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Quantum Chemical Calculation Of Uroidomethylgallate Based On Gallic Acid

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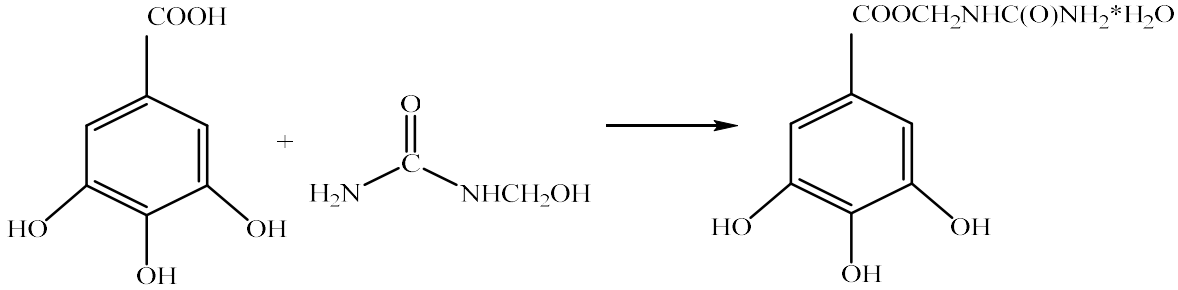
Abstract: *Typically, the synthesis of new potential drugs and drugs from complex organic molecules is carried out through multi-step chemical reactions. Recently, it has become relevant to obtain compounds based on existing biologically active compounds or compounds in fragments that include medicinal molecules. At the same time, attention is paid to the creation of structures with pharmacological properties. This route has a number of advantages, since the compounds included in these molecules are industrially available and their implementation in the pharmaceutical industry is quite simple [1]. Since the molecules of these substances contain fragments of amide and ether bonds, they can easily be broken down in the body under the action of enzymes. Thus, these molecules can either have an independent pharmacological effect after delivering them to the corresponding organs in the human body, or enhance the effect of each other, exhibiting synergy [1]. Thus, when these substances enter the body, they can exhibit certain activity. As is known, such substances exhibit unpredictable types of biological activity, which are often associated with the method and conditions of synthesis, the degree of purification, etc. It is known that derivatives of 4-hydroxybenzoic acid have an antimicrobial effect, and the antitumor activity of its derivatives has also been proven [2]. Derivatives of 4-hydroxybenzoic acid with heterocyclic compounds and their salts are used as drugs that promote the removal of uric acid from the body [3]. The authors in [4] indicate that 1,3-Bis(4-methoxybenzoyl)pyrimidine-2,4(1H,3H)-dione has activity that breaks the cross-links of glycated proteins and can be used in the treatment of diabetes and diseases associated with aging and neurodegenerative amyloid disease such as Alzheimer's*

disease. This, in turn, indicates the relevance and prospects of further research on this substance. Based on this, we for the first time studied the quantum chemical parameters of a hydroxybenzoic acid derivative using the example of a specific substance, 1,3-Bis(4-methoxybenzoyl) pyrimidine-2,4(1H,3H)-dione. GaussView software was used for calculations. This article aims to study the progress of the reaction of gallic acid obtained from pomegranate peel with monomethylolurea. The synthesized compound was also studied by modern quantum chemical method. Correlation between the obtained experimental and theoretical results was determined.

***Key words**: Pomegranate peel, uroidomethylgallate, tannins, synthesis, quantum-chemical method, IR-spectra.*

Introduction. The following were taken as the object of our research: gallic acid, a representative of the class of tannins [4,5] isolated from the composition of the fruit peel of pomegranate grown in Uzbekistan [1-3]. It is aimed to analyze its physico-chemical properties and the composition of compounds [6] obtained based on it from a theoretical and practical point of view. In the conducted scientific research, the course of chemical reactions was studied, and now the modern quantum-chemical calculation method was used in the theoretical study of the object. The mobility and reactivity of molecules in chemical reactions mainly depends on their chemical composition, properties, structure and energetics. It is important to know in advance the reaction centers and active groups of organic molecules. Today, the use of quantum-chemical methods allows practicing chemists to plan experimental experiments in advance and is of great importance in the synthesis of chemical products.

Literature review. "Gaussian 98" software package was used for quantum-chemical study of the composition and structure of the reaction mechanism of the substance obtained on the basis of gallic acid and monomethylolurea using quantum-chemical methods.



