QUANTUM-CHEMICAL CALCULATION OF PHYSICO-CHEMICAL PARAMETERS OF ANTHRACHINONE

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Abstract. In this article, the reactivity of the anthraquinone molecule, the electron density distribution in the molecule, the distance between the bonds, and the physicochemical parameters extracted from the root extract of the plant "Rubia tinctorum L" are studied using quantum chemical methods (DFT, PM3, , TS-DFT was performed in Gaussian 09 using the 6-31G basis set. The reactivity, bond energies, electron density distribution of the molecule were calculated, the structure was analyzed by IR spectroscopy and compared with the spectra obtained from the "Spectral Database for Organic Compounds SDBS" database. The degree of agreement between the quantum chemical calculations and the spectra obtained from the basis set was evaluated by finding the correlation coefficient by the method of least squares.

Keywords: anthraquinone, reactivity, electron density, Gaussian 09 program, bond energy, IR-spectroscopy.

Introduction

As a result of the development of science and technology, in the field of chemistry, the main attention is paid to the study of the connections between the "composition-structure" and "structure-property" of substances, at the same time, the structure and properties of the substance, the sizes of the particles that make up its molecule (nanoparticles), as a result of studying the relationship with their number and properties, it is usually possible to predict the composition, properties and molecular structure of a substance by studying the laws between "composition-structure-property". Currently, semi-empirical quantum-chemical (PM3, DFT, AM1) methods are used to determine the electronic structure and reactivity of substance molecules, competing donor centers, as well as energetic and electronic properties of molecules, angle and bond length values. As a result of determining the negative effective charges of the donor atoms of the substance molecule, it is possible to conclude about the ligand nature of this molecule. Taking this into account, in this research work, it was planned to carry out the targeted synthesis of new derivatives of anthraquinone, which is a derivative of anthracene, one of the plant substances, in order to ensure the wide possibilities of its ligand properties. The reactivity of substances is taken into account during the synthesis

Analysis of literature on the topic. Physico-chemical indicators such as the reactivity of the studied molecule, the distribution of electron density in the molecule, the distance between bonds, were studied using quantum chemical methods (DFT, PM3,) performed with the help of computer technology. Quantum chemical calculations are performed in the Gaussian 09 program using the TS-DFT 6-31G basis set.

The Gaussian calculation complex created by J.Pople has a wide range of possibilities, is designed to solve problems in almost all areas of chemistry and includes some semi-empirical and many non-empirical calculation methods [1-2]. The calculations were based on the electron density distribution in the molecule. Anthraquinone substance, whose quantum chemical parameters are being studied, is an odorless yellow crystalline substance that liquefies at 277 oC

and boils at 382 oC. Soluble in aniline, acetone, nitrobenzene and hot toluene. It is noted in the literature that anthraquinone is obtained by oxidizing anthracene or by reacting phthalic anhydride with benzene under the catalyst of aluminum chloride [3-6]. It can undergo various reactions, but it is very difficult to undergo replacement reactions. Anthraquinone is transformed into alizarin in an alkaline environment under the influence of various oxidizing agents. Due to the presence of carbonyl groups in anthraquinone, its properties are similar to those of ketones and quinones. It is slowly sulfonated even at 250 oC under the influence of dilute H_2SO_4. When sulfonation is carried out at 140 oC with 35-40% oleum content, β-anthraquinone sulfoacid is formed [4-10].

Research methodology. Using TS-DFT 6-31G basis sets in the Gaussian 09 program of information technologies for quantum-chemical calculations, the spectra obtained by IR-spectroscopy of the molecular structure were compared with the spectra obtained from the "Spectral Database for Organic Compounds SDBS" database.

