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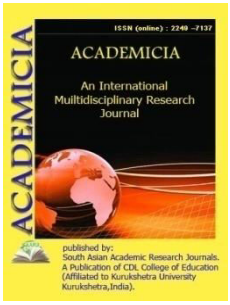

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QUANTUM CHEMICAL CALCULATION OF PIPERIDINE-BASED SYNTHESIZED COMPOUNDS USING THE PM-3 SEMIEMPIRICAL METHOD

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ABSTRACT

The article provides estimates of the geometry of molecules, calculation of the stability of intermediate products and transition states. Calculation of the results for the majority of reactions is carried out experimentally. Along with a multi-stage process, difficulties are inherent in the appearance of intermediate stages and the presence of intermediate reaction products in an extremely short time.

KEYWORDS: *semiempirical methods, RM3 and AM1, 3D structurepiperidine, acrylic acid, metacrylic acid .*

INTRODUCTION

Today, the methods of quantum chemistry and molecular dynamics are widely used in the numerical simulation of the electronic and atomic structures of complex systems of molecular, crystalline, and transitional (nano) sizes. This is due to the technological development of the corresponding software[1-2]. Nowadays, there are quite a few modern computational complexes operating in the world that implement the methods of quantum chemistry and molecular dynamics, however, for a wide range of users, the use of these methods is most accessible is

provided by the well-known quantum-chemical and molecular-dynamic program HyperChem[3-4].

RESEARCH METHODS AND TECHNIQUES

As is known, the physicochemical properties and reactivity of molecules are associated with their electronic structure and energy characteristics [5]. The rapid development of methods for quantum chemical calculations and the emergence of powerful computer tools have made it possible to determine many properties of complex organic substances. In this regard, in quantum chemical and molecular dynamics research, when obtaining information necessary to create certain patterns and mechanisms for the synthesis of organic compounds, these methods of physical and chemical research are of particular importance [6].Quantum chemistry makes it possible to explain experimental data on the reactivity of organic compounds and predict possible reactions. The basis of modern quantum chemistry is the Schrödinger equation, which is usually solved for stationary states in an adiabatic process [7]. Using the methods of quantum chemistry, it is possible to obtain data on electron density, electron density distribution, potential reaction regions and various spectroscopic calculations. Currently, the methods of quantum chemistry are the cheapest, simplest, and most versatile methods for studying the electronic structure of molecules. However, it is impossible to completely abandon the traditional experimental methods of studying substances. Since in traditional methods all external factors are taken into account. Due to the complex nature of substances, it is necessary to take into account the influence of temperature, the nature of the solvent, catalysts, etc. [8].

RESEARCH RESULTS AND DISCUSSION

This section presents the results of quantum chemical research on the geometric, electronic structure of synthesized compounds. The electronic and spatial structure of the synthesized compounds, the distribution of electrons, the optimal geometry, the bond lengths between the atoms, the charge values of the atoms were determined. Quantum chemical calculations of 1-chloro-3-piperidine-2-propanol, 1-chlorine-3-piperidine-2-propyl-acrylate and 1-chlorine-3-piperidine-2-propyl-methacrylate molecules,PM-3 semi-empirical was performed using the method (calculations in the program Hyper Chem 8.07)the results of quantum chemical calculations are given below (Figures 1, 2, 3).

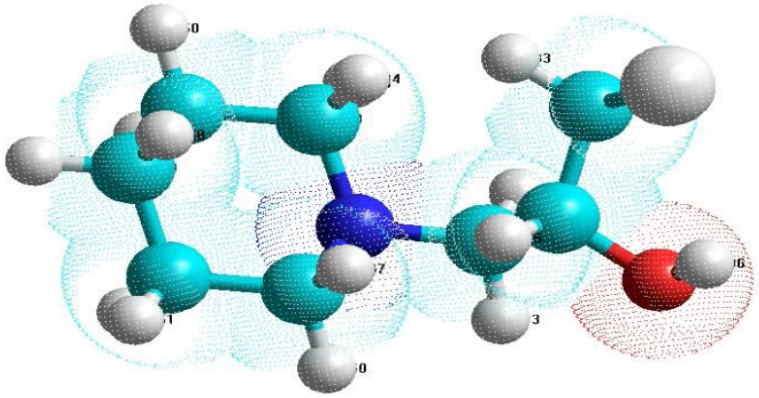

Figure 1.3D structure of 1-chloro-3-piperidine-2-propanol.

