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.

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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

us to calculate the electronic absorption spectrum of new compounds molecules [1]. Electronic spectrum of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol is calculated for 10 excited states in the region 276.79-595.40nm. The results of calculation of the absorption spectrum are given in the table.

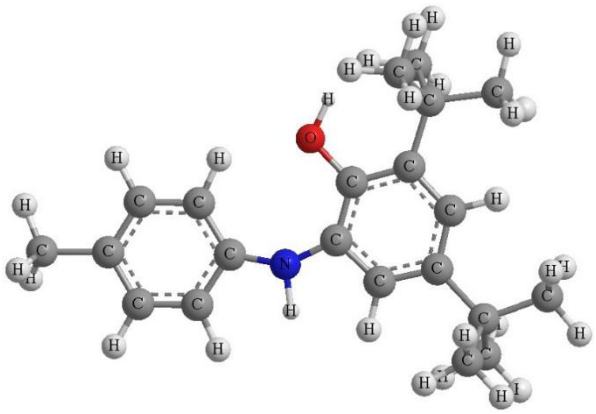


Figure 1 – Optimized molecule by PM6 method

The maximum wavelength with a high oscillator strength was observed at λ = 325.35 nm and f = 0.4911 (Table, Fig. 2, 3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 325.35 nm, which refers to the electron transition to the excited singlet state $S_0 \rightarrow S_6$. The remaining transitions have a small value of f and are forbidden by symmetry.

The theoretical absorption spectrum of the optimized molecule in a solvent medium was calculated using the Gaussian 16 software package by PM6 method. The calculated electronic absorption spectrum of a molecule in a solvent medium is shown in Figure 2.

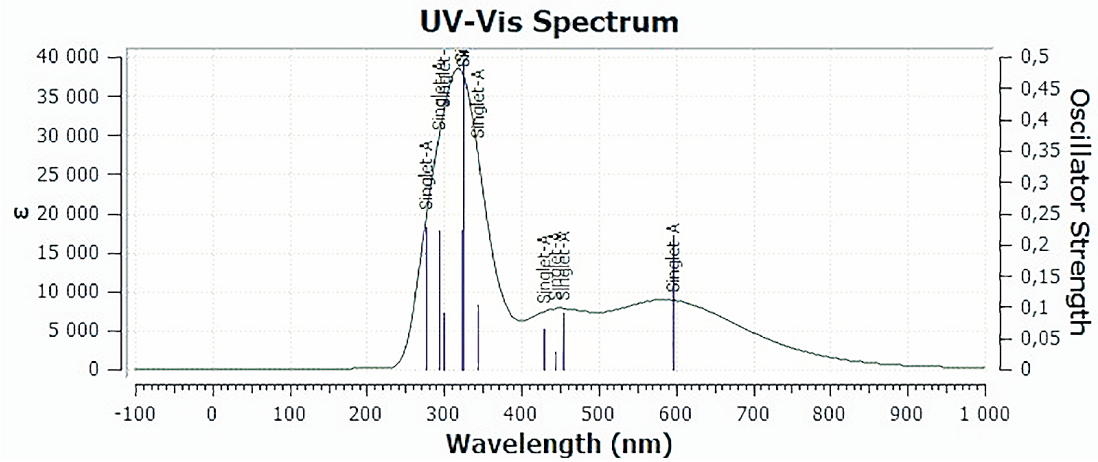
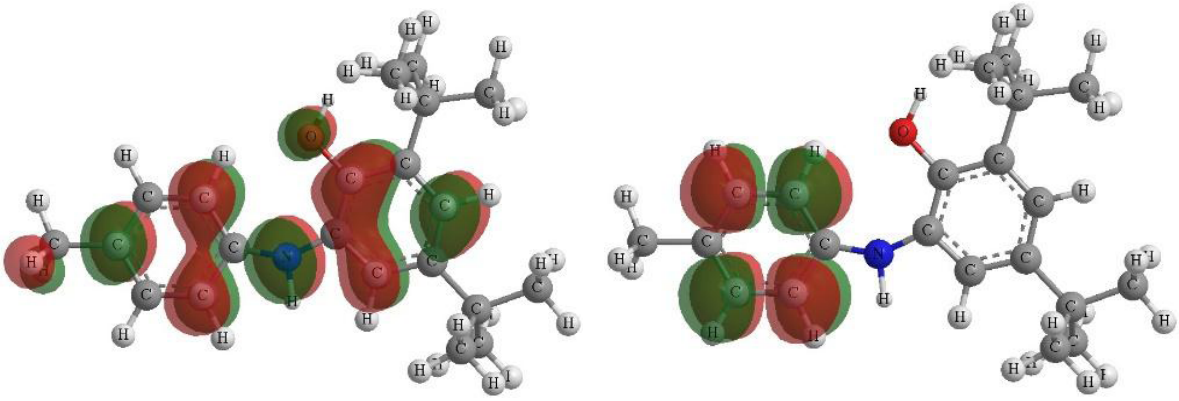


