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QUANTUM-CHEMICAL CALCULATION OF N-(3,5-di-tert-butyl-2-hydroxyphenyl) BENZENE SULFONAMIDE

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ N-(3,5-ди-трет-бутил-2-гидроксифенил) БЕНЗОЛСУЛЬФОНАМИДА

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This paper presents theoretical calculations related to N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide compound to determine its equilibrium geometry, total energy and calculation of molecular orbitals involved in formation of UV/Vis spectrum.

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

Keywords: Molecular orbital, PM3, UV/Vis spectrum.

Ключевые слова: Молекулярная орбиталь, PM3, УФ спектр.

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Preliminary quantum-chemical modeling of the N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide molecule. For calculation, we used a personal laptop with an Intel i7 processor (3.30 GHz CPU) with the Windows 10 operating system installed. We used ChemDraw 20.0 to build the 2D structure of the molecule shown in Figure 1. When calculating the initial geometry of a N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide molecule, the method of molecular mechanics (MM^+) of the ChemOffice 2020 software package was chosen. Calculation parameters depend on the specific task. The starting geometry of the molecule was additionally optimized in the solvent medium of H_2O (WATER) by the PM3 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 PM3 method is used to find optimized geometric configurations, the total energy of molecules, electronic properties, and the enthalpy of formation of substances [1].

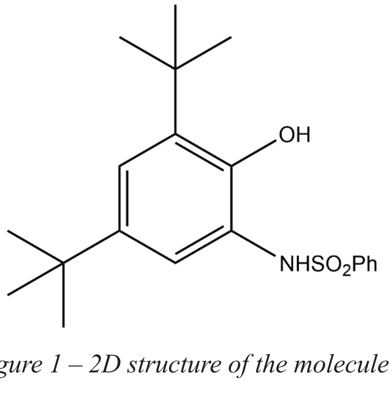


Figure 1 – 2D structure of the molecule

The GaussView 6.0 program was used to visualize the results. The equilibrium geometry of the molecule by the PM3 is shown in Figure 2.

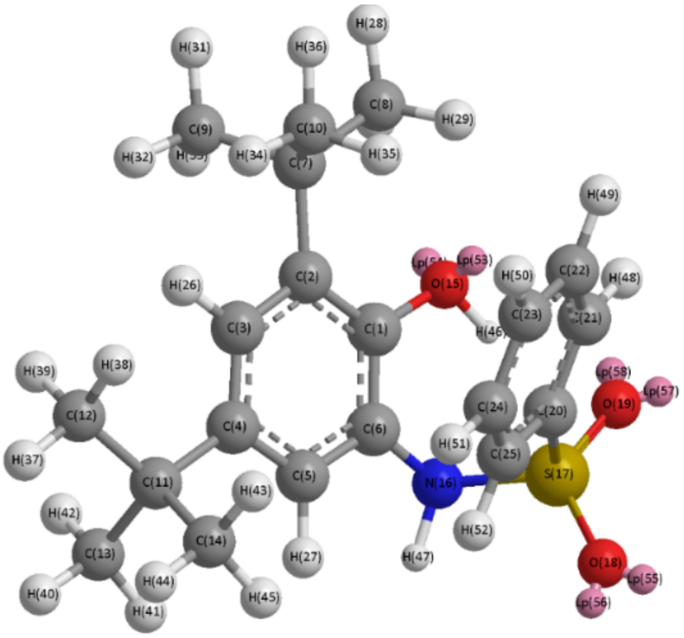


Figure 2 – Optimized molecule by PM3 method

Complete quantum-chemical simulation of the equilibrium geometry and electronic structure of the N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide molecule. Full optimization and calculation of the electronic structure were carried out by the PM3 method. This method is used to calculate optimized geometries, electronic absorption spectra, values of total energy and heat of formation [2]. We also applied it to calculate the electronic absorption spectrum of a molecule of N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide. The electronic spectrum of the molecule N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide (A) is calculated for 10 single-electron excitations in the range of 966.76 - 309.89 nm. The results of the absorption spectrum calculation are given in table 1.

Table 1 – Calculated electron absorption spectrum of the molecule (A)

Excited State	Wavelength (nm)	Transition energy (eV)	Decomposition of wave functions by a single excited configuration	Oscillator Strength (f)
$S_0 \rightarrow S_1$	966.76	1.2825	-0.21(64->69)+0.18(67->69)-0.60(68->69)+0.13(68->74)	0.0034
$S_0 \rightarrow S_2$	388.03	3.1952	-0.11(62->69)-0.22(67->73)-0.61(68->72)-0.12(68->73)	0.2140
$S_0 \rightarrow S_3$	371.72	3.3354	-0.27(67->72)-0.14(68->72)+0.59(68->73)	0.0498
$S_0 \rightarrow S_4$	338.00	3.6681	-0.17(58->69)+0.21(59->69)-0.13(60->69)+0.23(61->69)-0.14(62->69)-0.10(63->69)+0.13(64->69)-0.32(67->69)-0.18(68->69)	0.0158
$S_0 \rightarrow S_5$	335.55	3.6950	-0.21(58->69)-0.21(60->69)+0.13(61->69)-0.15(62->69)-0.15(64->69)+0.38(67->69)+0.19(68->69)	0.0687
$S_0 \rightarrow S_6$	332.48	3.7291	-0.41(59->69)-0.14(59->70)-0.10(59->75)+0.11(59->79)-0.12(60->69)-0.11(61->69)-0.23(62->69)-0.10(67->69)	0.0432
$S_0 \rightarrow S_7$	331.14	3.7442	-0.29(65->71)-0.36(66->69)+0.50(66->70)-0.12(66->74)	0.0585
$S_0 \rightarrow S_8$	322.54	3.8440	+0.34(58->69)+0.12(58->70)+0.10(58->75)+0.11(58->76)+0.13(61->69)-0.16(62->69)-0.10(62->76)-0.28(63->69)-0.11(63->76)	0.0589
$S_0 \rightarrow S_9$	311.86	3.9756	-0.10(55->69)-0.14(58->69)+0.13(59->76)+0.23(60->69)-0.23(61->69)-0.23(62->69)-0.10(63->69)-0.24(65->69)+0.10(66->71)+0.18(67->73)	0.2001
$S_0 \rightarrow S_{10}$	309.89	4.0010	-0.12(43->69)-0.15(60->69)+0.13(61->69)-0.50(65->69)+0.17(65->70)-0.17(65->74)+0.18(66->71)	0.0782

