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QUANTUM-CHEMICAL CALCULATIONS OF NEW AZOMETHINE COMPOUNDS WITH ANTIOXIDANT ACTIVITY

M. Atroshko

Belarusian State University, ISEI BSU,
Minsk, the Republic of Belarus
atroshkomikhail@gmail.com

This publication represents theoretical calculations applied to newly synthetized azometine compounds to de-fine their optimized state, predicts its free energy, and distinguishes molecular orbitals that involved in spectrum for-mation.

Keywords: PM6, B3LYP, semi-empirical, theoretical calculations.

Materials and methods

For calculations we used a personal computer with an Intel core i7 processor (2.21 GHz CPU), with the installed Ubuntu 18.04 operating system. When calculating the starting geometry of the molecule with an azomethine base, we selected the method of molecular mechanics (MM+) of the HyperChem 08 software package. The choice of the MM+ method is justified by the fact that it has developed for organic molecules, takes into account potential fields generated by all atoms of the calculated system, and allows you to flexibly modify the calculation parameters depending on the specific task. Starting geometry of the molecule was additionally optimized in a solvent medium of N, N-dimethylformamide (DMF) using the semi-empirical PM6 method of the Gaussian 16 software package to achieve a global minimum of the total energy of the systems under study. To find the global energy minimum and the most stable conformers, we analyzed all the stationary points on the surface of the potential energy of the molecules.

Full optimization and calculation of the electronic structure was carried out by the non-empirical DFT / B3LYP method in the basis 6-311++G. This method is used to calculate optimized geometries, electronic absorption spectra, total energy and heat of formation and we used to calculate the electronic absorption spectrum of azomethine mole-cules. Electronic spectrum of the molecule 4-((Z)-((4-((E)-phenyldiazenyl)phenyl)imino)methyl)benzoic acid ($C_{20}H_{15}N_3O_2$) was calculated for 20 single-electron excitations in the region of 242.29 - 514.56 nm in the basis of 6-31G *.

The theoretical absorption spectrum of the optimized molecule in a solvent medium was calculated using the Gaussian 16 software package using the theory level RB3LYP / 6-311 ++ G. The average scaling factor of the program in calculating the UV spectra is 0.99 [1,2].

Results and discussion

Using the PM6 method we had found optimized geometric configurations.

The maximum wavelength with a high oscillator strength was observed at $\lambda = 479.15$ nm и f = 2.0107 (Table 1, Fig. 2,3). The calculation showed that the strongest electron transition is observed at an absorption maximum of 479.15 nm, which refers to the transition of an electron to an excited singlet state $S_0 \rightarrow S_2$. The remaining transitions have a small value of f and forbidden by symmetry.

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