Web of Discoveries: Journal of Analysis and Inventions
webofjournals.com/index.php/3

QUANTUM-CHEMICAL ANALYSIS OF THE SYNTHESIZED ORGANOSILICON OLIGOMER BASED ON MONOMETHYLOLUREA

Rakhimov Firuz Fazlidinovich
Ph.D., Associate Professor of the Bukhara Engineering
Technological Institute, Uzbekistan, Bukhara
E-mail: feruz.raximov.1990@mail.ru

Djunaidov Khakimjon Hamrokulovich
Trainee Teacher of the Bukhara Engineering
Technological Institute, Uzbekistan, Bukhara
E-mail: hakim _75@mail.ru

Abstract
This article presents the quantum-chemical analysis of silicon organic substance synthesized on the basis of urea, formaldehyde and tetraethoxysilane based on the Gaussian Interface program. As a result of quantum-chemical calculations, the electronic structure and energetic properties of reagents and products, including total energy, energy of formation, heat of formation, electron energy, nuclear energy, dipole moment, and the values of the charges of oxygen atoms were determined in advance of the reaction centers. It has been confirmed that the results obtained on the basis of the analysis are consistent with the general laws. When planning chemical reactions, especially when determining the technological parameters of reactions and developing technology, it is important to carry out quantum chemical calculations of the initial chemical substances and carry out mathematical modeling of the results obtained.

Keywords: Urea, formaldehyde, tetraethoxysilane, electron energy, dipole moment.

Introduction

It is well known that the chemical properties and reactivity of molecules depend on their electronic structure and energy characteristics.

Currently, quantum chemical calculation methods are rapidly developing. As a result, it is possible to estimate the geometry of molecules, calculate the stability of intermediate and transition states. The experimental calculation of such results for many reactions is associated with difficulties caused by the simultaneous occurrence of intermediate stages in a multi-stage process and the presence of intermediate products in a very short time. The rapid development of computational methods of quantum chemistry, as well as the creation of modern computing equipment and programs, made it possible to find many properties of complex organic compounds. For this reason, molecular dynamic and quantum chemical tests are currently considered important physicochemical testing methods for obtaining data necessary to establish certain mechanisms and patterns of production of organic substances [3, p. 2; 4, p. 3].

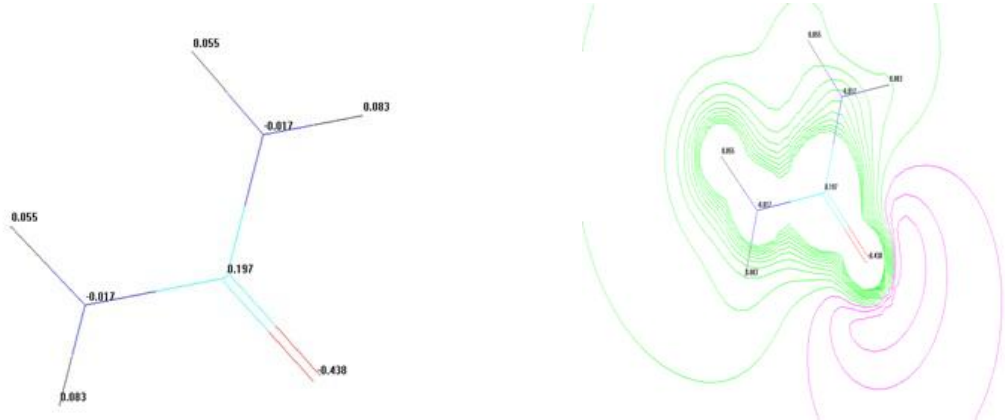
In the experimental evaluation and explanation of the reactivity of organic substances, quantum chemistry closely helps and makes it possible to predict probable reactions. The basis of today's

quantum chemistry is the Schrödinger equation, it is most often determined in a process without heat exchange for stationary states.

As a result of applying quantum chemistry methods, calculated information is obtained on the density of electron states, the arrangement of electron density, possible reaction surfaces and various spectroscopic quantities. Today, quantum chemistry methods are inexpensive, convenient and multipurpose methods for studying the electronic structure of molecules. However, it is impossible to completely abandon traditional experimental methods of testing substances [6, p. 2; 2, p. 2].

The activity of a molecule in any reaction depends largely on its structure and energy properties. With the development of quantum-chemical calculation methods, chemists have gained the opportunity to plan experimental work, carry out targeted synthesis of products and obtain substances with specified properties.