The structures and molecular structures of gallic acid and its compounds were optimized on the basis of 3-21G, and IR-spectra and Hartree energies were calculated based on the DFT/B3LYP hybrid method of this program.

Calculation of IR spectra was carried out using the "Optimization" commands of "Job type" in "Frequency" and "Gaussian calculation setup" sections, optimizing the structures of molecules. Calculation processes for molecules were carried out separately without solvent (in gas phase) and in chloroform and diethyl ether. Solvents were selected via the solvation section of the Gaussian calculation setup.

Monomethylolurea ester of gallic acid has been found to have biostimulant properties that are effective in the growth and development of plants. To determine the geometrical parameters and electronic structure of

urodomethylgallate, we performed quantum chemical calculations of uridomethylgallate ether using the state-of-the-art DFT-B3-LYP quantum chemistry method using the Gaussian program based on the 3-21G basis set. The initial matrix was prepared using GaussView software [7,8,9,10].

Experimental section and discussion of results. The numbering of atoms is conditionally selected by the Gaussian program, which simplifies the analysis of the calculated data (Fig. 1) and does not affect the results.

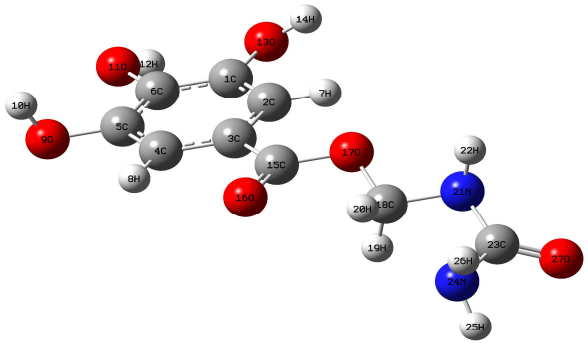


Figure 1. Conventional numbering of atoms of the uredomethylgallate molecule.

Modern quantum chemical programs, including the Gaussian-98 program, perform molecular calculations in spatial Cartesian coordinates. Distances between atoms (d, Å), valence angles (φ, ^{0}S), torsion angles (τ, ^{0}S) were obtained with high accuracy, within 1/10000 of a unit. These results of the Gaussian-98 program serve for easy comparison with the results of IR-, X-ray research methods in other methods of physical research methods (PRM).

Table 1.

Quantum-chemically calculated structural descriptions of the uredomethylgallate molecule.

№	Atomic numbers	Charge, e	Atoms	Interatomic distance, Å	Valent angle	The magnitude of the valence angle, °
1	1C	0.220	1C-13O	1.43000	1C-2C-3C	120.0000
2	2C	-0.182	1C-14H	1.9702	2C-3C-4C	120.0000
3	3C	-0.110	1C-2C	1.4014	3C-4C-5C	120.0000
4	4C	-0.207	1C-6C	1.4014	4C-5C-6C	120.0000
5	5C	0.249	2C-7H	1.0700	1C-13O-14H	109.46804
6	6C	0.256	2C-3C	1.4014	5C-9O-10H	109.47522
7	7H	0.215	3C-4C	1.4014	6C-11O-12H	109.46577

8	8H	0.230	3C-15C	1.5400	3C-15C-17O	120.0000
9	9O	-0.602	4C-5C	1.4014	3C-15C-16O	120.0000
10	10H	0.372	4C-8H	1.0700	15C-17O-18C	109.46835
11	11O	-0.57	5C-6H	1.07000	17O-18C-19H	109.47218
12	12H	0.377	5C-7H	1.07000	17O-18C-20H	109.47218
13	13O	-0.58	5C-6C	1.4014	19H-18C-20H	109.47218
14	14H	0.364	5C-9O	1.4300	17O-18C-21N	109.46390
15	15C	0.561	6C-11O	1.4300	18C-21N-23C	109.48011
16	16O	-0.47	11O-12H	0.9600	21N-23C-27O	120.0000
17	17O	-0.52	15C-16O	1.2584	21N-23C-24N	120.0000
18	18C	0.043	15C-17O	1.4300	23C-24N-25H	109.46390
19	19H	0.230	18C-17O	1.47001	18C-21N-22H	109.4712
20	20H	0.230	18C-19H	1.070	4C-5C-9O	120.00018
21	21N	-0.52	18C-20H	1.070	5C-11O-12H	109.4712
22	22H	0.300	18C-21N	1.4700	3C-4C-8H	109.4712
23	23C	0.630	21N-22H	1.000	23C-24N-26H	109.4712
24	24N	-0.690	21N-23C	1.4700	5C-6C-11O	120.0000
25	25H	0.300	23C-24N	1.4700	1C-2C-7H	120.0000
26	26H	0.300	23C-24O	1.2584	2C-3C-15C	120.0000
27	27O	-0.420	24N-25H	1.0000	5C-6C-1C	120.0000
28			24N-26H	1.40140	25H-24N-26H	109.4712

According to the data calculated by us (Table 1), the maximum absolute values of negative charges correspond to carbon, nitrogen and oxygen atoms.

