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STUDYING THE STRUCTURE AND ELECTRONS OF PIRACETAM MONOSULFATE BY QUANTUM CHEMICAL METHOD

Amrilloev Akbar Azamat o`g`li
Teacher of the Department of General Sciences of Asia International University

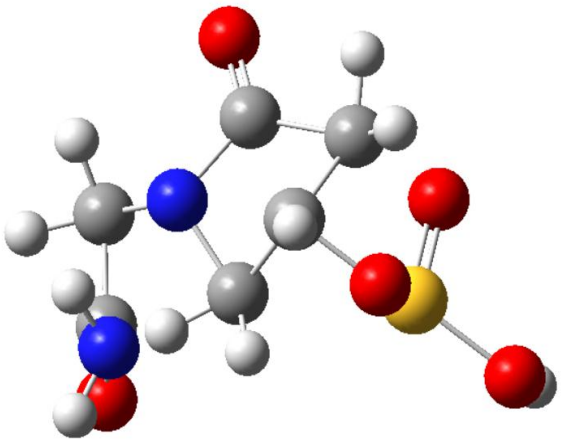
Abstract: This article describes the properties of piracetam derivatives, as well as the study of their compounds by physical methods.

Key words: infrared spectrum, coordination sphere, electron paramagnetic resonance spectroscopy.

Entroduction

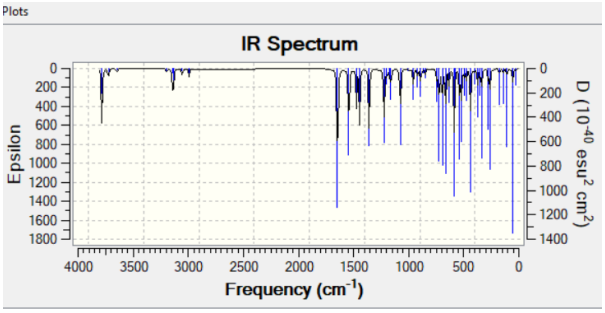
Today, the head of state pays great attention to the production of chemical industry products and their introduction into the sectors of the economy in our Republic. In the action strategy of the development of the Republic of Uzbekistan, "further modernization and diversification of the industry by transferring high-tech processing industries to a qualitatively new stage aimed at the rapid development of production of high-added-value finished products based on deep processing of local raw materials to do", "mastering fundamentally new types of products and technologies" and "further strengthening of the country's food security, expanding the production of ecologically clean products" are defined as important tasks.

The effect of power on the body is on them. When adjusting the pK of a beneficial substance to the body, various compounds are introduced and what kind of substances are formed as a result of their metabolism in the body.



Pic.1. Prepared in Gauss View program of Sulfopiracetam substance.

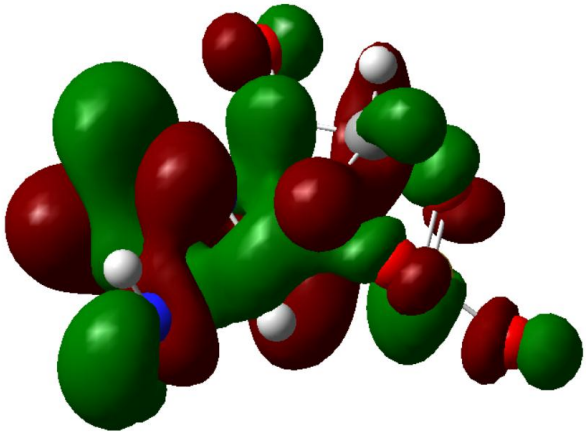
From the chemical structure, we can see that the sulfo group is located in the ring.



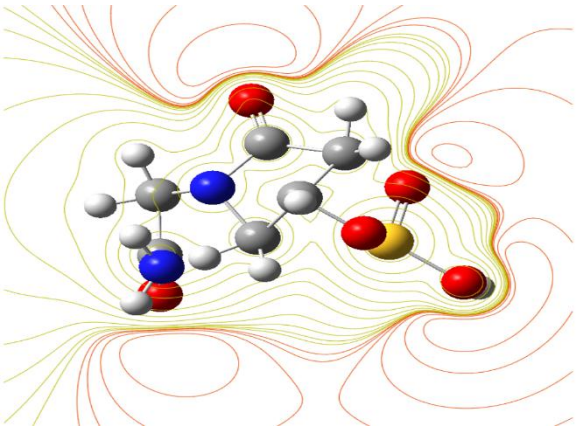
We can see the infrared spectrum of the substance, in the range of 1500-3000 cm-1 there are lines with high intensity indicating the bonds between sulfur and oxygen. Also, there were no lines indicating the formation of hydrogen bonds in the molecule.

The HOMO and LUMO states of the electrons of the substance are given.

The binding electrons in the green part are the free electrons in the red state. Most of the bonding electrons are located in the ring and are collected near the nitrogen atoms in it.



The state of the substance in the magnetic field lines of force is shown in the following calculations.



Also, it can be seen that the magnetic lines of force are denser on the side of atoms where oxygens are located in the calculation results. We can see that the oxygens in the sulfo group have a strong effect in the magnetic field.

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