Based on the above, the electronic structure of some intermediate substances used in scientific research was studied and quantum chemical calculations were performed [1, p. 1; 5, p. 2]. Results are presented on the electronic structure and spatial geometry of the starting substances urea, formaldehyde and tetraethoxysilane (TEOS), obtained semi-empirically using the RMZ and AM1 methods (Fig. 1, 2, 3).



A **B**

Fig. 1. A, B. Charge distribution in the urea molecule

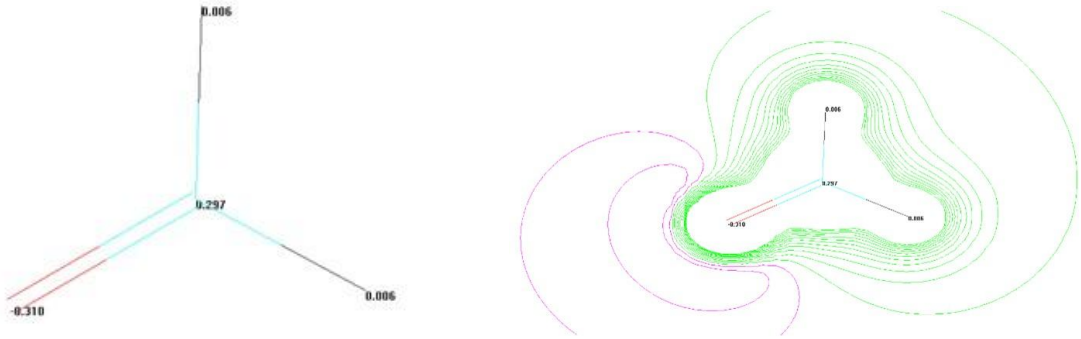
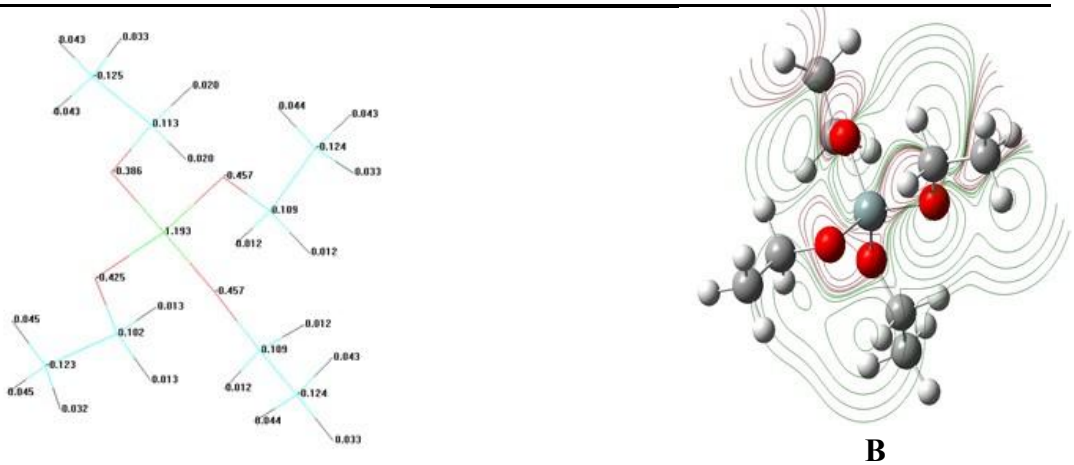


Fig. 2. Electron distribution of the formaldehyde molecule



A **B**

Fig. 3. A, B. Distribution of energy and electrons in the tetraethoxysilane molecule

The separation of atomic charges in the studied molecules shows that, based on the distribution of the negative and positive charges of the molecules of the starting materials, their reactivity is high and they can react with various compounds.

Based on the above, the electronic structure and charge distribution were studied taking into account that the addition of tetraethoxysilane to the monomethylol derivative formed by urea with formaldehyde is considered an intermediate state in our experiments (Fig. 4).

