI: doi:10.1016/j.molliq.2018.05.070

Reference: MOLLIQ 9125

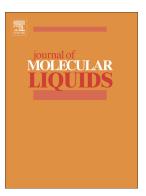
To appear in: Journal of Molecular Liquids

Received date: 22 December 2017

Revised date: 15 May 2018 Accepted date: 16 May 2018

Please cite this article as: M.A. Krestyaninov, E.G. Odintsova, A.M. Kolker, M.G. Kiselev, The structure of water – Acetamide hydrogen bonded complexes. Quantum chemical analysis. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2018.05.070

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



ACCEPTED MANUSCRIPT

The structure of water – acetamide hydrogen bonded complexes.

Quantum chemical analysis.

Krestyaninov M.A., Odintsova E. G., Kolker A.M. and Kiselev M.G.

G.A. Krestov Institute of Solution Chemistry of the RAS,

153045, 1, Academicheskaya st., Ivanovo, Russian Federation

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 $T=108~\rm K^{3,4}$.

The results of *ab-initio* calculations of acetamide structure, torsional potential of CH₃ 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 earlier⁷, and the refined crystal structure was determined.

Download English Version:

https://daneshyari.com/en/article/7842145

Download Persian Version:

https://daneshyari.com/article/7842145

<u>Daneshyari.com</u>