Figure 2 – Absorption spectrum of the title molecule



HOMO (N=62) [-8.544eV] LUMO (N=63) [0.430eV]

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of the title molecule (A) at λ = 325.35 nm

Table – Calculated electronic absorption spectrum of the title molecule (A)

Excited State	Wavelength (nm)	Excitation Energy(Ev)	Configurations Composition(corresponding transition orbitals)	Oscillator Strength (f)
$S_0 \rightarrow S_1$	595.40	2.0824	-0.11(60→64)-0.13(60→66)+0.19(61→66)+ 0.60(62→63)	0.2067
$S_0 \rightarrow S_2$	455.17	2.7239	0.22(60→63)+0.15(61→63)+0.27(61→64)- 0.17(61→65)+0.11(61→66)+0.13(62→63)+0.36(62→64)-0.32(62→65)- 0.13(62→66)	0.0905
$S_0 \rightarrow S_3$	443.41	2.7962	-0.15(59→64)-0.19(59→65)-0.14(60→63)- 0.10(60→64)+0.14(60→65)+0.12(60→66)+0.34(61→63)- 0.11(61→64)+0.22(62→64)+ 0.38(62 → 66)	0.0282
$S_0 \rightarrow S_4$	429.10	2.8894	0.15(59→63)-0.17(59→66)-0.15(60→64)- 0.15(60→65)+0.16(61→64)+0.25(61→65)-0.31(62→64)- 0.42(62→65)+0.12(62→66)	0.0656
$S_0 \rightarrow S_5$	342.66	3.6183	0.11(59→65)-0.19(60→64)+0.14(60→65)- 0.18(61→64)+0.12(61→65)+0.10(61→66)-0.14(62→63)+0.49(62→67)- 0.13(62→68)	0.1044
$S_0 \rightarrow S_6$	325.35	3.8108	-0.14(59→64)-0.20(59→65)-0.26(60→63)+ 0.11(60→64)-0.11(60→66)-0.26(61→63)+ 0.15(61→64)-0.14(61→65)-0.19(61→66)+ 0.17(62→63)+0.13(62→64)+0.27(62→67)	0.4911
$S_0 \rightarrow S_7$	322.72	3.8419	0.21(60→63)+0.22(60→64)-0.15(60→65)+ 0.11(60→66)+0.28(61→63)+0.12(61→64)- 0.20(62→64)+0.18(62→65)+0.22(62→67)-0.25(62→68)	0.2219
$S_0 \rightarrow S_8$	298.56	4.1528	-0.22(59→64)-0.27(59→65)+0.11(61→63)+ 0.10(61→68)+0.13(61→69)-0.37(62→66)+ 0.17(62→68)+0.18(62→69)+0.14(62→71)	0.0897
$S_0 \rightarrow S_9$	293.00	4.2316	0.15(59→64)+0.16(59→65)+0.12(60→64)+0.11(61→63)+0.12(61→67) +0.21(61→68)+0.17(61→69)+0.25(62→66)+0.15)62→67)+0.28(62→68)+0.20(62→69)+0.10(62→70)	0.2230
$S_0 \rightarrow S_{10}$	276.79	4.4793	-0.43(59→63)+0.43(59→66)-0.15(62→64)-0.21(62→65)	0.2285

Conclusion. Full optimization and calculation of electronic structure of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol were carried out by PM6 method. Electronic spectrum of the 2,4-di-tert-butyl-6-(p-tolylamino) phenol was calculated for 10 excited states in the region of 276.79-595.40 nm. The maximum wavelength 325.35 nm and high oscillator strength 0.4911 were calculated. The calculation showed that the strongest electron transition is observed at the absorption maximum of 325.35 nm which refers to the electron transition to the excited state $S_0 \rightarrow S_6$. The HOMO (N=62) energy is -8.544 eV. The LUMO (N=63) energy is 0.430 eV.

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