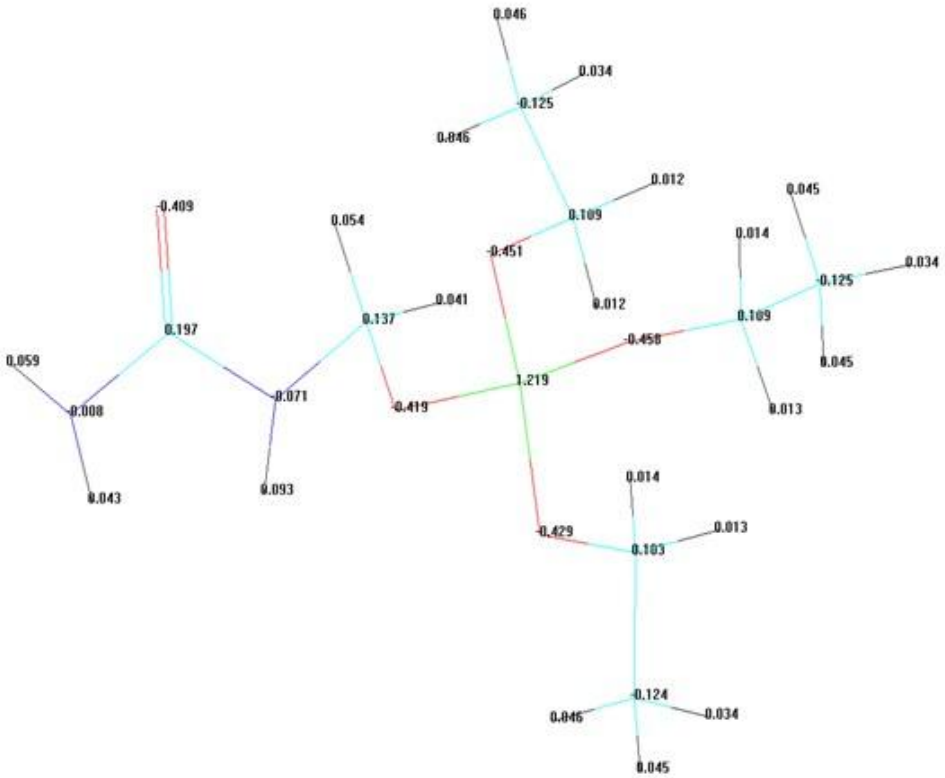


Fig. 4. Distribution of electronic charge in the intermediate state of monomethylol urea with tetraethoxysilane.

Quantum-chemical calculations of the selected substances for the synthesis of organosilicon compounds were studied, the obtained data are presented in Table No. 1. The energy properties

Web of Discoveries: Journal of Analysis and Inventions
webofjournals.com/index.php/3

of the molecules taken (total energy, formation energy, formation heat, electron energy, nuclear energy, dipole moment, oxygen atom charge) and the electronic structure, as well as the reaction the center in them can be determined in advance[7].

Table No. 1

Quantum-chemical calculations of the compounds used

Compounds	Total energy kcal/mol	Energy of formation, kcal/mol	Heat of formation, kcal/mol	Electron energy eV	Nuclear energy kcal/mol	Dipole moment (D)	Charge of the oxygen atom
Primary substances							
Urea	-18418	-705	-41,04	-54689	36270	4,071	0,1017
Formaldehyde	-10209	-368	-34	-19246	9037	2,164	0,06
TEOS	-57886	-3082	-326	-338530	280644	2,678	0,08734
Synthesized intermediates							
Intermediate state	-72148	-3402	-361	-444066	371918		0,4244

Analyzed values of total energy, energy of formation, heat of formation, electron energy, nuclear energy, dipole moment, atomic charge oxygen also indicate that the results obtained are consistent with general laws.

When selecting chemical reactions, especially when identifying technological conditions for reactions and creating technology, it is important to carry out quantum-chemical calculations of the initial chemical compounds, and to carry out mathematical modeling with the data obtained.

References

1. Аминов Ф., Рахимов Ф., Ахмедов В. Гидрофобизатор на основе мочевинаформальдегида и тетраэтоксилана //Збірник наукових праць ΛΌГОΣ. – 2020. – С. 69-71.
2. Бахромов Х. К., Ниязов Л. Н. Квантово-химический расчет производной салициловой кислоты с пиримидином //Universum: химия и биология. – 2020. – №. 3-2 (69). – С. 36-38.
3. Игнатов С. К. Квантово-химическое моделирование молекулярной структуры, физико-химических свойств и реакционной способности //Нижн. Новгород. – 2006. С. 35-37.
4. Рахимов Ф. Ф., Беков У. С. Квантово-химические расчёты зарядов кремниорганических соединений-как основа устойчивости промежуточного и переходного состояний //Universum: химия и биология. – 2022. – №. 5-2 (95). – С. 47-50.
5. Рахимов Ф. Ф. Технология получение поливинилетинилтриэтоксисила на основе тетраэтоксисилана //Universum: технические науки. – 2021. – №. 10-3 (91). – С. 97-100.
6. Цирельсон В. Г. Квантовая химия. Молекулы, молекулярные системы и твердые тела. – 2010. С. 26-28.

