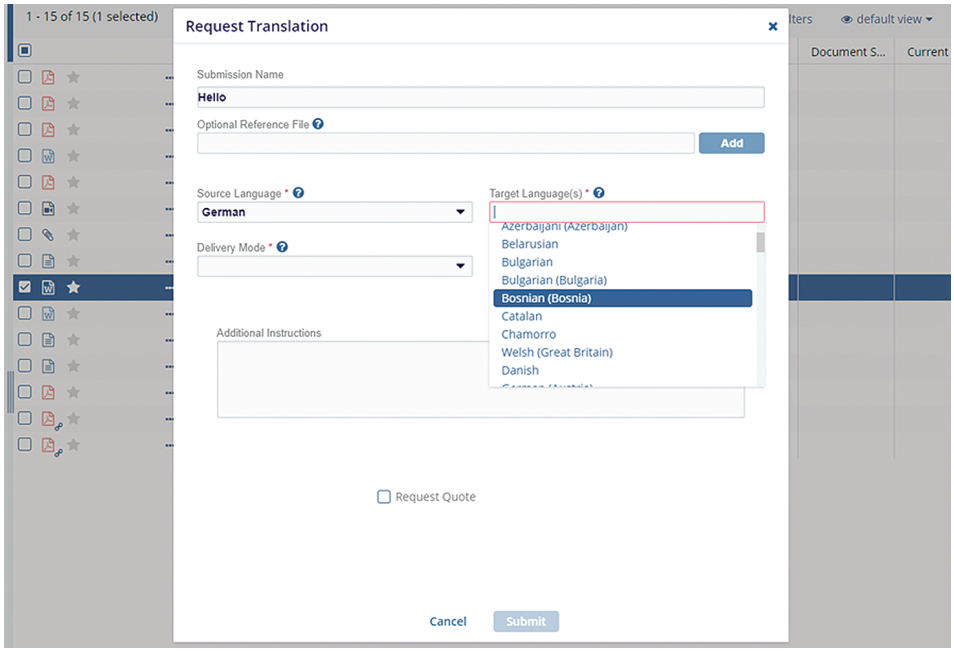

Рисунок 3 – Диалоговое окно с подготовкой отправки запроса на перевод документа

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QUANTUM-CHEMICAL CALCULATION OF 2,4-DI-TERT-BUTYL-6-MORPHOLINOPHENOL COMPOUND

КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ 2,4-ДИ-ТРЕТ-БУТИЛ-6-МОРФОЛИНОФЕНОЛ

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This publication presents theoretical calculations applied to 2,4-di-tert-butyl-6-morpholinophenol compounds to determine their optimized state, predict its free energy, and determine the molecular orbitals involved in spectrum formation.

В данной работе представлены теоретические расчеты соединения 2,4-ди-трет-бутил-6-морфолинофенола с целью определения его равновесной структуры, полной энергии и вида молекулярных орбиталей, участвующих в формировании спектра поглощения.

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

Ключевые слова: компьютерная химия, PM6, УФ спектр.

https://doi.org/10.46646/SAKH-2022-2-370-373

Preliminary quantum chemical modeling of the 2,4-di-tert-butyl-6-morpholinophenol compound. For calculation, we used a personal laptop with an Intel i5 processor (2.71 GHz CPU) with the Windows 10 operating system installed. When calculating the initial geometry of a molecule with a 2,4-di-tert-butyl-6-morpholinophenol base, the method of molecular mechanics (MM+) of the ChemOffice 2020 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 PM6 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 PM6 method is used to find optimized geometric configurations, the total energy of molecules, electronic properties, and the enthalpy of formation of substances. The GaussView 6.0 program was used to visualize the results. The equilibrium geometry of the molecule by the 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-morpholinophenol Molecule. Full optimization and calculation of the electronic structure were carried out by the PM6 method. This method is used to find optimized geometric configurations, the total energy of molecules, electronic properties, and the enthalpy of formation of substances. The electronic spectrum of the molecule 2,4-di-tert-butyl-6-morpholinophenol was calculated for 10 one-electron excitations in the range of 246.88-595.60 nm. The results of calculation of the absorption spectrum are given in the table [1].

The maximum wavelength with a high oscillator strength was observed at $\lambda = 333.95$ nm and $f = 0.2034$ (Table 1, Fig. 2,3). The calculation showed that the strongest electron transition is observed at the absorption maximum of 333.95 nm, which refers to the electron transition to the excited state $S_0 \rightarrow S_4$.