For example, in 2C , 3C , 4C , 9O , 11O , 13O , 16O , 17O , 21N , 24N , 27O atoms, the magnitude of electronic charges is respectively equal to q= -0.182e, -0.110e, -0,207e, -0.602e, -0,570e, -0,580e, -0,470e, -0.520e, -0.520e, -0.690e, -0.420e. The analysis of the geometrical parameters of the molecule, i.e. the

interatomic distances, shows that the lengths of the C1-C2,C2-C3, C3-C4, C4-C5, C5-C6, C6-C1 bonds in the aromatic ring are almost the same and meet the requirements of aromaticity, and has a planar view.

Analyzing the reaction mechanism of monomethylolurea gallate formed by gallic acid with monomethylolurea, the formation of ether as a result of the reaction was concluded based on the analysis of bond energies of -NH_2 and -OH groups in gallic acid -NH2 and -OH groups. The analysis of this mechanism was based on the theory of Coulomb's electrostatic effect.

$F=kq_1q_2/r^2$

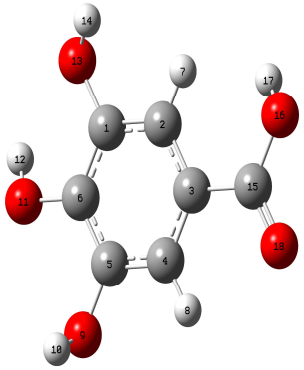


Figure 2. Conventional numbering of atoms in a gallic acid molecule.

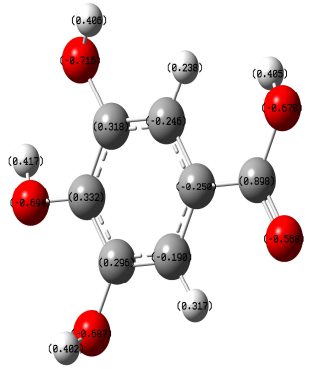
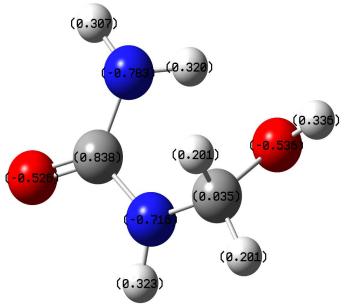


Figure 3. Charge of atoms in gallic acid molecule.

Due to the small bond energy of the aromatic ring in gallic acid – OH groups ($F_{O9H10}=0.3387$, $F_{O11H12}=0.3534$, $F_{O13H14}=0.33947$) and the acid (–COOH) group and the – OH bond energy of –COOH in the carboxyl group $F_{O15H17}=0.31904$ it can be theoretically justified that there is less energy consumption for breaking the bond.

If we analyze the bond energies of -NH_2 and –OH groups in monomethylol urea ($F_{N9H10}=0.2268$, $F_{N9H11}=0.2268$, $F_{O4H5}=0.1790$),



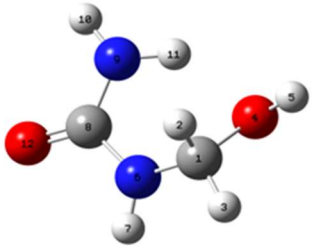


Figure 4. Conventional numbering of atoms in the molecule of monomethylolurea.

Figure 5. Charges of atoms in a molecule of monomethylolurea.

the small value of –OH in the carboxyl group of – OH F_{O4H5} =0.1790 indicates that less energy is spent on the bond chain.