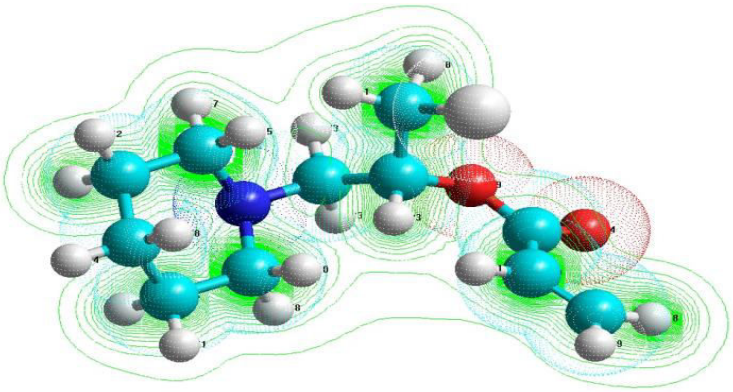

Figure 2. 1-chlorine-3-piperidine-2-propyl acrylate 3D structure

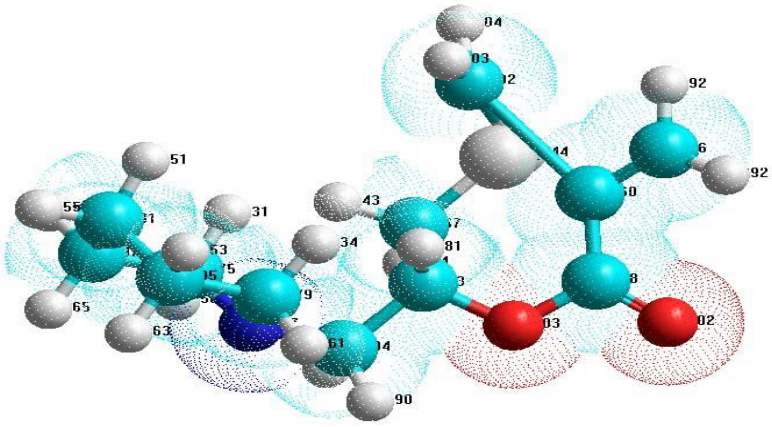

Figure 3. 3D structure of 1-chlorine-3-piperidine-2-propylmethacrylate

Based on the analysis of the charge distribution in the atoms of the molecules of the synthesized substances, it can be seen that the negative charge values are slightly more concentrated in the oxygenatoms (Figures 4, 5., And 6).

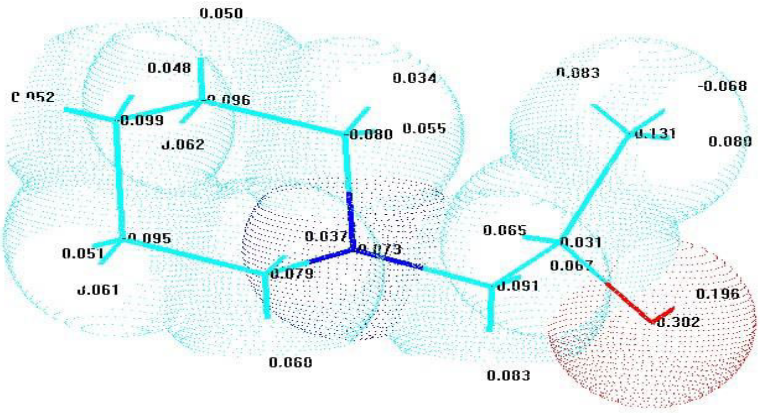

Figure 4. Charge distribution in the 1-chloro-3-piperidine-2-propanol molecule

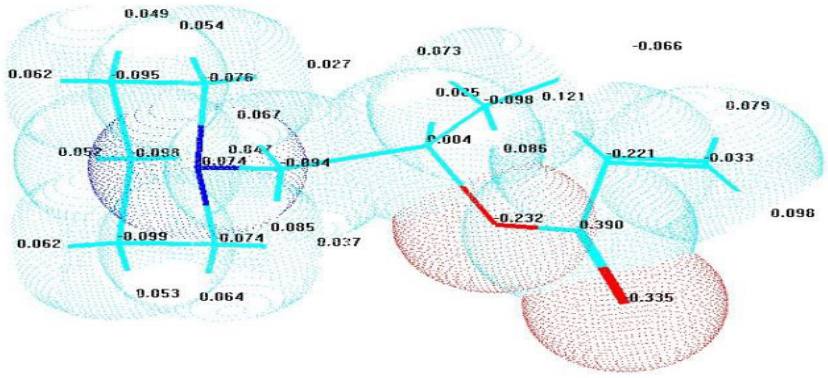

Figure 5. Charge distribution in the 1-chlorine-3-piperidine-2-propylacrylate molecule

