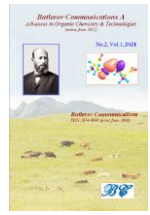
BUTLEROV HERITAGE

Butlerov Communications A
Advances in Organic Chemistry & Technologies
ISSN 2074-0948 (print)

2021. Vol.1, No.2, Id.17.
Journal Homepage: https://a-journal.butlerov.com/



Thematic section: Theoretical Study.
Subsection: Quantum Chemistry.

Full Paper

The Reference Object Identifier – ROI-jbc-A/21-1-2-17
The Digital Object Identifier – DOI: 10.37952/ROI-jbc-A/21-1-2-17
Received 6 June 2021; Accepted 8 June 2021

Hydrogen bonds in molecular crystalsserine: Morokuma method and NBO analysis

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Keywords: amino acids, serine, hydrogen bonding, intermolecular interaction, modeling, Mokoruma method, NBO analysis.

Abstract

Quantum-chemical modeling by the Morokuma methods (HF/6-31G (PC GAMESS)) and the DFT/B97D/6-31++G** method (Gaussian 03) was carried out, as well as the study of the nature and energy characteristics of hydrogen bonds (H-bonds) N–H···O and O–H···O in molecular crystals of serine. The calculation of the interaction energy and its decomposition using the Morokuma method allowed us to estimate its components such as electrostatic, exchange repulsion, polarization, charge transfer, and mixing. It is shown that the main contribution to the interaction energy is provided by the electrostatic component. According to their energy characteristics, the eight H-bonds are divided into three different types – N–H···O and one O–H···O. In the framework of the NBO analysis, the stabilization energies of the formed hydrogen bond and the value of the transferred charge are calculated. It is shown that in serine dimers, the main factor affecting the H-bond stabilization energy is the geometric parameters and, above all, ∠(N–N···O). It is established that the binding σ-orbital of the hydrogen bond is the result of the interaction of the hybrid NBO of the lone electron pairs the oxygen atom and the loosening σ*-NBO of the N−H bond. It was found that the nature of the formation of bonds in all three cases is the same. According to the strength of the H-bond, it can be correlated as follows: in the first it is average, in the other two it is weak. The NBO results show that of the two unequal hydrogen bonds present in the second dimer formed by one H atom (according to X-ray diffraction analysis), only one is realized. This is indicated by the amount of charge transfer. The H-bonds between the hydroxo groups formed by the interaction of the hybrid NBO of the unshared pair of the oxygen atom and the loosening σ*-NBO O–H bond are weak.

For citation: Tatiana G. Volkova, Irina O. Talanova, Iroda M. kizi Abdukhalimova. Hydrogen bonds in molecular crystalsserine: Morokuma method and NBO analysis. *Butlerov Communications A*. **2021**. Vol.1. No.2. Id.17. DOI: 10.37952/ROI-jbc-A/21-1-2-17.

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