

**QUANTUM-CHEMICAL CALCULATION  
OF THE N-(2-hydroxy-3,5-DIISOPROPYLPHENYL)METHANESULFONAMIDE  
КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ N-(2-ГИДРОКСИ-3,5-ДИИЗОПРОПИЛФЕНИЛ)  
МЕТАНСУЛЬФОАМИДНА**

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This paper presents theoretical calculations applied to N-(2-hydroxy-3,5-diisopropylphenyl)methanesulfonamide to determine its optimal free energy state and the shape of the molecular orbitals involved in the formation of the UV/Vis spectrum.

В данной работе представлены теоретические расчеты, примененные к N-(2-гидрокси-3,5-диизопропилфенил)метансульфонамиду для определения его оптимального состояния свободной энергии и формы молекулярных орбиталей, участвующих в формировании УФ/Вис спектра.

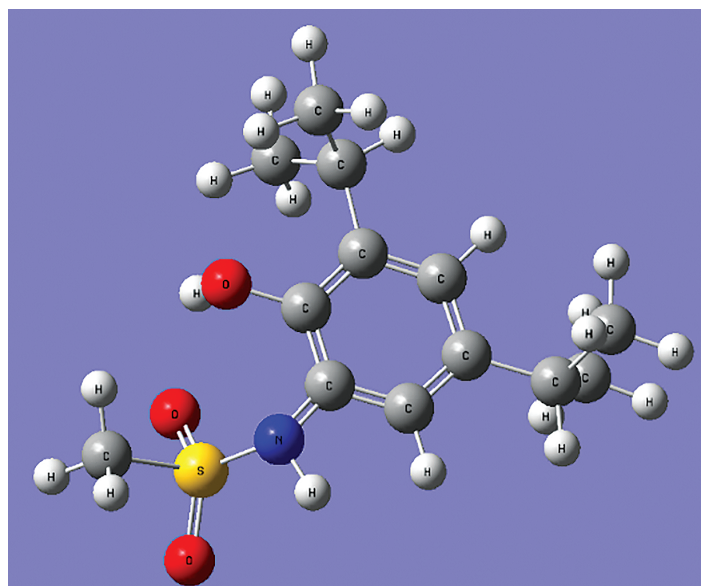
*Keywords:* computer chemistry, DFT, UV spectrum.

*Ключевые слова:* компьютерная химия, ДФТ, УФ спектр.

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**Preliminary quantum-chemical modeling of N-(2-hydroxy-3,5-diisopropylphenyl)methanesulfonamide.**

A personal computer with an intel core i7 processor (CPU 2.21 GHz) and Ubuntu 18.04 operating system was used for the calculations. The initial geometry of the N-(2-hydroxy-3,5-diisopropylphenyl)methanesulfonamide molecule was calculated using the molecular mechanics (MM+) method of Hyper Chem 17. The calculation parameters depend on the specific problem. In an aqueous solvent environment, the initial geometry of the molecules was optimized using the semiempirical PM6 method from the Gaussian 16 package until a global minimum of the total energy of the system under study was reached. All rest points of the molecular potential energy surface were analyzed to find the global energy minimum and the most stable conformer. The PM6 method was used to find the optimized geometric configuration, total energy of the molecule, electronic properties and enthalpy of formation of the substance [1]. The results were visualized using Gauss View 06 software. The molecular equilibrium geometries obtained by the semiempirical PM6 method are shown in Figure 1.



*Figure 1 – Optimized molecule by PM6 method*

**Optimized structure of N-(2-hydroxy-3,5-diisopropylphenyl)methanesulfonamide.** We performed conformational analysis for compounds 8 using the PM6 method. All quantum chemistry calculations were performed using the Gaussian 09 software package and the GaussView 05 visualization program on a Pentium IV/4.02 GHz personal computer. IEFPCM (Integral Equation Formalism PCM) combined with UAKS rays is the method that was used to calculate solvent (DMF) effects. The Integral Equation Formalism PCM, developed by Kance, Mennucci, and Thomas, is the most popular version of the PCM. It uses a molecular-shaped cavity consisting of spheres centered on nuclei, and the reaction field is modeled by placing charges on the surface of the cavity. It has been observed that the calculated parameters show a good approximation and can be used as a basis for calculating other parameters for the title compounds.

