QUANTUM-CHEMICAL CALCULATION OF N-(5-(TERT-BUTY1)-2-HYDROXYPHENYL)METHANESULFONAMIDE WITH ANTIOXIDANT ACTIVITY

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ N-(5-(ТЕРТ-БУТИ1)-2-ГИДРОКСИФЕНИЛ) МЕТАНСУЛЬФОНАМИДА С АНТИОКСИДАНТНОЙ АКТИВНОСТЬЮ

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This paper represents theoretical calculations related to newly synthesized methanesulfonamide compounds for defining their optimized state, predicting its free energy, and distinguishing molecular orbitals participating in spectrum formation.

В этой статье представлены теоретические расчеты нового соединения метансульфонамида с целью определения его равновесной геометрии, свободной энергии и видов молекулярных орбиталей, участвующих в формировании спектра поглощения.

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

Ключевые слова: компьютерная химия, ДФТ, УФ спектр.

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Preliminary quantum chemical modeling of the N-(5-(tert-buty1)-2-hydroxyphenyl) methane sulfonamide molecule. For calculations, a personal computer with an intel core i7 processor (2.21 GHz CPU) with the Ubuntu 18.04 operating system installed was used. When calculating the starting geometry of a molecule with an azomethine base, the method of molecular mechanics (MM*) of the HyperChem 08 software package was chosen. The choice of the MM* method is justified by the fact that it was developed for organic molecules, takes into account the potential fields formed by all atoms of the calculated system, and allows flexible modification of the parameters calculation depending on the specific task. The starting geometry of the molecule was additionally optimized in the solvent medium of water (H_2O) by the semi-empirical PM6 method of the Gaussian 16 software package until the global minimum of the total energy of the studied systems 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]. To visualize the results, the Gauss View 06 program was used. The equilibrium geometry of the molecule by the semi-empirical method PM6 is shown in Figure 1.

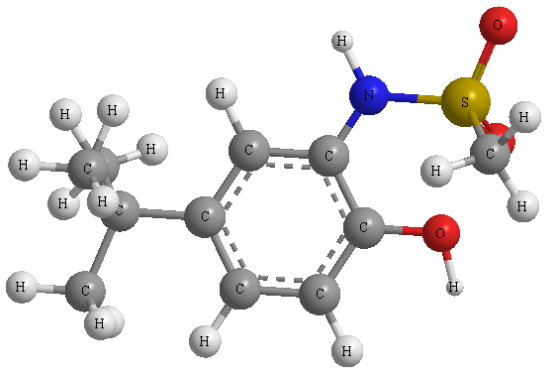


Figure 1 – Optimized molecule for PM6 method

Complete quantum chemical modeling of the equilibrium geometry and electronic structure of the azomethine molecule. Full optimization and calculation of the electronic structure were carried out by the PM6 method. This method is used to calculate optimized geometries, electronic absorption spectra, values of the total energy and heat of formation, and we have applied it to calculate the electronic absorption spectrum of new azomethine molecules. The electronic spectrum of the molecule the N-(5-(tert-buty1)-2-hydroxyphenyl)methanesulfonamide (A) was calculated for 20 one-electron excitations in the region of 228.46-499.99 nm. The results of calculation of the absorption spectrum are given in the table.

The maximum wavelength with high oscillator strength was observed at 298.78 nm and f = 0.5411 (Table, Fig. 2.3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 298.78 nm, which refers to the electron transition 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 the optimized molecule in the solvent medium was calculated using the Gaussian 16 software package using the PM6 methods. The average scaling factor of the program when calculating UV spectrum is 0.99. The calculated electronic absorption spectrum of a molecule in a solvent medium is shown in Figure 2 [1,2].

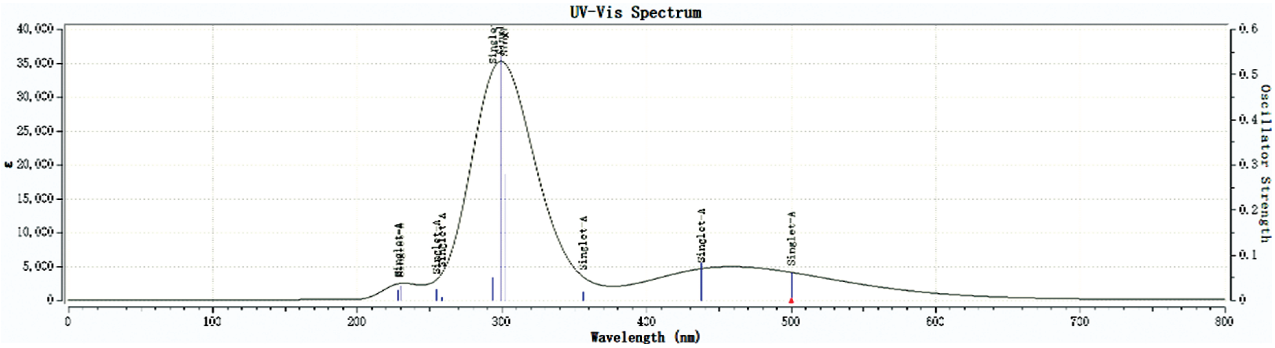
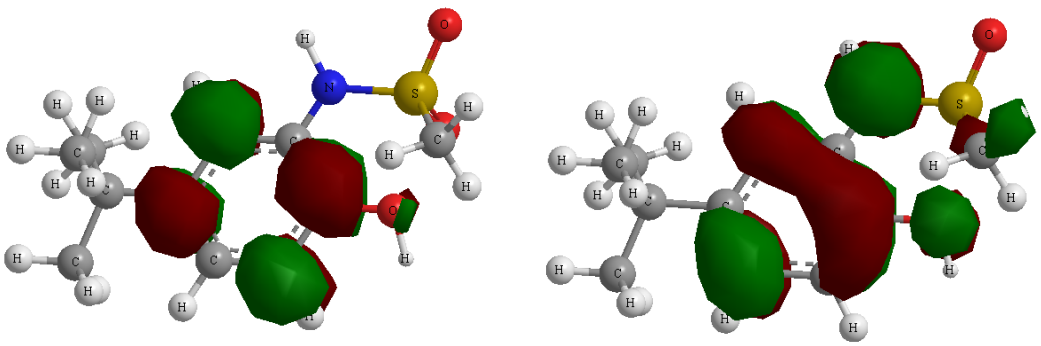


