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QUANTUM-CHEMICAL EVALUATION OF THE MECHANISM OF CONDENSATION AND CYCLIZATION REACTIONS BETWEEN HOMOVERATRYLAMINE AND GLYCINE

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Abstract

The mechanism of condensation and cyclization reactions between homoveratrylamine and glycine has been studied by semi-empirical, ab initio calculation methods. During quantum-chemical calculations HyperChem, Gaussian and ChemOffice softwares were used. Thermodynamic and kinetic objective laws of the synthesis process have been studied by building energetic profiles of the reactions of condensation and cyclization between homoveratrylamine and glycine. As well as in quantum-chemical calculations IR-spectra of the reagents and products were taken and they were compared with standard IR-spectra on their suitability degree studied by least squares methods.

Keywords: homoveratrylamine, phenylalanine, condensation, cyclization, quantum-chemical calculation, energetic line, IR-spectrum.

Introduction. It is known that studying any reaction thoroughly depends on the determination of the products formed stage by stage during a reaction and on the determination of their amount, the quantum-chemical calculations have a significant role in accomplishment of abovementioned works. Fulfillment of the quantum-chemical calculations based on the mechanism of condensation and cyclization reactions of homoveratrylamine with aminoacids and researching optimal ways for the planned synthesis of isoquinoline derivates by mathematic evaluation of the results is one of the actual problems at present time. With this purpose the proceeding mechanism of condensation and cyclization reactions between homoveratrylamine and glycine was studied by quantum-chemical methods.

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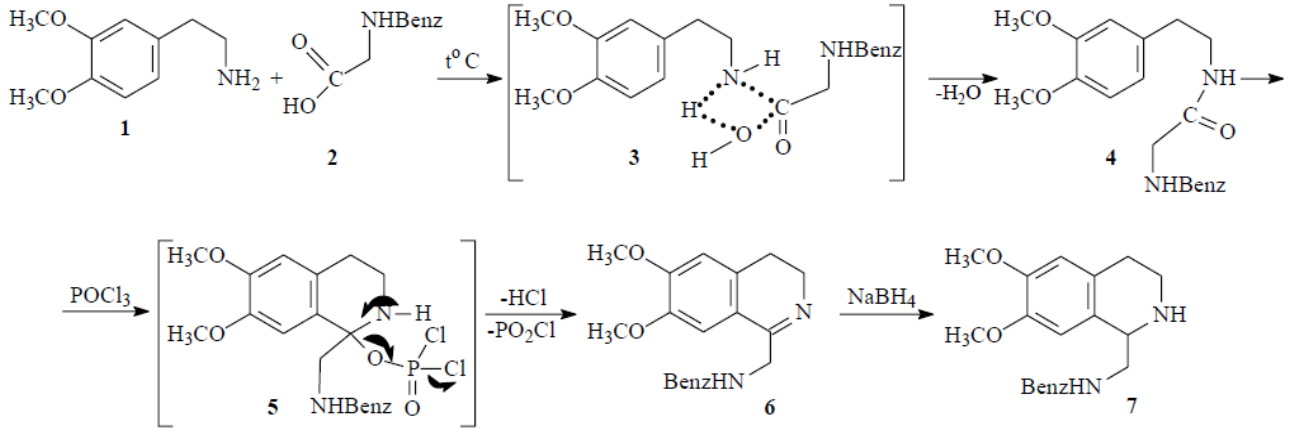
Purpose of the research

Quantum-chemical study of the proceeding of the reactions of condensation and cyclization between homoveratrylamine and glycine.

Object of the research: homoveratrylamine, glycine, quantum-chemical calculation softwares, IR-spectra.

Methods of the research: IR-spectroscopy, semi-empirical and Ab initio methods, GAUSSIAN 09 software.

The reactions of condensation and cyclization between homoveratrylamine and glycine proceed on the following mechanism:



It is shown from the reaction mechanism that homoveratrylamine (1) forms its amide (4) by the condensation reaction through transfer state (3) with glycine (2). The formed acid amide (4) in its turn, is transferred to (6) through intermediate complex (5) with the influence of water absorbing agent and finally isoquinoline derivative (7) of oleic acid is prepared as a result of hydrogenation by $NaBH_4$. Every stage of above mentioned reactions was separately analyzed by quantum-chemical calculation method.