**Electronic Structure and Excited States of N-(2-hydroxy-3,5-diisopropylphenyl)methanesulfonamide.** The electronic spectrum of the N-(2-hydroxy-3,5-diisopropylphenyl) methanesulfonamide molecule was calculated for 10 one-electron excitations in the 228.72-493.83 nm region. The results of the calculation of the absorption spectrum are shown in the table. The maximum wavelength with high oscillatory strength was observed at  $\lambda = 303.26$  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  $S_4 \rightarrow S_5$ . Other 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 with the Gaussian 16 software package using the PM6 method. The average scaling factor of the program in calculating the UV spectra is 0.99. The calculated electronic absorption spectrum of the molecule in the solvent medium is shown in Figure 2.

Table 1

Estates	Wavelength (nm)	Excitation Energy(V)	Configurations Composition (corresponding transition orbitals)	Oscillator Strength(f)
$S_0-S_1$	493.83	2.5106	0.10884 (49->56)+0.19563(50->52)+0.25934(50->53)+ 0.47609(51->52)-0.30544(51->53)+0.18846(51->54)	0.0435
$S_1-S_2$	436.83	2.8383	-0.24160(50->52)+0.10935(50->53)-0.15681(50->54)+ 0.36790(51->52)-0.50905(51->53)	0.0659
$S_2-S_3$	352.78	3.5145	0.13734 (49->52)-0.11943(49->54)-0.20403(50->53)+ 0.24289(51->52)-0.53382(51->54)-0.11080(51->55)+0.14128(51->57)	0.0270
$S_3-S_4$	306.58	4.0442	0.28835 (50->52)+0.48804(50->53)-0.19296(51->52)+ 0.20867(51->53)-0.25232(51->54)	0.4025
$S_4-S_5$	303.26	4.0884	0.46773 (50->52)-0.30538(50->53)+0.26716(50->54)+ 0.28726(51->53)+0.11871(51->54)	0.5239
$S_5-S_6$	291.86	4.2481	0.16403(50->55)-0.49108(51->55)-0.30900(51->57)+ 0.20771(51->58)-0.12180(51->63)-0.10916(51->68)	0.0065
$S_6-S_7$	261.01	4.7502	-0.32446 (51->55)-0.12490(51->56)+0.10030(51->57)- 0.46225(51->58)+0.23391(51->63)-0.10634(51->66)	0.0045
$S_7-S_8$	255.42	4.8542	-0.15393 (49->52)+0.18889(49->53)-0.14583(49->54)- 0.57641(51->56)+0.14828(51->58)	0.0297
$S_8-S_9$	234.67	5.2833	0.27084 (49->52)+0.22823(49->53)+0.11139 (50->52)- 0.29890(50->54)+0.41239(50->56)+0.10088(51->54)	0.0410
$S_9-S_{10}$	228.72	5.4207	0.10682 (45->54)-0.10003(49->52)-0.18460(49->53)- 0.11412(49->54)+0.16277(50->52)-0.34018(50->54)-0.26637 (50->56)+0.15388(50->57)+0.13677(51->54)- 0.12155(51->64)-0.12507(51->66)	0.0036