7. Frisch, M. J. Gaussian 09, Revision A.02, [electronic resource] // M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox – Wallingford CT : Gaussian, Inc., 2009.
8. Karimov J. S., Djunaidov X. X. Salitsil kislotaning tiomachevina fragmenti saqlagan birikmalari sintezi tahlili //Kimyo va tibbiyot: nazariyadan amaliyotgacha. – 2022. – С. 183-184.
9. Niyazov L. N., G'apurov U. U., Djunaidov X. X. P-aminobenzoy kislotasining 4-gidrooksibenzoy kislotasi bilan hosilasining termik tahlili //Kimyo va tibbiyot: nazariyadan amaliyotgacha. – 2022. – С. 181-182.
10. Жумаев Қ. К., Комилов М.З., Джунаидов Х. Х. ЙЎЛДОШ ГАЗЛАРНИ ОЛТИНГУГУРТЛИ БИРИКМАЛАРДАН ТОЗАЛАШ АБСОРБЕРИДА ЖАРАЁННИ // НАУКА И ИННОВАЦИОННЫЕ ТЕХНОЛОГИИ В ПРОИЗВОДСТВЕ ПРОДУКТОВ ПИТАНИЯ. – 2022. – С. 574-577.
11. Джунаидов Х. Х. Создание более рентабельной абсорбционной установки для очистки природного газа от серосодержащих соединений //INTERNATIONAL SCIENTIFIC-PRACTICAL CONFERENCE ON" MODERN EDUCATION: PROBLEMS AND SOLUTIONS". – 2023. – Т. 2. – №. 2.
12. Jumaev K., Kh D. Development of a highly saving technology for purifying natural gas from sulfur-containing compounds //Sciences of Europe. – 2022. – №. 107. – С. 132-136.
13. Karimovich D. K., Khamrokulovich D. H. High Performance Natural Gas Treatment Technology //Scholastic: Journal of Natural and Medical Education. – 2023. – Т. 2. – №. 4. – С. 67-71.
14. Shamsiyeva N. F., Djunaidov H. H. Polimer chiqindilari asosida xom-ashyo olish qurilmalarida energosistemalar o'rnatish va uning samaradorligi. Zamonaviy ta'limda fan va innovatsion tadqiqotlar ilmiy–uslubiy jurnal 1-son 3-to'plam 2023 yilhttp //zamtadqiqot. uz/index.
15. Каримович Ж. Қ., Джунаидов Х. Х., Хайдарович Қ. Ж. УЮРМАЛИ АБСОРБЕРДА МОДДА АЛМАШИНИШ ЖАРАЁНИ САМАРАДОРЛИГИНИ ТАДҚИҚ ҚИЛИШ //PEDAGOGS jurnali. – 2023. – Т. 31. – №. 1. – С. 111-119.
16. Жумаев Қ. К., Джунаидов Х. Х. ТАБИИЙ ГАЗНИ НОРДОН КОМПОНЕНТЛАРДАН ТОЗАЛАШ ТЕХНОЛОГИК ТИЗИМИ // НАУКА И ИННОВАЦИОННЫЕ ТЕХНОЛОГИИ В ПРОИЗВОДСТВЕ ПРОДУКТОВ ПИТАНИЯ. – 2022. – С. 577-580.

17. Рахимов Ф. Ф., Акмалов М., Джунаидов Х. Х. Некоторые аспекты использования полимерных композиций на основе сельскохозяйственных отходов в производстве строительных материалов на основе гипса //SCientific aspects and trends in the field of scientific research International scientific-online conference. – 2022. – Т. 9. – №. 30. – С. 13-15.
18. Джунаидов Х. Х. Рост научных исследований в области экологии //Проблемы экологии и экологического образования. – 2022. – С. 53-54.
19. Shamsieva N. F. Djunaidov H.H COMPOSITES REINFORCED WITH FIBERS OR FIBROUS CRYSTALS //International Multidisciplinary Research in Academic Science (IMRAS) September. – 2024.
20. Shamsiyeva N.F., Raximov F.F., Junaidov H.H. METALL KOMPOZITSION QURILISH MATERIALLARNING TURLARI VA QO'LLANILISHI // INTERDISCIPLINE INNOVATION AND SCIENTIFIC RESEARCH CONFERENCE 3 (25), 164-167
21. Shamsiyeva N.F., Raximov F.F., Djunaidov H.H. ZAMONAVIY QURILISH MATERIALLARI ISHLAB CHIQARISH SANOATIDA ALYUMINIY VA POLIMERLARNING O'RNI // FORMATION OF PSYCHOLOGY AND PEDAGOGY AS INTERDISCIPLINARY SCIENCES 3 (34), 6-13

Web of Discoveries: Journal of Analysis and Inventions
webofjournals.com/index.php/3