The theoretical absorption spectrum of an optimized molecule in a solvent medium is calculated using the Gaussian 09W software package by the PM6 method. The calculated electronic absorption spectrum of a molecule in a solvent medium is shown in Figure 2 [2].

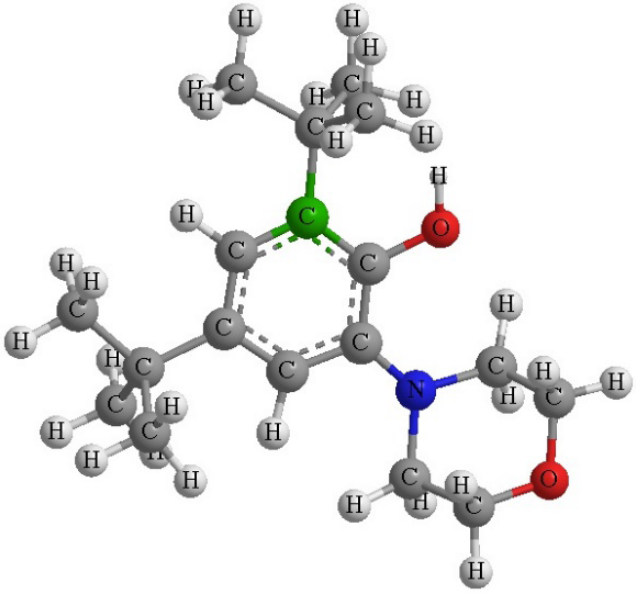


Figure 1 – Optimized molecule by PM6 method

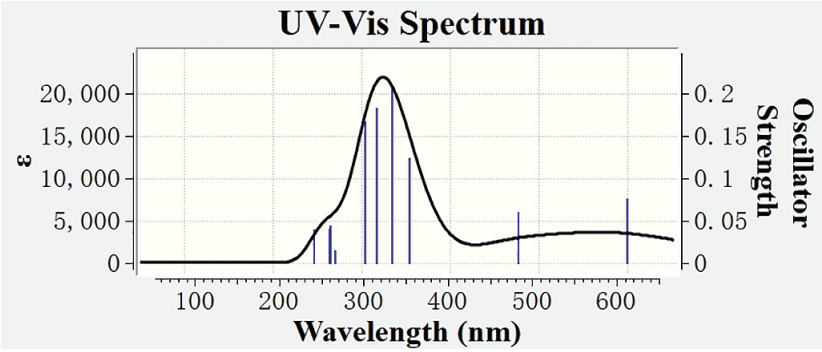
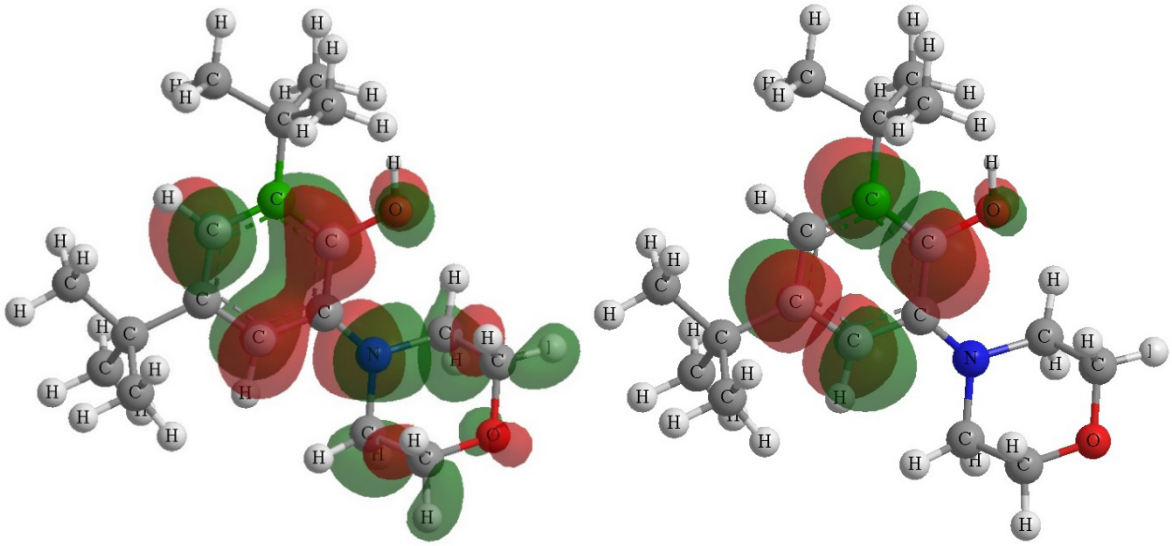


