Structure of water-N-methylacetamide, -N,N-dimethylacetamide complexes. Quantum chemical analysis.

Mikhail Krestyaninov[1], Ekaterina Odintsova[1], Mikhail Kiselev[2], and Arkadiy Kolker[1]

[1]G A Krestov Institute of Solution Chemistry Russian Academy of Sciences
[2]Institute of solution chemistry

May 5, 2020

Abstract

The structure of N-methylacetamide and N,N-dimethylacetamide dimers and hydrogen-bonded complexes of N-methylacetamide and N,N-dimethylacetamide with water molecules (1-3 molecules in the complex) has been studied by the quantum chemical method based on the 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.

Hosted file

`W-NMA,DMA_2018-3-eng-rev.doc` available at https://authorea.com/users/297519/articles/426682-structure-of-water-n-methylacetamide-n-n-dimethylacetamide-complexes-quantum-chemical-analysis