Synthesis of ureidomethylgallate. The mixture of substances resulting from the reaction of gallic acid with monomethylolurea was separated by column chromatography. The productivity of ureidomethylgallate was 42%. T.c.=155ºC. *IR spectrum (Fig. 6).* δ_{NH_2} strong 580 cm^{-1}, valence vibration δ_{NH} medium 765 cm^{-1}, deformation vibration $\delta_{Ar(as)}$ medium 880 cm^{-1}, aromatic ring in aromatic ring $\delta_{Ar(s)}$ strong 940 cm^{-1}, r_{CH_2} medium 990 cm^{-1}, $v_{C(O)-O}$ strong 1035 cm^{-1}, τ_{NH_2} strong 1090 cm $^{-1}$, v_{H_2C-O} very strong 1110 cm^{-1}, $r_{CH(Ar)}$ broad, strong 1130 cm^{-1}, deformation vibration δ_{OH} broad, strong 1190 cm^{-1}, τ_{CH_2} strong 1260 cm^{-1}, $v_{C(O)=O}$ strong 1570 cm^{-1}, $v_{C(NH_2)=O}$ strong 1650 cm^{-1}, δ_{NH_2} weak, shoulder 1670 cm^{-1}, $v_{CH_2(s)}$ weak 3280 cm^{-1}, $v_{CH_2(as)}$ weak 3355 cm^{-1}, valence vibration in the aromatic ring $v_{CH(Ar)}$ weak 3370 cm^{-1}, valence vibration $v_{NH_2(s)}$ weak 3720 cm^{-1}, valence vibration v_{NH} weak 3770 cm^{-1}, $v_{NH_2(as)}$ weak 3830 cm^{-1} , valence vibration v_{OH} broad, weak 3890-3900 cm^{-1} special lines were detected [3] and the IR spectrum of uroidomethylgallate (Fig. 7) obtained as a result of quantum-chemical calculations is compared in Table 2.

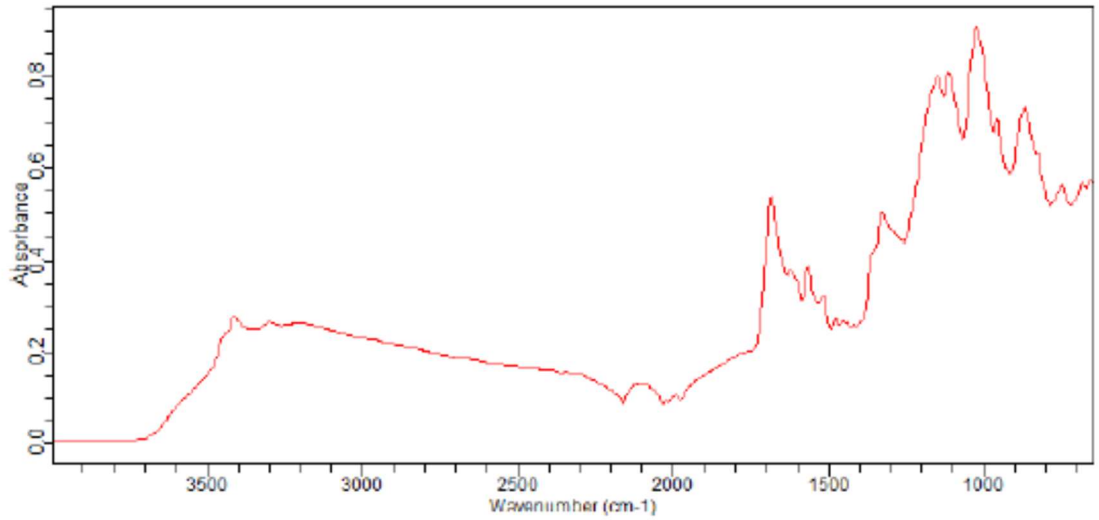


Figure 6. Experimental IR spectrum of uroidomethylgallate.

