Preliminary Quantum Chemical Analysis of Synthesized Monomers with the Participation of Vinylacetylene

Преаварительный Квантово-Химический Анализ Синтезированных Мономеров С Участием Винилацетилена

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Abstract – It known that the physicochemical properties and reactivity of all molecules depend on their electronic structure and energy state. Today the discovery of various mathematical modeling methods in chemistry has opened up the possibility of planning and predicting any chemical reactions in science especially in chemistry as well as conducting targeted studies of organic compounds. Based on this the article examined the electronic structure of paracresol and its vinyl derivative from monohydric phenols and quantum chemical calculations were performed. This paper examines and presents the results of quantum chemical calculations of paracresol and its vinyl derivative β-(4-methyl phenoxy) butadiene-1,3 molecules, the spatial geometry and electronic structure obtained using the semi-empirical method PM3.

Keywords – Vinilacetylene, Paracresol, PM3 Semi-Empirical Method, Monomer, Polymer, Monohydric Phenol.

Аннотация – Известно, что физико-химические свойства и реакционная способность всех молекул зависят от их электронной структуры и энергетического состояния. Сегодня открытие различных методов математического моделирования в химии открыло возможность планирования и прогнозирования любых химических реакций в науке, особенно в химии, а также проведения целевых исследований органических соединений. На основании этого в статье исследована электронная структура паракрезола и его винилового производного из одноатомных фенолов и выполнены квантово-химические расчеты. В данной статье исследуются и представлены результаты квантово-химических расчетов паракрезола и его винилового производного β-(4-метилфенокси) бутадиен-1,3 молекул, пространственная геометрия и электронная структура, полученные с помощью полумпирического метода PM3.

Ключевые слова – винилацетilen, пара-крезол, полумпирический метод PM3, мономер, полимер, одноатомный фенол.

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I. INTRODUCTION

Quantum chemical methods provide a great opportunity to understand accurate data on the reaction activity of organic substances and to predict the reactions. As a result of the application of quantum chemical methods, it is possible to obtain information on electron density, electron density distribution and calculations of various spectroscopic quantities. Today quantum chemical methods are cheap, convenient and universal for studying the electronic structure of molecules [1-3]. But it is also impossible to deny traditional experimental methods for studying substances. Because in traditional methods all external factors are taken into account. The reason is that the nature of the substances is complex and the effects of temperature, solvent nature, catalysts, etc. must also be taken into account. Quantum chemical methods only analyze the results based on theories [3-6].

II. MATERIALS AND METHODS

Based on the above, the three-dimensional appearance, electronic structure were studied and quantum-chemical calculations were carried out, proving the compatibility of practical and theoretical knowledge of the substances used for synthesis. The results obtained by semiempirical PM3 and AM1 methods on the spatial geometry and electronic structure of phenol molecules were studied using the example of ortho- and paracresols and their vinyl esters.

III. RESULTS

The distribution of charges in the atoms in the molecules studied above showed that the negative charge value on the oxygen atom in the hydroxyl group of the molecules of the starting materials was high (-0.228). Therefore, under the reaction conditions studied in phenols, the vinyl reaction takes place at the expense of their hydroxyl group (Figures 4-8).
Figure 4. Distribution of charges in atoms in a vinylacetylene molecule

Figure 5. The distribution of charges on the atoms of the orthocresol molecule

Figure 6. Distribution of charges on atoms of a paracresol molecule
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Figure 7. Electron density distribution in a vinylacetylene molecule

Figure 8. Electron density distribution in the orthocresol molecule
Based on the data obtained due to the high electronegativity of oxygen in the hydroxyl group in the starting material the electron cloud distribution is relatively dense and the electrophilic reagent is a possible reaction center and the vinylation process takes place in these centers. Quantum chemical calculations of synthesized vinyl compounds were also performed to provide a more complete description of the substances and to be used as a database (Figures 10-11).
The electronic structure and energy properties of the molecules obtained for synthesis (total energy, formation energy, heat of formation, electron energy, nuclear energy, dipole moment, charge of the oxygen atom) allow to analyze aromatic phenol molecules and determine in advance the reaction centers in them.

IV. CONCLUSION

In the planning of chemical reactions, especially in the determination of technological parameters of reactions and the development of technology it is important to perform quantum chemical calculations of primary chemicals and mathematical modeling of the obtained results. Quantum chemical calculations of source materials and compounds used for synthesis: spatial 3D structure of the molecule, distribution of charges and electron densities in the atoms of the molecule, total energy of the molecule, energy of formation, heat of formation, electron energy, nuclear energy, dipole moment and important calculations the charge of the oxygen atom is determined. Based on the analysis of the results, it was scientifically hypothesized that the vinylation process is due to the oxygen of the hydroxyl group and the results of the experiment were proved on the basis of spectral analysis.

V. ACKNOWLEDGMENTS

The author of this work acknowledges the gratitude to the rector of the Bukhara Engineering and Technology Institute N.R. Barakaev for his supporting the development of science and created conditions for doctoral students and scientific researchers at the educational institution, and the head of the department of Bukhara State Medical Institute PhD L.N. Niyazov for his assistance in organizing and conducting laboratory and measuring work regarding the determination of activated sludge concentration by mass and optical methods. And also we want to express special gratitude to our colleagues for the invaluable experience transferred to us in the process of research and mentoring.

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