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ELECTRONIC STRUCTURE AND QUANTUM-CHEMICAL ACCOUNT OF FURFUROLIDENUREA

FURFUROLIDENKARBAMIDNING ELEKTRON TUZILISHI VA KVANT-KIMYOVIY HISOBI

ЭЛЕКТРОННАЯ СТРУКТУРА И КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ ФУРФУРОЛИДЕНКАРБАМИДА

Mukhammedov Saidmurod[1], Askarov Ibrokhim[2], Isakov Khayatulla[2], Mamarakhmonov Mukhamatdin[2]

[1]Mukhammedov Saidmurod	*− Basic doctoral student of Fergana Polytechnic Institute*
[2]Askarov Ibrokhim	*− Professor of the Department of Chemistry, Andijan State University, DSc*
[2]Isakov Khayatulla	*− Professor of the Department of Chemistry, Andijan State University, DSc*
[2] Mamarakhmonov Mukhamatdin	*− Associate Professor of Chemistry, Andijan State University, PhD.*

Аннотация

Bugungi kunda yuqori molekulyar birikmalar xossalari va ular ishtirokidagi kimyoviy reaksiyalarni nazariy jihatdan yuqori aniqlikda aniq aytib berish sohasida olib borilayotgan tadqiqotlar muhim hisoblanadi.Ushbu maqolada furfurolidenkarbamid olish uchun kerakli furfurol va karbamid molekulalarining reaksion qobiliyatlari zamonaviy Gaussian98 kompyuter dasturi yordamida xisoblangan natijalari keltirilgan. Furfurolidenkarbamid molekulasining elektron tuzilishi, optimallashgan geometrik parametrlari, atom zaryadlarini yuqori aniqlikda hisoblandi. Birikmaning reaksion qobiliyati bo'yicha nazariy jihatdan kerakli natijalar olindi.

Аннотация

В настоящее время проводятся важные исследования в области точного описания свойств высокомолекулярных соединений и протекающих в них химических реакций с высокой теоретической точностью.В данной работе представлены результаты расчета реакционной способности молекул фурфурола и мочевины, необходимой для получения фурфуралиденкарбамида, с использованием современной компьютерной программы Gaussian98. Электронное строение молекулы фурфуралиденкарбамида, оптимизированные геометрические параметры, заряды атомов рассчитаны с высокой точностью. Были получены теоретически необходимые результаты по реакционной способности соединения.

Abstract

Today, important research is being conducted in the field of accurately describing the properties of high-molecular compounds and the chemical reactions involved in them with high theoretical accuracy.This paper presents the results of the reactivity of furfural and urea molecules required to obtain furfuralidenurea calculated using a modern Gaussian98 computer program. The electronic structure of the furfuralidenurea molecule, optimized geometric parameters, atomic charges were calculated with high accuracy. Theoretically necessary results were obtained on the reactivity of the compound.

Kalit so'zlar: *furfurol, karbamid, furfurolidenkarbamid, kvant-kimyoviy hisob, atom zaryadi, bog' uzunligi, Gaussian.*

Key words: *furfural, urea, furfuralidenurea, quantum chemical calculation, atomic charge, bond length, Gaussian.*

Ключевые слова: *фурфурол, мочевина, фурфуралиденкарбамид, квантово-химический расчет, заряд атома, длина связи, Gaussian.*

INTRODUCTION

It is known that the physicochemical properties of molecules and their reactive activity are related to their electronic structure and energy properties [1]. In modern chemistry, the method of quantum chemical calculation to determine the interatomic and intermolecular interactions of a molecule of matter, its spatial structure is widely used. Quantum chemical calculation is the fastest, most accurate, and most convenient method for determining the molecular properties of a complex organic substance [2]. Quantum chemistry makes it possible to explain experimental data on the

reactivity of organic compounds and to theoretically determine possible reactions. The Gaussian program is widely used in performing these calculations.

MATERIALS AND METHODS

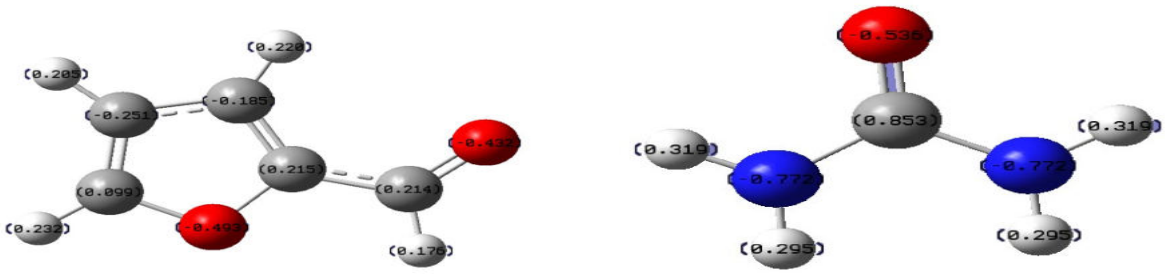
One of the important tasks of research in the field of predicting the properties of high molecular weight systems is to expand the possibilities of describing and determining the properties of high molecular weight compounds using mathematical and computer computational methods [3].

The reactivity of substances depends on many factors, the existence of a number of functional groups is a general concept, and now in the context of modern quantum chemistry there is a need to clarify the fundamental concepts of this problem [4].

