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QUANTUM CHEMICAL CALCULATIONS AND ELECTRON NATURE OF DRUG SUBSTANCES

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Abstract: This article describes the study of various substances with the help of computer programs. Work was carried out to determine the changes in the phenomenon of tautomerism occurring in such a molecule.

Key words: drugs, piracetam, ketone, enol, tautomerism, HOMO, LUMO, infrared spectroscopy, comparison.

Introduction

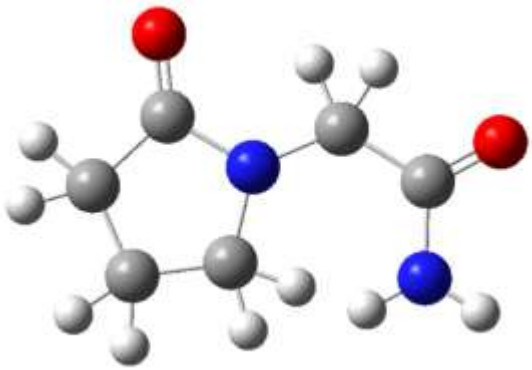
Quantum chemical calculations and biological activity calculations in the synthesis of drugs and determination of their biological activity are made easier by the Online Pass program.

The biological activity of newly synthesized substances and the functional groups showing this activity are thoroughly studied using the online pass program.

The substance piracetam contained in the drug piracetam was studied using quantum chemical programs.

The substance was modeled in the Gaussian 09 program and calculated using the RB3LYP calculation method and the 6-311G Basis set.

Piracetam molecule. Pic. 1



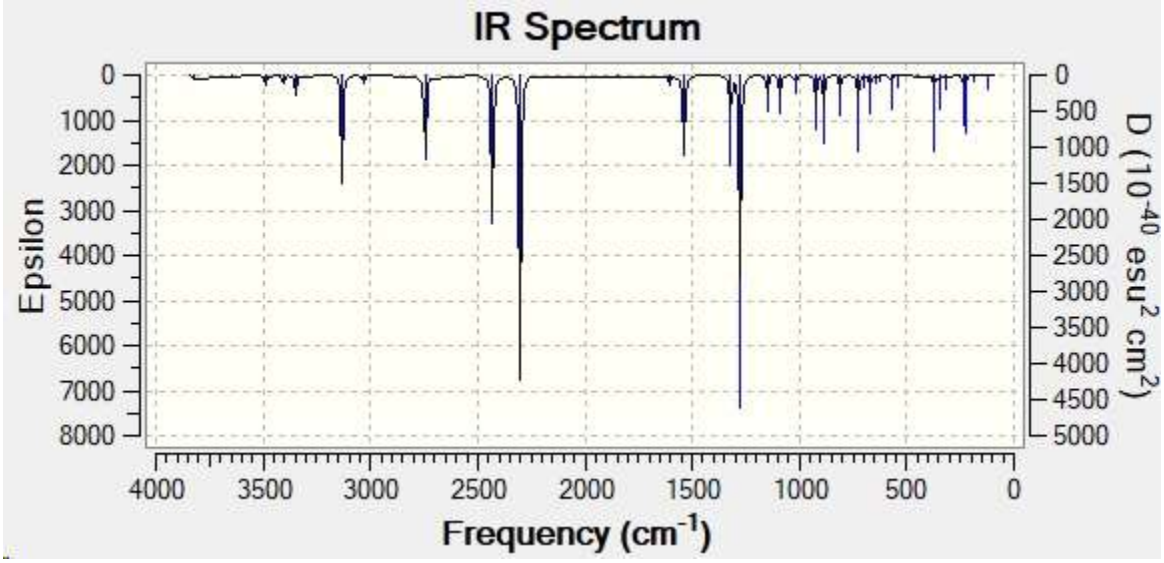
Calculation Type	FREQ	
Calculation Method	RB3LYP	
Basis Set	6-311G	
Charge	0	
Spin	Singlet	
Total Energy	-493.61749823	a.u.
RMS Gradient Norm	0.05264278	a.u.
Imaginary Freq	17	
Dipole Moment	7.6877	Debye
Point Group		

It was determined that the total energy in the molecule is -493.617 J and the dipole moment is 7.6877 debays.

Below we can see between which atoms the electron densities of the free and binding electrons of the molecule are.