Figure 2 – Absorption spectrum of the title molecule

Table – Calculated electronic spectrum of the molecule (A)

State	Wavelength, nm	Energy transition, eV	Decomposition of wave functions by singly excited configuration	Power oscillator(f)
$S_0 \rightarrow S_1$	499.99	2.4797	-0.15(44->46)-0.25(44->47)-0.52(45->46)0.25(45->47) -0.18(45->48)	0.0615
$S_0 \rightarrow S_2$	437.69	2.8327	0.23(44->46)0.15(44->48)-0.30(45->46)-0.56(45->47)	0.0828
$S_0 \rightarrow S_3$	356.22	3.4806	-0.12(43->46)0.18(44->47)-0.22 (45->46)0.54(45->48) 0.10(45->49)-0.15(45->51)	0.0191
$S_0 \rightarrow S_4$	301.77	4.1085	-0.41(44->46)-0.36(44->47)-0.10(44->48)0.14(45->46) -0.25(45->47)0.17(45->48)-0.14(45->49)-0.10 (45->51)	0.2794
$S_0 \rightarrow S_5$	298.78	4.1497	0.35(44->46)-0.44(44->47)0.23(44->48)0.14(45->46) 0.17(45->47)0.18 (45->48)	0.5411
$S_0 \rightarrow S_6$	293.70	4.2215	-0.15(44->46)-0.11(44->48)-0.13(44->49)-0.10(45->47) 0.48(45->49)0.12(45->50)0.25(45->51)-0.22(45->53)	0.0500
$S_0 \rightarrow S_7$	258.58	4.7947	-0.27(45->49)-0.15(45->50)0.11(45->51)0.19(45->52) -0.49(45->53)0.10(45->54)0.14(45->56)	0.0072
$S_0 \rightarrow S_8$	254.52	4.8712	-0.15(43->46)0.15(43->47)-0.13(43->48)-0.10(44->47) 0.14(45->49)-0.57(45->50)0.10(45->53)	0.0236
$S_0 \rightarrow S_9$	229.66	5.3986	0.23(43->46)0.22(43->47)0.11(44->46)-0.30(44->48) -0.11(44->49)0.38(44->50)	0.0324
$S_0 \rightarrow S_{10}$	228.46	5.4270	0.10(43->48)-0.15(44->49)0.11(45->48)-0.15(45->49) 0.33(45->51)0.20(45->52)0.22(45->53)-0.18(45->54) 0.27(45->57)	0.0217



LUMO (N=46) [0.379 eV] HOMO (N=45) [-8.797 eV]

Figure 3 – Types of molecular orbitals involved in the formation of the absorption spectrum of the molecule (A) at 298.78 nm

Conclusion. Using the PM6 method to measure this the molecule the N-(5-(tert-buty1)-2-hydroxyphenyl) methanesulfonamide in the solvent medium of water (H_2O), and the maximum wavelength with high oscillator strength was observed at 298.78 nm and f=0.5411. Results of molecular orbitals are LUMO (N=46) [0.379eV] and HOMO (N=45) [-8.797eV].

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ПРОГРАММА ЕЖЕДНЕВНОЙ ПРОЦЕДУРЫ ГАРАНТИИ КАЧЕСТВА НА ЛИНЕЙНОМ УСКОРИТЕЛЕ ЭЛЕКТРОНОВ

PROGRAM OF THE DAILY QUALITY ASSURANCE PROCEDURE ON THE ELECTRON LINEAR ACCELERATOR

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Осуществление мероприятий по контролю качества работы медицинских линейных ускорителей – один из элементов радиационной защиты пациентов, подвергающихся медицинскому терапевтическому облучению, который в то же время является важнейшим из составляющих программы гарантии качества лучевой терапии. Контроль качества линейных ускорителей позволяет полностью выдержать заданные параметры плана облучения каждого пациента и избежать его переоблучения или недооблучения, а также тяжелых радиационных аварий.

The implementation of quality control measures for the operation of medical linear accelerators is one of the elements of radiation protection of patients undergoing medical therapeutic radiation, which at the same time is the most important component of the radiotherapy quality assurance program. The quality control of linear accelerators makes it possible to fully comply with the specified parameters of the exposure plan for each patient and avoid overexposure or underexposure, as well as severe radiation accidents.

Ключевые слова: лучевая терапия, гарантия качества, линейный ускоритель электронов, доза, онкология, медицинская физика.

Keywords: radiation therapy, quality assurance, linear electron accelerator, dose, oncology, medical physics.

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Наиболее важным аспектом контроля качества линейных ускорителей электронов является проведение ежедневной процедуры гарантии качества, которая проводится утром инженерами или медицинскими физиками, перед тем, как отдать аппарат в лечебную практику.

Все проверки, которые входят в программу проверки ежедневного контроля качества линейных ускорителей, можно разделить на четыре процедуры:

1. Дозиметрические,
2. механические,
3. безопасность,
4. изображение.