QUANTUM-CHEMICAL CALCULATION OF THE N-(3,5-DI-TERT-BUTYL-2-HYDROXYPHENYL) METHANESULFONAMIDE COMPOUNDS WITH ANTIOXIDANT ACTIVITY

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ N-(3,5-ДИ-ТРЕТ-БУТИЛ-2-ГИДРОКСИФЕНИЛ) МЕТАНСУЛЬФОНАМИДА С АНТИОКСИДАНТНОЙ АКТИВНОСТЬЮ

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This publication presents theoretical calculations applied to N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide compounds to determine their optimized state, predict its free energy, and determine the molecular orbitals involved in spectrum formation.

В работе представлены теоретические расчеты соединения N-(3,5-ди-трет-бутил-2-гидроксифенил)метансульфонамида с целью определения его равновесной геометрии, полной энергии и видов молекулярных орбиталей, участвующих в формировании спектра поглощения.

Keywords: PM6, Molecular orbital, HOMO.

Ключевые слова: PM6, молекулярная орбиталь, ВЗМО.

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Preliminary quantum chemical modeling of the N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide molecule. For calculation, we used a personal computer with an Intel i5 processor (3.10 GHz CPU) with the Windows 10 operating system installed. When calculating the initial geometry of a molecule with a N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide base, the method of molecular mechanics (MM^{+}) of the ChemOffice 2020 software package was chosen. Calculation parameters depending on the specific problem. The starting geometry of the molecule was additionally optimized in the solvent medium of Water by the semi-empirical PM6 method of the Gaussian 09W software package until the global minimum of the total energy of the systems under study was reached. To find the global energy minimum and the most stable conformers, we analyzed all stationary points on the potential energy surface of molecules. The PM6 method is used to find optimized geometric configurations, the total energy of molecules, electronic properties, and the enthalpy of formation of substances [2]. The GaussView 6.0 program was used to visualize the results. The equilibrium geometry of the molecule by the PM6 semi-empirical method is shown in Figure 1.

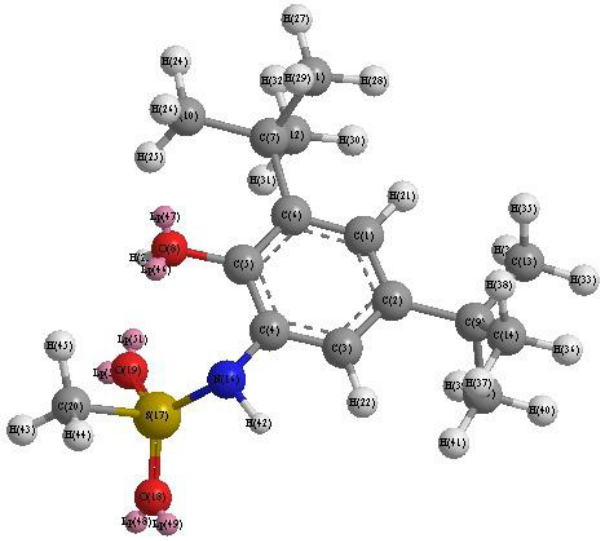


Figure 1 – Optimized structure of the title molecule by PM6 method

Complete Quantum Chemical Simulation of the Equilibrium Geometry and Electronic Structure of the N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide Molecule. Full optimization and calculation of the electronic structure were carried out by PM6 method [1,2]. This method is used to calculate optimized geometries, electronic absorption spectra, values of total energy and heat of formation, and we applied it to calculate the electronic absorption spectrum of molecules of new N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide. The UV/Vis spectrum of the molecule N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide is calculated for 10 single-electron excitations in the range of 493.62-228.60 nm. The results of the absorption spectrum calculation are given in the table.

The maximum wavelength with a high oscillator strength was observed at λ = 302.06 nm and f = 0.5154 (Table, Fig. 2.3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 302.06 nm, which refers to the transition of the electron to the excited singlet state S0→S5. The remaining transitions have a small value of f and are forbidden by symmetry.