Figure 2 – UV/Vis spectrum of the compound in the solvent water

Table 1 – Electronic absorption spectrum of the compound

Excited State	Wavelength (nm)	Excitation Energy (eV)	Configurations Composition (corresponding transition orbitals)	Oscillator Strength(f)
$S_0 \rightarrow S_1$	596.60	2.0782	0.22(58→61) +0.62(59→60) +0.12(59→61)	0.0742
$S_0 \rightarrow S_2$	476.16	2.6038	0.12(57→61)-0.27(58→60)-0.15(59>60) +0.60(59→61)	0.0606
$S_0 \rightarrow S_3$	354.27	3.4997	0.12(56→60)-0.10(57→60)+0.11(57→61)-0.26(58→60)-0.40(58→61)+0.14(59→60) +0.35(59→62)-0.12(59→63)+0.14(59→64)	0.1294
$S_0 \rightarrow S_4$	333.95	3.7127	-0.14(57→60)+0.52(58→60)-0.15(58→61)-0.10(58→64)+0.26(59→61)+0.15(59→62)-0.10(59→63)-0.14(59→64)+0.10(59→65)	0.2034
$S_0 \rightarrow S_5$	318.24	3.8960	0.10(57→61)-0.12(58→60)-0.32(58→61) +0.10(58→62)+0.15(59→60)-0.32(59→62)-0.37(59→64)-0.13(59→66)	0.1806
$S_0 \rightarrow S_6$	304.07	4.0774	-0.16(58→60)+0.23(58→61)-0.15(58→64)-0.13(59→60)-0.11(59→61)+0.27(59→62)-0.18(59→63)-0.33(59→64)+0.21(59→65)-0.15(59→66)	0.1707
$S0 \rightarrow S_7$	271.42	4.5679	0.11(56→62)+0.22(56→63)+0.29(57→62) +0.36(57→63)+0.16(58→62)+0.13(58→63) +0.31(59→63) +0.14(59→66)	0.0141
$S_0 \rightarrow S_8$	266.05	4.6602	-0.13(56→62)-0.18(57→63)+0.12(58→62)-0.14(58→63)-0.25(59→64)-0.12(59→65) + 0.43(59→66)+0.12(59→72)-0.15(59→74)-0.10(59→79)	0.0425
$S_0 \rightarrow S_9$	264.57	4.6863	-0.17(56→60)+0.21(57→60)-0.11(58→61) +0.10(58→65) +0.51(59→65) +0.20(59→66)	0.0401
$S_0 \rightarrow S_{10}$	246.88	5.0201	0.26(56→60)-0.38(57→60)+0.13(58→61)-0.20(58→62)+0.13(58→63)+0.14(58→65)-0.14(59→62)+0.12(59→65)+0.16(59→66)+0.10(59→76)	0.0439



HOMO (N=59) [-7.456eV] LUMO (N=60) [1.835eV]

Figure 3 – Form of molecular orbitals involved in the formation of absorption spectrum of the molecule at λ = 333.95 nm by PM6 method

Conclusion. We chose the method of molecular mechanics (MM+) of the ChemOffice 2020 software package to calculate the initial geometry of the 2,4-di-tert-butyl-6-morpholinophenol. We also chose the PM6 method of the Gaussian 09W software to additionally optimized in the water solvent medium. The electronic spectrum of the 2,4-di-tert-butyl-6-morpholinophenol was calculated for 10 one-electron excitations in the range of 246.88-595.60 nm .The calculation showed that the strongest electron transition is observed at the absorption maximum of λ = 333.95 nm and f = 0.2034 which refers to the electron transition to the excited state $S_0 \rightarrow S_4$. The LUMO (N=60) energy is 1.835 eV and the HOMO (N=59) energy is -7.456 eV.

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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].

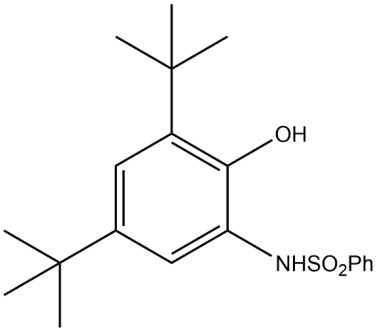

Figure 1 – 2D structure of the molecule