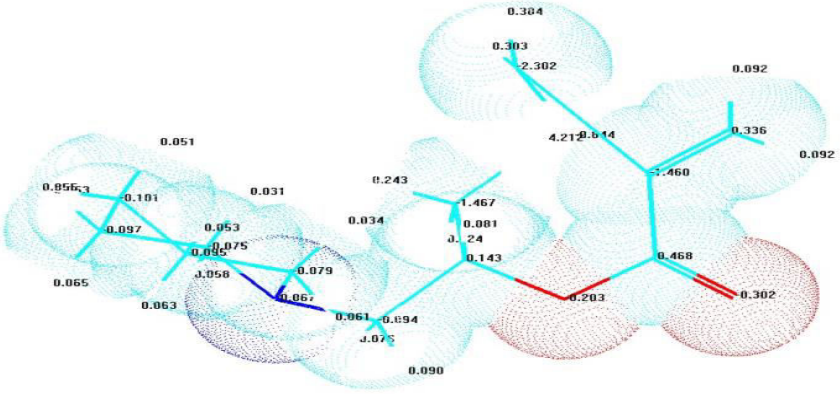

Figure 6. Charge distribution in 1-chlorine-3-piperidine-2-propylmethacrylate molecule

The distribution of electron densities in the molecules of the above substances is also calculated.

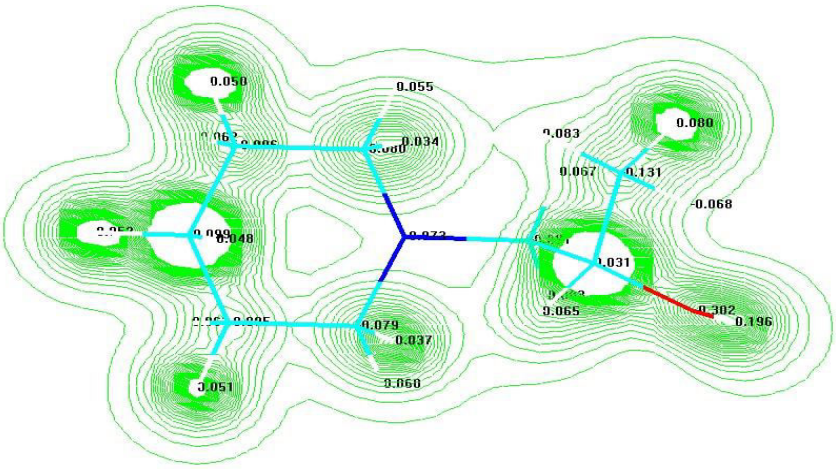

Figure 7. Electron density distribution in the 1-chlorine-3-piperidine-2-propanol molecule

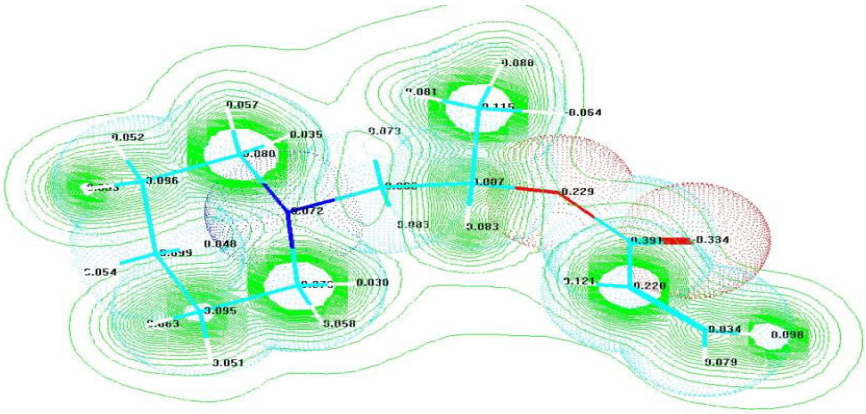

Figure 8. Electron density distribution in the 1-chlorine-3-piperidine-2-propylacrylate molecule

