Quantum-Chemical Studies of Optical Properties of Pirydynsteryl

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Quantum mechanical simulation was performed using the software package Gaussian 09. Molecular optimization was performed using Hartree-Fock HF / 6-31G (d, p), DFT / B3LYP / 6-31G (d, p) methods. Characteristics of electronic transitions calculated by ZINDO / S and TD SCF methods.

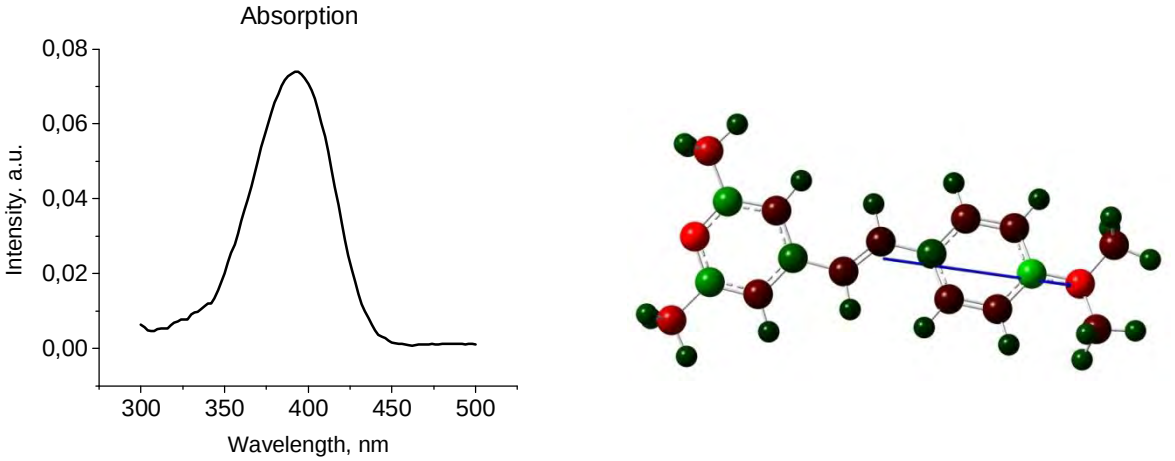

Fig.1. Optimized geometry of pirydynsteryl and calculated absorption spectrum. Perin charge distribution (red - negatively charged, green - positively charged particles). The arrow shows the magnitude and direction of the dipole moment. Also on figure depicted in acetonitrile absorption spectra of the molecule pirydynsterylu.

Calculations show There is a peak in the vicinity of 328 nm and experimental 392 nm.

The magnitude of dipole moment equal to 5.22 Debye charge distribution is due, in particular, as a result of having two nitrogen atoms that have large negative charges -0.5 electronic units, compared with the carbon atoms.

The most negatively charged nitrogen atoms of the molecule can react with pirydynsteryl electron acceptor group other molecules and atoms with a deficit of electron density.

Explain the nature peaks can using quantum-chemical calculations of electronic transitions in the molecule pyridine. The most pronounced is the transition between HOMO and LUMO levels, this level has much more power oscillator. Ionization potential of the molecule that is responsible for transferring electrons to other compounds, calculated by AM1, HF and DFT is 8.26, 7.44 and 6.2 eV, respectively.