Results and discussion

The electron density distribution in the anthraquinone molecule is shown in Fig. 1.
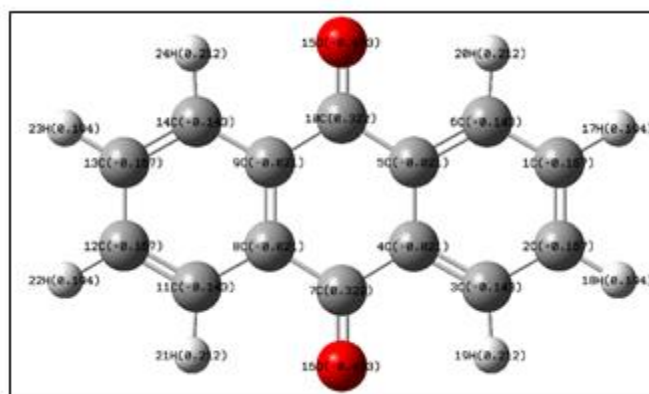
Figure 1. Mullican distribution of electron density in anthraquinone molecule

From the figure, the electron density in 3-C, 6-C, 11-C, and 14-C atoms due to the transfer of electron density to oxygen in carbon (7-C, 10-C) atoms, which are interconnected with element-oxygen atoms with high electronegativity in the molecule, can be seen can be seen to have high values of This, in turn, increases the mobility of hydrogen atoms bound to these carbon atoms and acts as a nucleophilic center for electrophilic substances in reaction processes [10-15]. Also, the energies of the interatomic bonds forming the reaction centers in the aromatic ring were calculated using quantum chemical (Ab initio, HatriFok) methods (Table 1).

Table 1

*Energy of interatomic bonds in anthraquinone molecule calculated by Ab initio method*

Bonds	3C and 19H,	6C and 20H	11C and 21H	14C and 24H
Energy (kcal/mol)	60,248	54,152	70,115	70,242

As can be seen from the table, the bond energies in the molecule are thermodynamically compatible with the reactions it undergoes. This indicates that these bonds are reactively active centers in the anthraquinone molecule.

