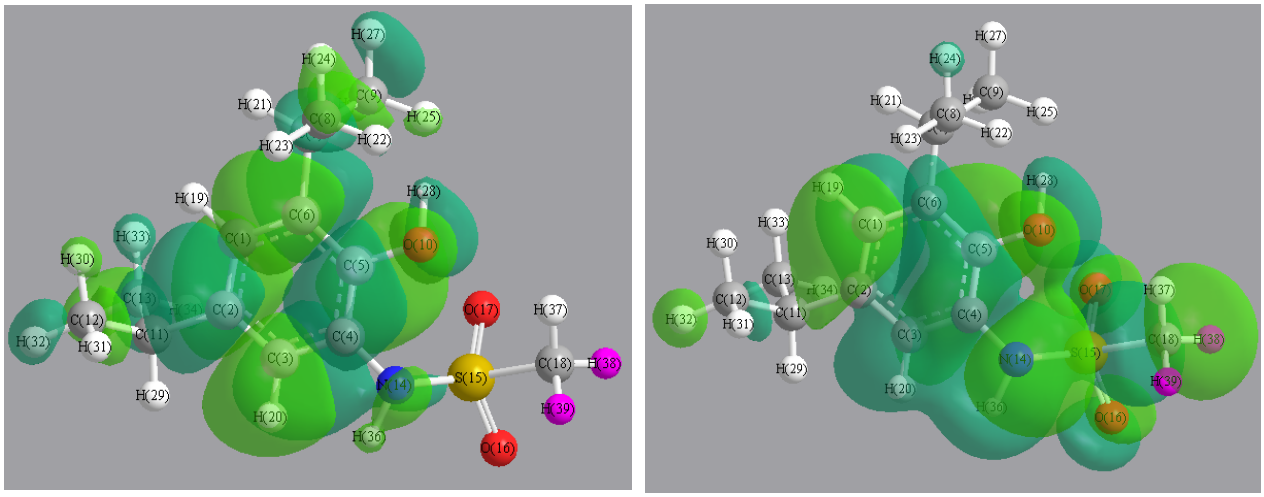

HOMO (N=54) [-10.723eV] LUMO (N=55) [23.810eV]

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of a molecule (A) at λ = 303.26 nm

Conclusion. We used a personal computer with an intel core i7 processor (CPU 2.21 GHz) with the Ubuntu 18.04 operating system installed. The molecule initial geometry with the base compound N-(2-hydroxy-3,5-diisopropylphenyl) methanesulfonamide was computed using the molecular mechanics (MM+) method of the Hyper Chem 08 software package. A maximum high oscillatory wavelength was observed at λ = 303.26 nm and f = 0.5239 (Table Figs. 2,3). The calculation showed that the strongest electronic transition is observed at the absorption maximum of 303.26 nm, which refers to the electronic transition to the excited singlet state $S_0 \rightarrow S_5$. Other transitions have a small value of f and are forbidden by symmetry.

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QUANTUM-CHEMICAL CALCULATION OF THE N-(3,5-NI-TERT-BUTYL-2-HYDROXYPHENYL)-4-METHYLBENZENESULFONAMIDE WITH ANTIOXIDANT ACTIVITY

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ N-(3,5-НИ-ТРЕТ-БУТИЛ-2-ГИДРОКСИФЕНИЛ)-4-МЕТИЛБЕНЗОЛСУЛЬФОНАМИДА С АНТИОКСИДАНТНОЙ АКТИВНОСТЬЮ

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This paper represents theoretical calculations applied to newly synthetized of N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide compounds for defining their optimized state, predicting its free energy, and distinguishing molecular orbitals participating in spectrum formation.

В данной статье представлены теоретические расчеты соединения N-(3,5-ди-трет-бутил-2-гидроксифенил)-4-метилбензолсульфонамида для определения его равновесного состояния, полной энергии и визуализации молекулярных орбиталей, участвующих в спектре поглощения.

Keywords: computer chemistry, PM6, UV/Vis spectrum.