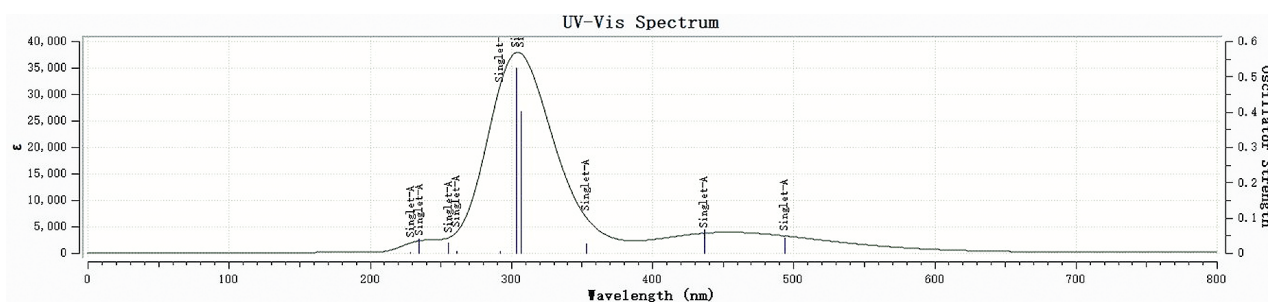
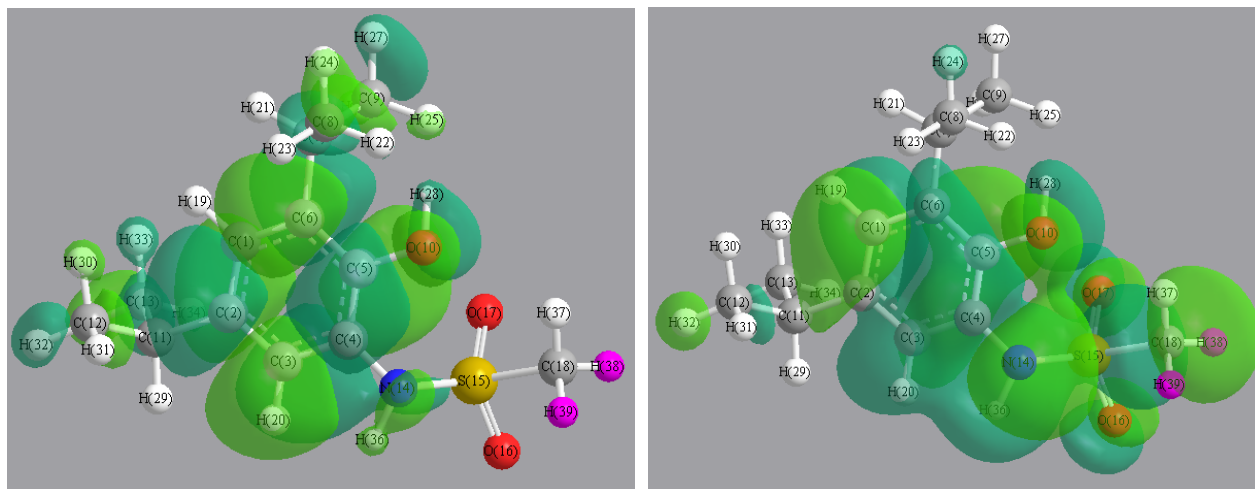


Figure 2 – Absorption spectrum of a molecule



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  $\lambda = 303.26$  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  $\lambda = 303.26$  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  $S_0 \rightarrow S_1$ . Other transitions have a small value of  $f$  and are forbidden by symmetry.

#### REFERENCES

1. Sheikhi, M., Shahab, S., Filippovich, L., Khaleghian, M., Dikumar, E., Mashayekhi, M. Interaction between new synthesized derivative of (E,E)-azomethines and BN(6,6-7) nanotube for medical applications: Geometry optimization, molecular structure, spectroscopic (NMR, UV/Vis, excited state), FMO, MEP and HOMO-LUMO investigations // Journal of Molecular Structure. – 2017. – No. 1146. – P. 881–888.

### QUANTUM-CHEMICAL CALCULATION OF THE N-(3,5-DI-TERT-BUTYL-2-HYDROXYPHENYL)-4-METHYLBENZENESULFONAMIDE WITH ANTIOXIDANT ACTIVITY КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ N-(3,5-ДИ-ТРЕТ-БУТИЛ-2-ГИДРОКСИФЕНИЛ)-4-МЕТИЛБЕНЗОЛСУЛЬФОНАМИДА С АНТИОКСИДАНТНОЙ АКТИВНОСТЬЮ

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This paper represents theoretical calculations applied to newly synthesized 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.