Quantum chemical calculations to find the geometric parameters of furfuralidencarbamide and the reagents required to obtain furfural, urea molecules were performed in a computer program Gaussian 98 with a density function DFT / B3LYP method with a set of 3-21 G bases [5].

RESULTS AND DISCUSSION

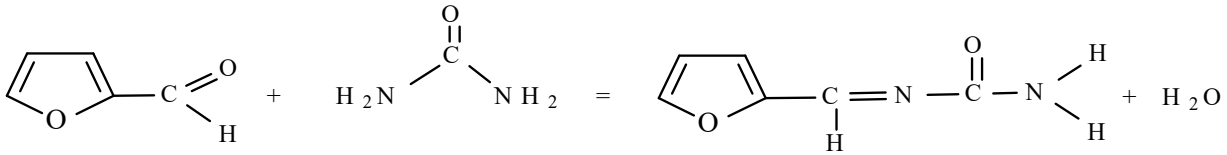
Using a Gaussian 98 computer program, data were first obtained on the interaction of furfural and urea molecules as a result of calculations. Figure 1 below shows an image of the charges of the atoms they form.



a) furfural ***b***) urea

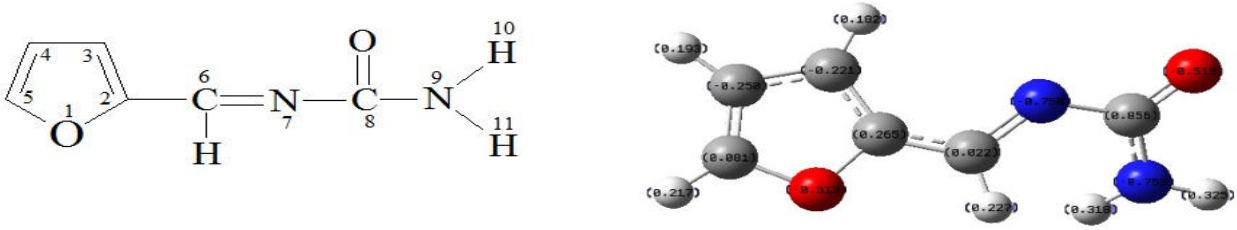
Figure 1. Charge distribution in the atoms of the reagent molecule:

Based on the calculation of the reactive activity of the reagent molecules in the program, we theoretically evaluated the formation of a furfuralidenurea compound, which reacts as follows when they are taken in a ratio of 1: 1. Potential reaction centers were identified based on the redistribution of electron charges in reagents.



It can be seen from this reaction that the furfuralidenurea compound is formed as a result of the accumulation of urea instead of the oxygen atom in the aldehyde group in the furfural molecule. In this process, the oxygen in the aldehyde group interacts with the hydrogen in the urea to form water.

The optimized geometry of the resulting furfuralidenurea molecule was determined. The results



obtained are shown in figure 2 and table 1.

Figure 2. Conditional numbering of atoms in the furfuralidenurea molecule and electron charge distribution

Table 1

Geometric parameters and charges of atoms of furfuralidenurea molecule

№	Атом	Atomic charge, e	Bond	Link length, Å
1	*O1*	-0,513	*O1-C2*	1,416
2	*O9*	-0,515	*C2-C3*	1,401
3	*C2*	0,265	***C3-C4***	**1,425**
4	*C3*	-0,221	*C4-C5*	1,369
5	*C4*	-0,250	*C5-O1*	1,404
6	*C5*	0,081	*C2-C6*	1,368
7	*C6*	0,022	*C6-N7*	1,390
8	***C8***	**0,856**	*N7-C8*	1,405
9	***N7***	**-0,758**	*C8-O9*	1,237
10	***N9***	**-0,765**	*C8-N10*	1,376
11	*H3*	0,182	***N10-H11***	**1,011**
12	*H4*	0,193	***N10-H12***	**1,012**
13	*H5*	0,217	*C3-H3*	1,076
14	*H6*	0,227	*C4-H4*	1,076
15	*H11*	0,328	*C5-C6*	1,074
16	*H12*	0,316	*C6-H6*	1,081

From the results obtained, we can see that the negatively charged O1, O9, C4, N7, N9 atoms in the optimized furfuralidenurea molecule exhibited their states (q ≈ -0.513; -0.515; -0.221; -0.758, -0.765 e), respectively. The highest negative charges were observed on the N7 and N9 atoms. All other atoms were positively charged, and the highest charge (q ≈ 0.856 e) was found to be in the C8 atom. The C3-C4 bond length in the furan ring has the largest value (d ≈ 1,425Å) and the shortest bond length corresponds to the $d_{N10\text{-}N11}$ and $d_{N10\text{-}N11}$ bonds (d ≈ 1,011 and 1,012Å), respectively. Based on the calculated charge distribution and the length of the bonds, it was found that the probability of electrophilic exchange of the nitrogen atom in the amide group in the molecule is high and that the oxygen atom in the furan ring is the center of the electrophilic attack [6].

CONCLUSION

The electronic structure of the furfuralidenurea molecule was determined, and the distribution of electron charges and geometric quantities in the atoms were calculated with high accuracy using the Gaussian program. The reactivity of molecular atoms to obtain furfuralidencarbamide complexes was determined. Based on the results obtained, the potential derivatives of the reaction were evaluated and the yield of furfuralidencarbamide-based products with high yield was theoretically substantiated.

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