Ключевые слова: компьютерная химия, PM6, УФ спектр.

https://doi.org/10.46646/SAKH-2022-2-383-385

Preliminary quantum chemical modeling of the N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide. 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. When calculating the initial geometry of a molecule with N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide base, the method of molecular mechanics (MM+) of the HyperChem 08 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 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.

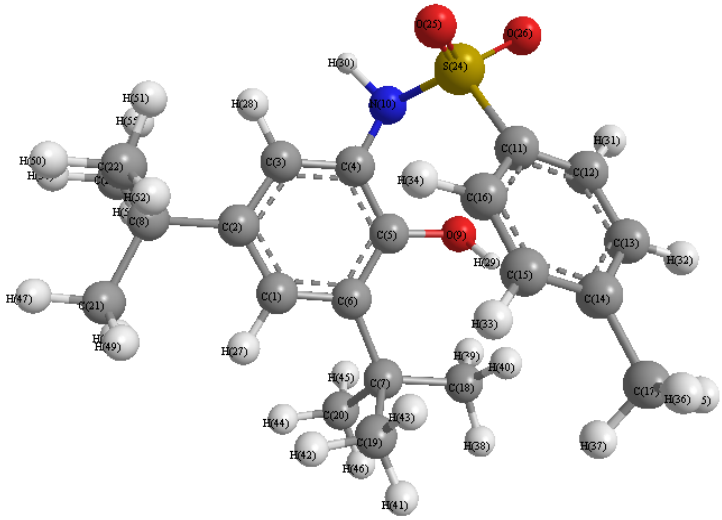

Figure 1 – Optimized molecule by PM6 method

Quantum Chemical Simulation of the Equilibrium Geometry and Electronic Structure of N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide Molecule. Full optimization and calculation of the electronic structure were carried out by the 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 the molecules. Electronic spectrum of the N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide molecule is calculated for 10 one-electron excitations in the region 275.99-501.97nm. The results of calculation of the absorption spectrum are given in the table.

The maximum wavelength with a high oscillator strength was observed at λ= 275.99 nm and f = 0.5795 (Table, Fig. 2, 3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 275.99 nm, which refers to the electron transition to the excited singlet state $S_0 \rightarrow S_{10}$. The remaining transitions have a small value of f and are forbidden by symmetry.

