QUANTUM-CHEMICAL ANALYSIS OF SOME PHYSICOCHEMICAL PROPERTIES OF AURINTRICARBONIC ACID AND ACETAMIDES DURING THE SYNTHESIS OF A COMPLEX COMPOUND WITH A MIXED LIGAND

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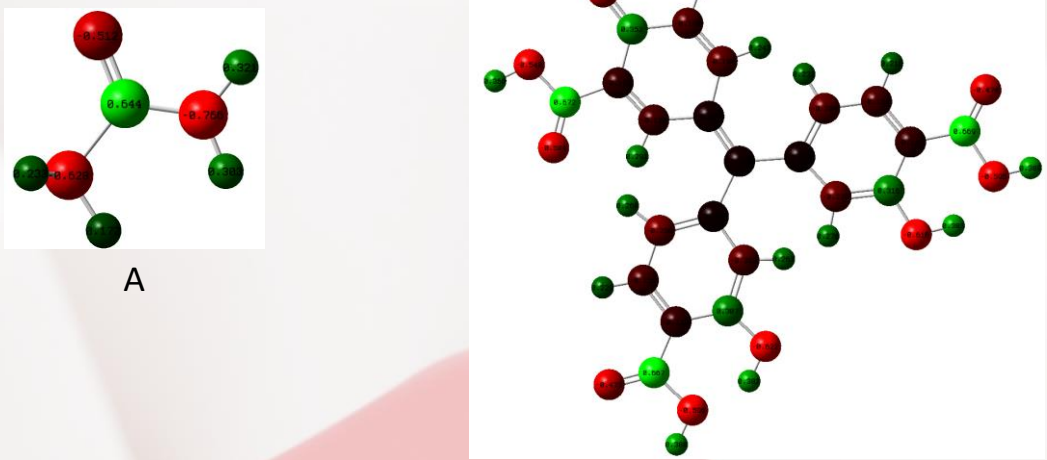
Abstract
This paper presents a quantum chemical analysis of some physicochemical properties of aurintricarbonic acid and acetamide. The purpose of the work is to carry out the synthesis of complex compounds on the basis of the theoretically obtained information and to study the physical and chemical properties of the synthesized complex compounds.

Keywords:aurintricarbonic acid, acetamide, electronic orbitals, electron densities and effective charges.

As a result of the high ability of ligands containing carbonyl groups to form coordination compounds, various complex compounds were synthesized and their composition and properties were studied. If O and N-containing ligands, including amides, are included in compounds with such characteristics, it is of theoretical and practical importance to study how they form a complex compound together. Because the reactivity of ethanolamines is high, it exhibits both amine and alcohol properties. As a result of their different denaturation properties, complex compounds with mixed ligands can be synthesized.



A b

Figure 1. Optimized electronic structure of ligands and distribution of Mulliken charges: acetamide (a), aurintricarbonic acid (b)

Aurintricarbonic acid and amidesVarious physico-chemical properties were analyzed quantum-chemically using Gaussian 09 software package. Calculations were performed using the B3LYP method within the DFT theory. HyperChem, GausView programs were used to create and visualize model systems [1-3].

The system was optimized at the initial stage of theoretical research. At the next stage, basic calculations were carried out. In fig.1 the optimized electronic structure of the ligands and the Mulliken charge distribution are described [4-6].

Also, within the framework of quantum-chemical calculations, the free state of the ligand molecule (NOMO[1]) and excited-state (LUMO) electronic orbital states were investigated. The results of the calculations are presented in Fig. 2.

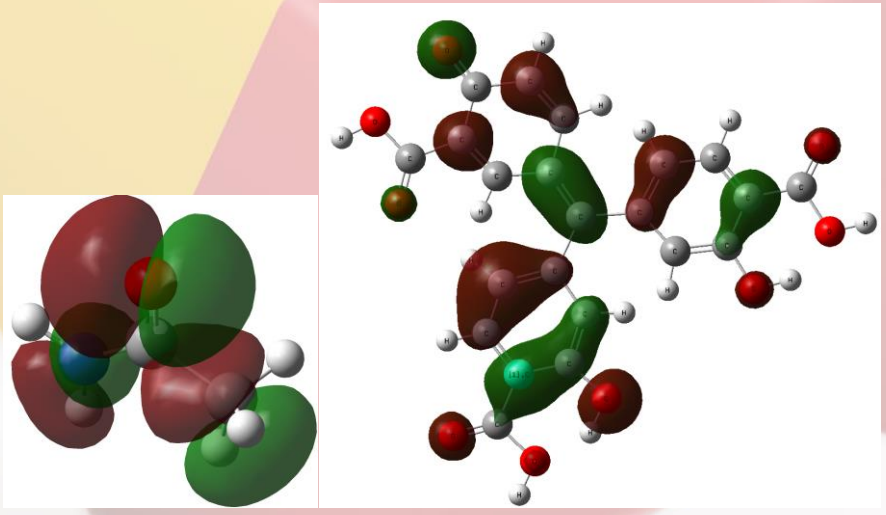


Figure 2. The position of electronic orbitals in the free state and in the excited state of the acetamide and aurintricarboxylic acid molecules

[1]HOMO - High occupied molecular orbital, LUMO - Low unoccupied molecular orbital

Calculations show that the energy difference between the free state (NOMO) and the excited state (LUMO) is 2.232 eV in acetamide and 3.199 eV in aurintricarbonic acid.

The surface represented by the electrostatic potential of the ligand molecules was calculated using DFT / B3LYP / 6–311 G (d, p) {C, H, N, O} / Lanl2DZ at 0.02 isovalue and 0.004 density values.

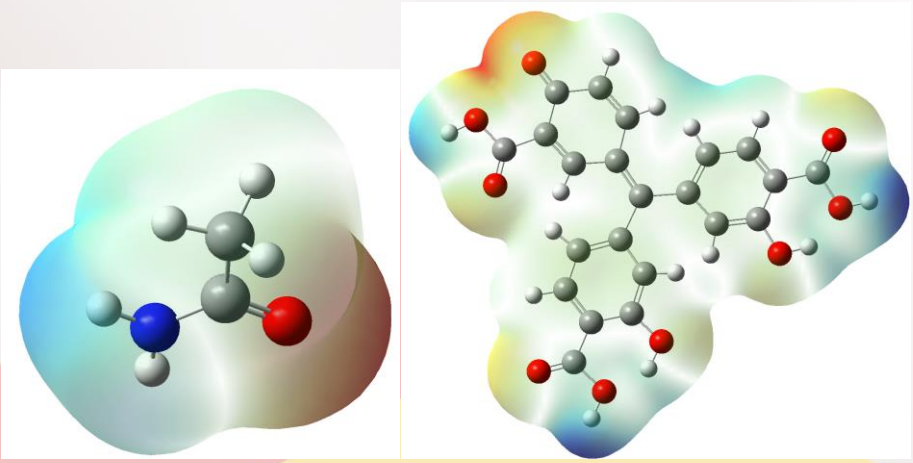


Figure 3. Acetamide and aurintricarboxylic acid geometric structure and MEP distribution of molecules

The MEP (molecular electrostatic potential) plots in red and blue are the negative and positive electrostatic potentials, respectively. In the color scheme of the MEP graph, the red area indicates atoms with an unshared electron pair or a negative electrostatic potential; the intensity of the color is proportional to the absolute value of the potential energy [7-8]. Positive electrostatic potentials are shown in the blue/yellow areas and characterize the polar hydrogen in the E–N bonds. The green areas cover the parts of the molecule with electrostatic potentials close to zero (C – C, C – N).

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