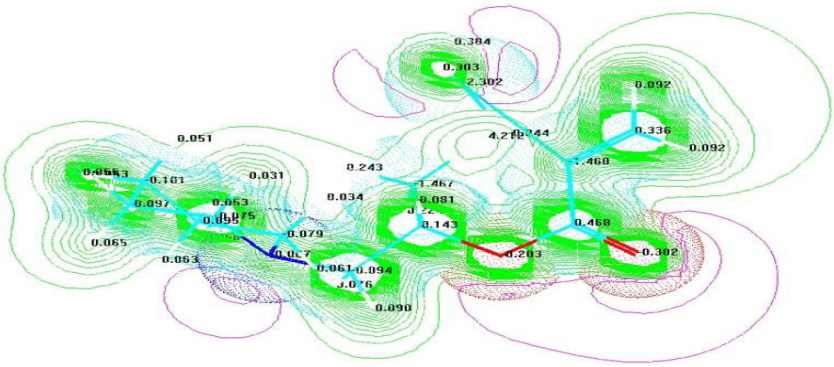

Figure 9. Electron density distribution in 1-chlorine-3-piperidine-2-propylmethacrylate molecule

From the data obtained, it can be seen that the oxygen atom in the studied substances has a high electro negativity value and it is denser than other atoms. It is possible to determine the reaction center of heterocyclic molecules by quantum chemical calculations of the electronic structure and energy properties of the selected molecules (total energy, formation energy, heat of formation, electron energy, dipole moment) (Table 1).

TABLE 1 QUANTUM CHEMICAL CALCULATION OF SYNTHESIZED COMPOUNDS

Name of compounds Total energy is kcal/mol	The energy of formation is kcal/mol	Heat of formation, kcal/mol	Heat of formation, kcal/mol	Electronic energy, eV	Nuclear energy, kcal/mol	Dipole moment (D)
1-chloro-3-pipyridine-2-propanol	-45396,29	-2476,10	-73,80	-254839,69	209443,40	0,9793
1-chlorine-3-piperidine-2-	-61054,94	-3165	-85,33	-392416,96	331362,17	3,653

propyl acrylate						
1-chlorine-3-piperidine-2-propyl methacrylate	-58345,7	-3019,91	-112,06	-360759,54	302413,83	3,906

In conclusion, it can be said that the results of the study show that the value of the negative charge in the compounds is heterocyclic. Concentrated slightly more in the oxygen atom located in the side chain than in the ring.

This can be explained by the electro negativity values of the atoms of the element, as the oxygen atoms in the substance perform the function of electro donation because they exhibit a high electro negativity value[9].

An amino alcohol was synthesized on the basis of piper dine and epichlorohydrin. The esterificationreaction of acrylic and meth acrylic acids with the obtained amino alcohol was studied. The kinetic laws of radical polymerization reactions of synthesized 1-chlorine-3-piperidine-2-propylacrylates and 1-chlorine-3-piperidine-2-propyl methacrylates were studied. The order of the monomer and initiator of the reaction, the activation energy of the process were calculated, and the average characteristic viscosity of the polymers was determined using the viscometric method. Polymer hydro gels based on 1-chlorine-3-piperidine-2-propylacrylate were synthesized at relatively high temperatures. Their degree of swelling and physicochemical parameters under the influence of various conditions was determined.

IN CONCLUSION

Quantum chemical calculations of 1-chlorine-3-piperidine-2-propanol, 1-chlorine-3-piperidine-2-propylacrylate and 1-chlorine-3-piperidine-2-propyl methacrylate selected using modern computer programs(atomic charge, 3D structure, distribution of electron clouds, dipole moment, etc.) were performed. It was shown that the negative charge values in the molecules were slightly higher in the C atoms near oxygen and the double bond. Based on the results obtained by literature sources and physicochemical methods, the reaction mechanism for the formation of complex ether obtained on the basis of piper dine was proposed [10].Based on the results obtained, the mechanisms of radical polymerization of 1-chlorine-3-piperidine-2-propyl acrylate and 1-chlorine-3-piperidine-2-propyl methacrylate were presented.

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