The maximum wavelength with a high oscillator strength was observed at λ = 388.03 nm and f = 0.214 (Table 1, Fig.3,4). The calculation showed that the strongest electron transition is observed at the absorption maximum of 388.03 nm, which refers to the transition of the electron to the excited state $S_0 \rightarrow S_2$. 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 PM3 method. The calculated electronic absorption spectrum of the title molecule in solvent medium water is shown in Figure 3.

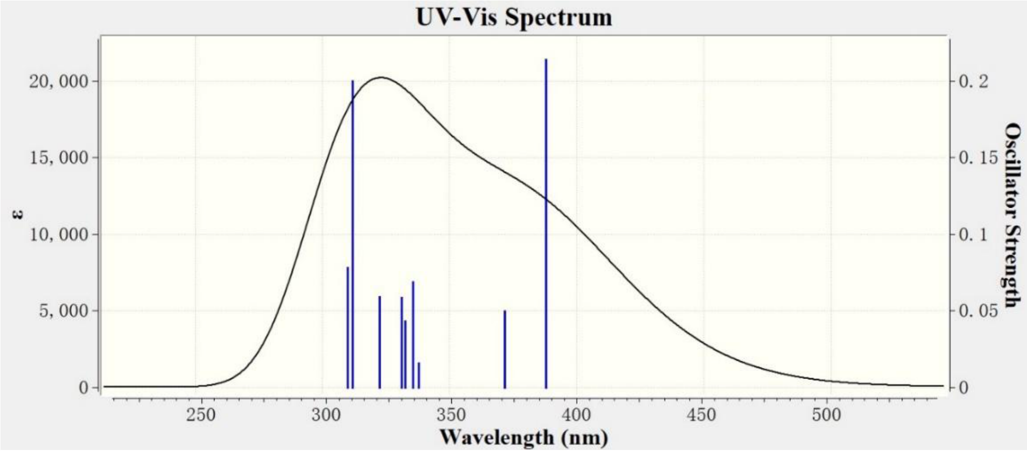
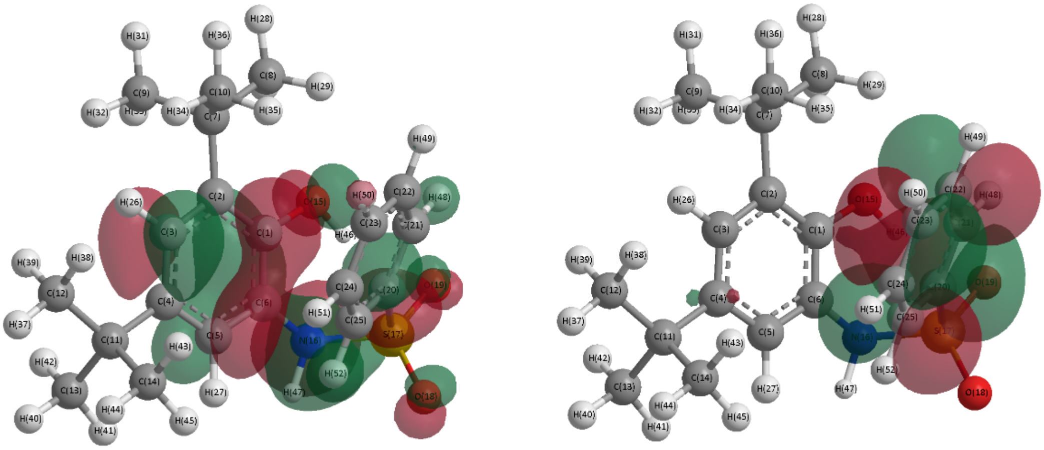


Figure 3 – UV-Vis spectrum of the compound in the solvent water



HOMO (N=68) [-8.857 eV] LUMO (N=69) [0.265 eV]

Figure 4 – Types of molecular orbitals involved in absorption spectrum formation of the molecule at λ = 388.03 nm

In this study, quantum-chemical calculations were carried out for N-(3,5-di-tert-butyl-2-hydroxyphenyl) benzene sulfonamide compound with PM3 method in the water solvent medium. The strongest electron transition is observed at the absorption maximum of 388.03 nm, which refers to the transition of the electron to the excited state $S_0 \rightarrow S_2$. Energy of HOMO (N=68) is -8.857 eV and the LUMO (N=69) is 0.265 eV.

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