The theoretical absorption spectrum of an optimized molecule in a solvent medium is calculated using the Gaussian 09W software package, using the PM6 method. The calculated electronic absorption spectrum of a molecule in a solvent medium is shown in Figure 2.

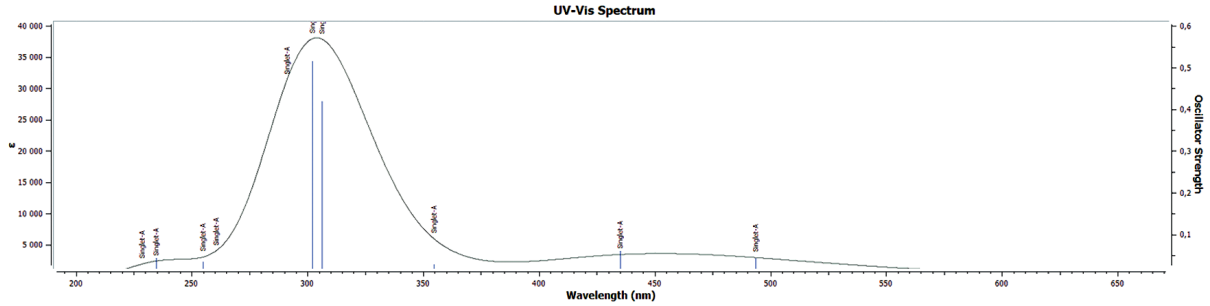
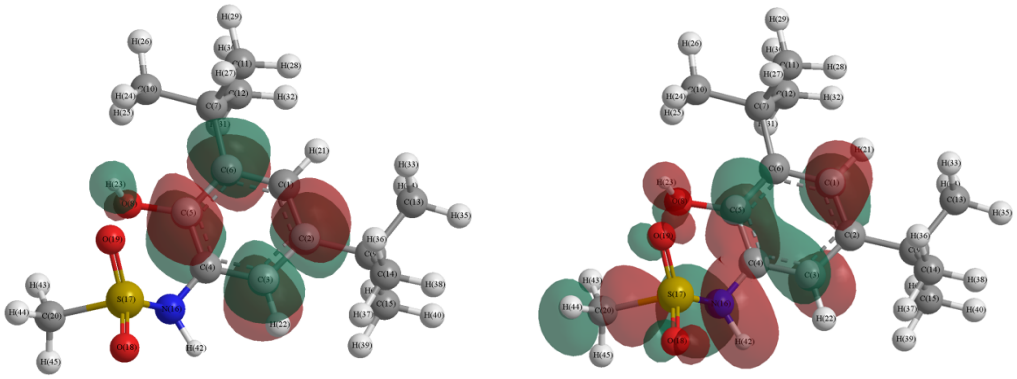


Figure 2 – Absorption spectrum of the title molecule

Table – Calculated electron absorption spectrum of the molecule

State	Wavelength (nm)	Transition energy (eV)	Decomposition of wave functions by a single excited configuration	Oscillator Strength (f)
$S_0 \rightarrow S_1$	493.62	2.5117	+0.10(55->62)+0.18(56->58)+0.26(56->59)+0.47(57->58) +0.29(57->59)+0.18(57->60)	0.0418
$S_0 \rightarrow S_2$	435.15	2.8493	-0.23(56->58)+0.11(56->59)+0.16(56->60)+0.34(57->58) +0.52(57->59)	0.0618
$S_0 \rightarrow S_3$	354.68	3.4957	+0.13(55->58)-0.11(55->60)-0.20(56->59) +0.25(57->58) -0.52(57->60)-0.10(57->61) +0.14(57->63)	0.0280
$S_0 \rightarrow S_4$	306.35	4.0472	+0.18(56->58)+0.53(56->59)-0.21(57->58) +0.15(57->59) -0.27(57->60)	0.4203
$S_0 \rightarrow S_5$	302.06	4.1046	+0.51(56->58) -0.20(56->59)+0.27(56->60)+0.31(57->59)	0.5154
$S_0 \rightarrow S_6$	291.15	4.2584	-0.16(56->61)+0.49(57->61)+0.29(57->63)-0.19(57->64)	0.0051
$S_0 \rightarrow S_7$	260.57	4.7581	-0.32(57->61)+0.11(57->63)-0.45(57->64) +0.18(57->69)+0.18(57->71)	0.0038
$S_0 \rightarrow S_8$	254.82	4.8656	+0.15(55->58)-0.19(55->59)+0.13(55->60) +0.5(57->62) -0.12(57->64)	0.0348
$S_0 \rightarrow S_9$	234.63	5.2842	+0.24 (55->58)+0.24 (55->59)+0.11 (56->58)-0.28 (56->60)+0.41 (56->62)	0.0442
$S_0 \rightarrow S_{10}$	228.60	5.4237	-0.10(51->60)+0.10(52->60)+0.10(55->58) +0.17(55->59)-0.18(56->58) +0.35(56->60)+0.12(56->61)+0.23(56->62)-0.16(56->63)-0.17(57->60)	0.0021