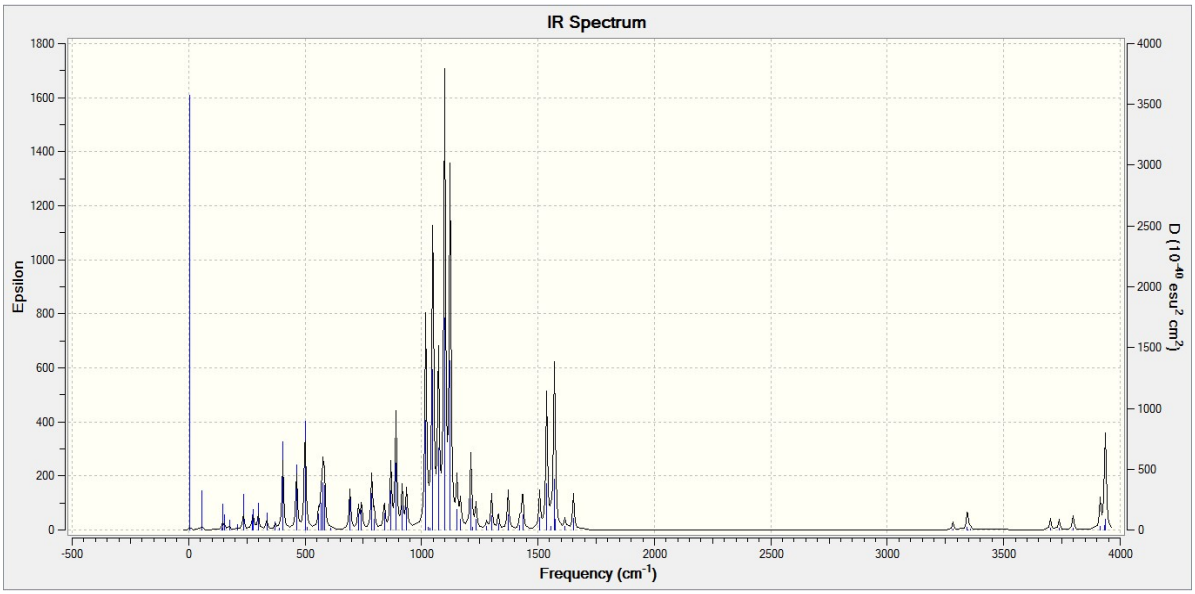


Figure 7. Quantum-chemically calculated IR spectrum of uroidomethylgallate.

Comparison of the IR spectra of uroidomethylgallate.

Table 2.

	Name of groups	IR spectra	
		Taken from experiment	Quantum-chem
1	δ_{NH_2}	strong 580 см$^{-1}$	569,48 см$^{-1}$
2	δ_{NH}	medium 765 см$^{-1}$,	742 см$^{-1}$
3	$\delta_{Ar(as)}$	medium 880 см$^{-1}$,	890 см$^{-1}$
4	$\delta_{Ar(s)}$	strong 940 см$^{-1}$	936 см$^{-1}$
5	r_{CH_2}	medium 990 см$^{-1}$	1011,12 см$^{-1}$
6	$v_{C(O)-O}$	strong 1035 см$^{-1}$	1048 см$^{-1}$
7	τ_{NH_2}	strong 1090 см$^{-1}$	1178 см$^{-1}$
8	v_{H_2C-O}	strong 1110 см$^{-1}$	1122 см$^{-1}$
9	$r_{CH(Ar)}$	strong 1130 см$^{-1}$	1152 см$^{-1}$
10	δ_{OH}	strong 1190 см$^{-1}$	1167,32 см$^{-1}$
11	τ_{CH_2}	strong 1260 см$^{-1}$,	1280 см$^{-1}$
12	$v_{C(O)=O}$	strong 1570 см$^{-1}$	1570 см$^{-1}$
13	$v_{C(NH_2)=O}$	strong 1650 см$^{-1}$	1570,12 см$^{-1}$
14	δ_{NH_2}	weak 1670 см$^{-}$	1652 см$^{-1}$
15	$v_{CH_2(s)}$	weak 3280 см$^{-1}$,	3281 см$^{-1}$

16	$\upsilon_{CH_2(as)}$	weak 3355 см$^{-1}$	3345 см$^{-1}$
17	$\upsilon_{CH(Ar)}$	weak 3370 см$^{-1}$	3358 см$^{-1}$
18	$\upsilon_{NH_2(s)}$	weak 3720 см$^{-1}$,	3738, strong 3700
19	υ_{NH}	weak 3770 см$^{-1}$,	3798 см$^{-1}$
20	$\upsilon_{NH_2(as)}$	weak 3830 с	3818 см$^{-1}$

If we compare the obtained results, the IR-spectrum of uroidamethylgallate formed in the synthesis of gallic acid and monomethylolurea, obtained on the basis of experimental experience, and the results of quantum-chemical calculations show that they are almost close to each other.

Conclusion. Based on gallic acid and monomethylolurea, the course of the chemical reaction and the formation of uroidomethylgallate were determined. It has been proved that this process can be carried out by the carboxyl group in gallic acid and the hydroxyl groups in monomethylurea molecule based on the changes in bond energies using the quantum-chemical method.

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