The IR spectra formed by the vibration of the bonds in anthraquinone were calculated using the Gaussian 09 program and compared with the spectra obtained from the "Spectral Database for Organic Compounds SDBS" database.
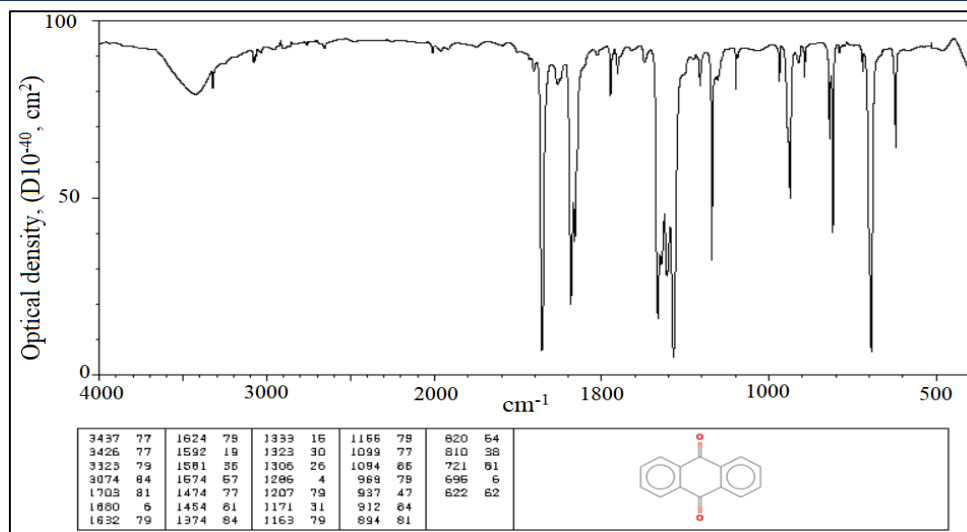
Figure 2. IR spectra of anthraquinone from the SDBS IR spectrum database.
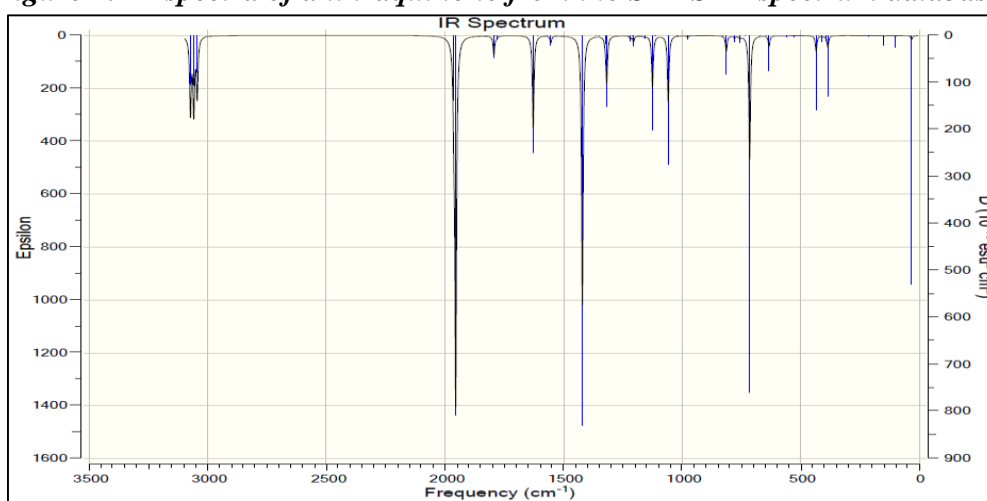
Figure 3. IR spectrum of anthraquinone obtained using Gaussian 09 software.
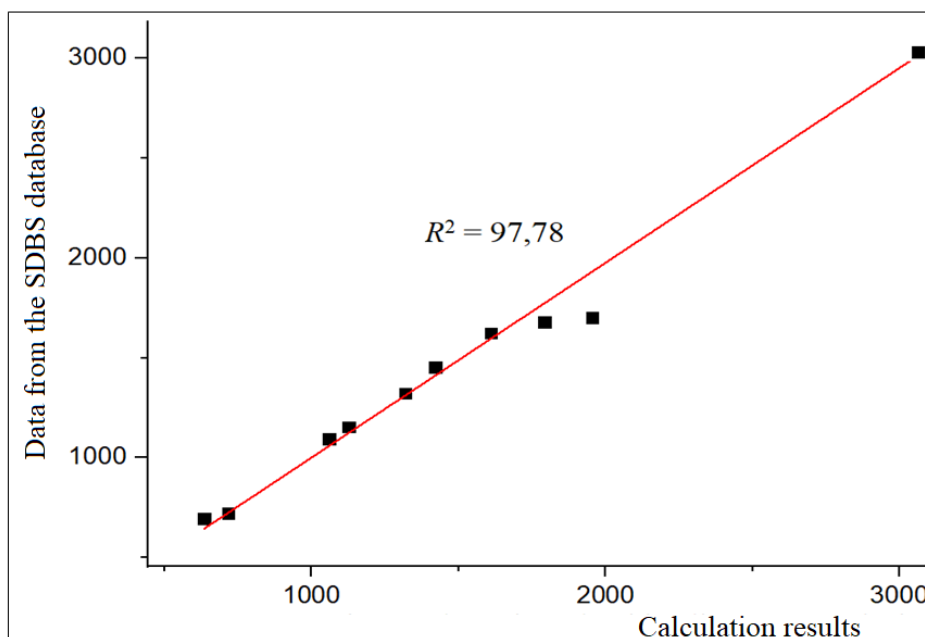
Figure 4. The level of agreement of the IR spectra obtained in the experiment and in the Gaussian 09 program.

From Figures 2 and 3, the peaks in the 3500-3000 cm^{-1} range in the IR spectra of anthraquinone are due to dimorphic vibrations of C=O bonds, and the high-intensity peaks in the 1600-1000 cm^{-1} range are due to the valence vibration of C-H bonds in the aromatic rings. it can be seen that it is formed due to Also, the peaks in the 1000-500 cm^{-1} range of the spectra were formed by the dimorphic vibration frequencies of the C=C bird bonds in the aromatic ring, and in the 500-400 cm^{-1} range by the valence vibrations of the C-C bonds. The degree of agreement between the quantum chemical calculations and the spectra obtained from the base was evaluated by finding the correlation coefficient by the method of short squares (Graph 1).

From the graph, it can be seen that the degree of agreement between the IR spectrum obtained from the "Spectral Database for Organic Compounds SDBS" and the results calculated in the Gaussian 09 program is R^2 = 97,78%.

Conclusion

Thus, the energies of the interatomic bonds that formed the reaction centers in the aromatic ring are thermodynamically compatible with spontaneous reactions, and according to the results of studying the structure of the molecule, the IR spectrum of the substance and the results calculated in the Gaussian 09 program are the same - was found to be consistent with one (R2 = 97.78 %).

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