LUMO (N=58) [1.688 eV] HOMO (N=57) [-9.098 eV]

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of the molecule (A) at λ = 302.06 nm

Conclusion. This publication presents theoretical calculations applied to N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide compound to determine its optimized state, predict free energy and determine the molecular orbitals involved in formation of UV/Vis spectrum. Quantum-chemical calculations were carried out for N-(3,5-di-tert-butyl-2-hydroxyphenyl) methanesulfonamide compound with PM6 method in the water solvent. The geometrical optimized bond lengths and bond angles were calculated.

REFERENCES

1. *Sheikhi, M., Koroleva, E., Shahab, S., Ignatovich, Z., Atroshko, M., Drachilovskaya, M. Filippovich, L., Pak, A.* spectroscopic (IR, excited states, UV VIS, polarization) properties, synthesis and quantum chemical studies of new azomethine derivatives // journal "dyes and pigments".

2. *Mikulsky D., Eder K. and Molsky M*. (2014). Quantum chemical study of the relationship between the structure and antioxidant properties of hepatoprotective compounds found in Cynara scolymus and Silybum marianum. Journal of Theoretical and Computational Chemistry, 13(01), 1450004.

QUANTUM-CHEMICAL CALCULATION OF 2,4-DI-TERT-BUTYL-6-(P-TOLYLAMINO) PHENOL

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ 2,4-ДИ-ТРЕТ-БУТИЛ-6-(П-ТОЛИЛАМИНО)ФЕНОЛА

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This paper represents theoretical calculations applied to newly synthesized 2,4-di-tert-butyl-6-(p-tolylamino) phenol compounds for defining their optimized state predicting its free energy and distinguishing molecular orbitals participating in spectrum formation.

В данной статье представлены теоретические расчеты нового соединения 2,4-ди-трет-бутил-6-(п-толиламино)фенола для определения его равновесной геометрии, полной энергии и вида молекулярных орбиталей, участвующих в формировании спектра поглощения.

Keywords: computer chemistry, UV/Vis spectrum.

Ключевые слова: компьютерная химия, УФ спектр.

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Preliminary quantum chemical modeling of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol molecule. For calculations, we used a personal computer with an intel core i7 processor (2.21 GHz CPU) with the Ubuntu 18.04 operating system installed. For calculation of initial geometry of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol the method of molecular mechanics (MM+) of the Chem Office 2020 software package was chosen. The starting geometry of the molecule was additionally optimized in the solvent medium of Water by the semiempirical PM6 method of the Gaussian 16 software package until the global minimum of the total energy of the systems under study was reached. To find the global energy minimum and the most stable conformers, we analyzed all stationary points on the potential energy surface of molecules. The PM6 method is used to find optimized geometric configurations, the total energy of molecules, electronic properties, and the enthalpy of formation of substances [2]. The Gauss View 06 program was used to visualize the results. The equilibrium geometry of the molecule by the PM6 semiempirical method is shown in Figure 1

Complete Quantum Chemical Simulation of the Equilibrium Geometry and Electronic Structure of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol compounds Molecule. Full optimization and calculation of electronic structure of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol were carried out by PM6 method. This method is used to calculate the optimized geometries, electronic absorption spectra, total energy and heat of formation, and was used by