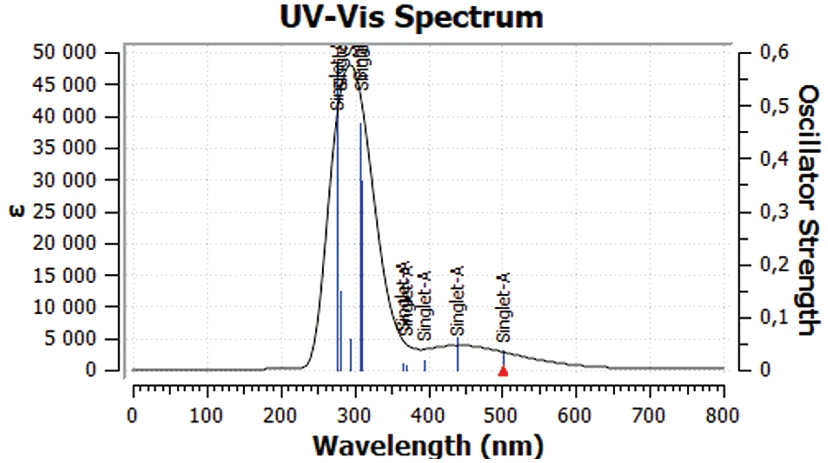

Figure 2 – Absorption spectrum of the title molecule

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

Excited State	Wavelength(nm)	Excitation Energy(eV)	Configurations Composition (corresponding transition orbitals)	***Oscillator Strength(f)***
S_0-S_1	501.97	2.4699	-0.14(70→73) -0.28024(0→75) +0.48(71→73) -0.22(71→75) +0.26(71→76)	0.0373
S_0-S_2	438.50	2.8274	+0.22(70→73)+0.19(70→76)+0.27(71→73) +0.57(71→75)	0.0609
S_0-S_3	394.57	3.1423	+0.12(68→72)+0.40(68→74) -0.50(69→72) +0.11(69→74)	0.0198
S_0-S_4	370.50	3.3464	+0.12(67→73) +0.16(70→75) -0.17(71→72) +0.27(71→73) -0.50(71→76) -0.14(71→80)	0.0090
S_0-S_5	365.48	3.3923	+0.55(68→72)+0.15(69→72)+0.39(69→74)	0.0128
S_0-S_6	309.61	4.0045	+0.56 (70→75)+0.20(71→73)+0.27 (71→76)	0.3578
S_0-S_7	307.15	4.0366	-0.49(70→73)-0.30(70→76)+0.30(71→75) -0.14(71→78)	0.4671
S_0-S_8	293.35	4.2265	+0.11(70→73)+0.13(70→76)-0.13(70→78) -0.45(71→78)-0.19(71→79)-0.25(71→80) +0.11(71→81) -0.21(71→82)	0.0577
S_0-S_9	279.78	4.4314	-0.26(68→74)-0.15(69→72)+0.58(71→72) +0.16(71→73)	0.1490
S_0-S_{10}	275.99	4.4924	-0.43(68→74)-0.40(69→72)-0.28(71→72)	0.5795

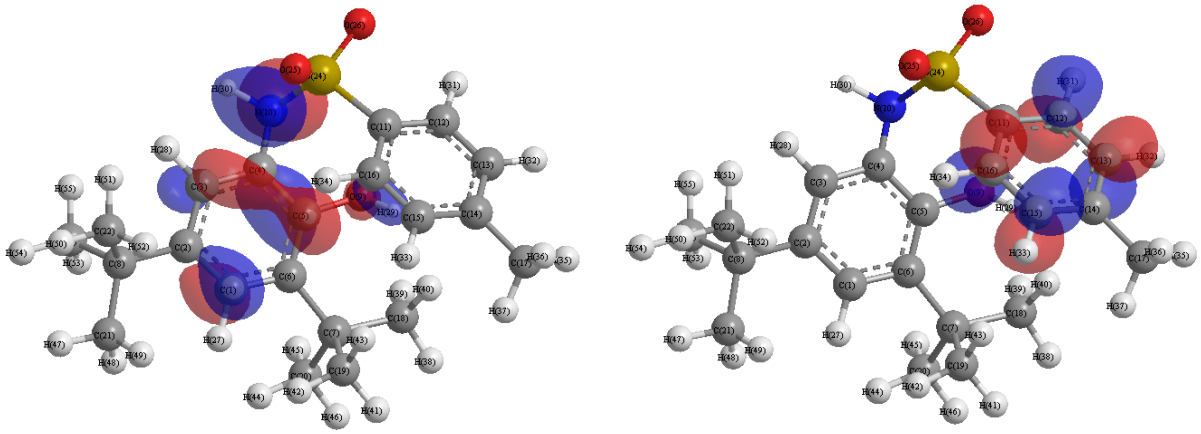

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of the title molecule (A) at λ= 275.99 nm

The theoretical absorption spectrum of the optimized molecule in a solvent medium was calculated using the Gaussian 16 software package by PM6. The calculated electronic absorption spectrum of a molecule in a solvent medium is shown in Figure 2 [1, 2].

Full optimization and calculation of the electronic structure of the N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide were carried out by the PM6 method. The calculated electronic absorption spectrum(UV/VIS) of the compound in solvent water was observed. Electronic spectrum of the N-(3,5-di-tert-butyl-2-hydroxyphenyl)-4-methylbenzenesulfonamide molecule was calculated for 10 one-electron excitations in the region 275.99-501.97 nm. The maximum wavelength with a high oscillator strength was observed at λ= 275.99 nm and f = 0.5795. The calculation showed that the strongest electron transition is observed at the absorption maximum of 275.99 nm which refers to the electron transition to the excited singlet state $S_0 \rightarrow S_{10}$. The HOMO (N=71) energy is -9.584 eV and the LUMO (N=72) energy is 0.363 eV.

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