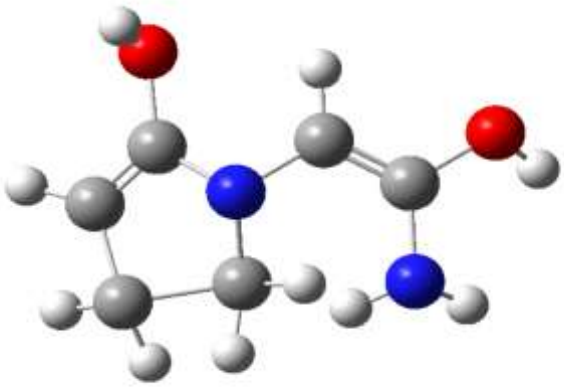
Between oxygen and nitrogen atoms, the density of binding electrons is high, and it can be observed that the density of free electrons is high in the carbons bound to these atoms.

Theoretically, the infrared spectrum of the molecule was obtained and analyzed, where we can see the vibrations of amine and keto groups.



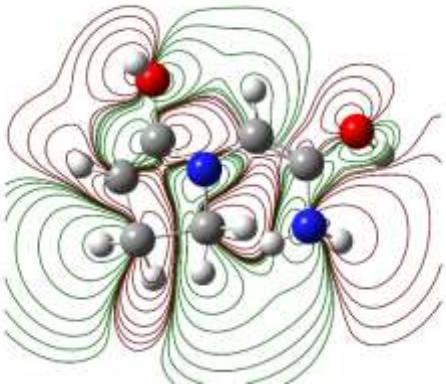
Absorption at 3820 cm-1 shown in this spectrum reflects deformational vibrations of hydrogen atoms bound to nitrogen in acid amide. Deformation vibrations of hydrogens attached to carbon in the 3400 - 3487-cm-1 ring are also reflected. Deformation vibrations of ketone groups correspond to 1535-1541 cm-1.

The following results were obtained when piracetam was studied in its enol state.

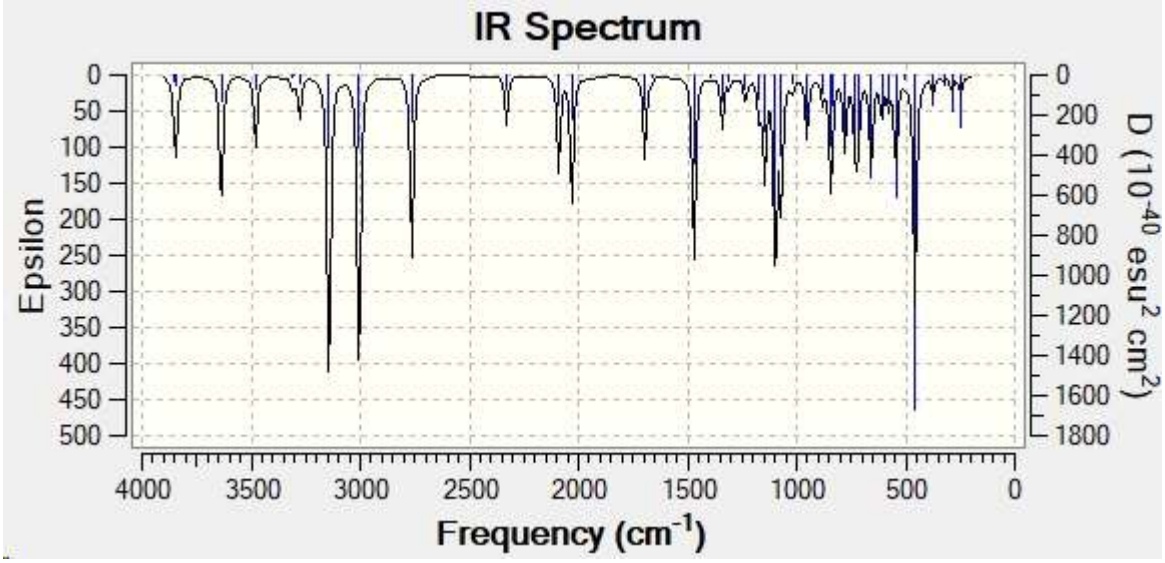


Total energy of the molecule: -493.88461246; and the dipole moment is: 1.7091 debay. At the same time, we considered it permissible to mention that the dipole moment in the enol state is reduced by 5 times compared to the ketone state. HOMO and LUMO states of binding and relaxing orbitals in the molecule are shown.

HOMO and LUMO of the enol form of piracetam. Pic. 3



We compare the results obtained in the infrared spectrum of the enol state of piracetam.



When we observe the absorption in the spectrum, we can see that new absorption lines appear. At 3843cm-1, the deformation vibration of the -OH group attached to the ring appeared. Vibrations of hydrogens in amide correspond to 3476-3637 cm-1. The absorption spectrum of the OH group, which is not in the ring, corresponds to 3851 cm-1, and these are newly formed vibrations.

In the enol state, various changes in the molecule and a change in reactivity were observed.

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