Quantum-chemical calculation is done by functional density method using VZLYP/6-31G(d,r) basis, which is valent-separated by Ab initio method.

In calculation process, thermodynamic and kinetic objective laws of the synthesis process were studied by building energetic profiles of the reagents and products. Activation energy of the reactions ΔE_a and rate constant of the process – k have been determined by the linear transformation method on time using Arrhenius equation:

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$$\frac{d(lnk)}{dT} = -\frac{\Delta E}{RT^2}$$

The dependence chart of formation time on the temperature $lnt_0^{-1}=f(1/T)$ was plotted and calculated ΔE_a value to determine activation energy of the reactions. The results are presented in table 1.

Table 1

№	Activation energy ΔE_0 (kJ/mol)	Rate constant $k=[c]^{-1}\cdot[t]^{-1}$
Condensation reaction	60,7	$2,3\cdot10^{-3}$
Cyclization reaction	52,6	$1,26\cdot10^{-3}$

It is shown from the data in the table that the condensation reaction goes with difficulty than the cyclization reaction and this stage (stage 1) plays a limiting role in consecutive reaction.

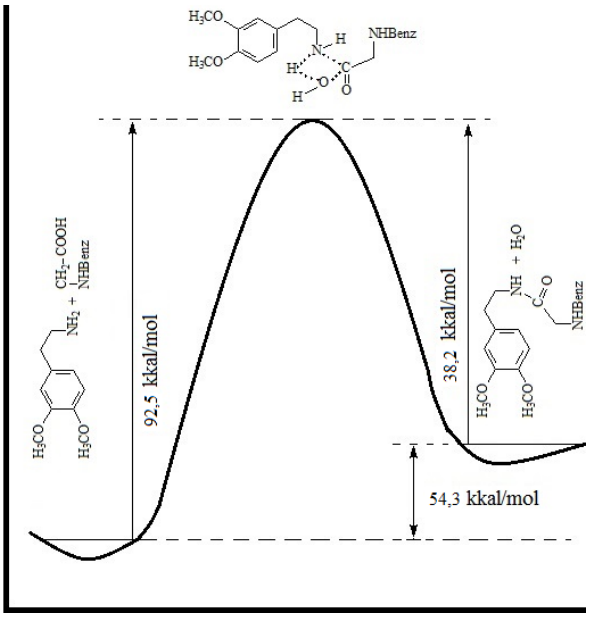

Figure 1. Energetic profile of condensation reaction

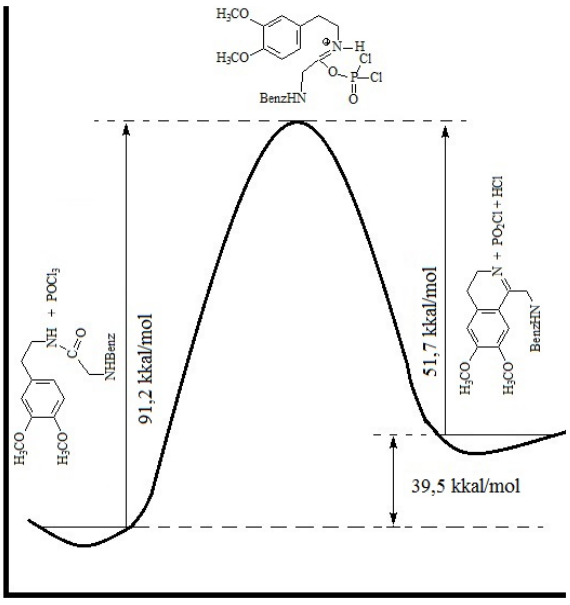

Figure 2. Energetic profile of cyclization reaction

It can be noted from the reactions data the activation energy for condensation reaction is ΔE_0=60,7 (kJ/mol), for cyclization reaction ΔE_0=52,6 (kJ/mol).

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Also IR-spectra of the products of the reactions of condensation and cyclization have been calculated through quantum-chemical method. The suitability degree of the calculated spectra with the standard IR-spectra was evaluated by calculating correlation coefficient on the least squares method. According to that the value of the correlation coefficient is respectively r=0.981 for amine, r=0.959 for glycine, r=0,982 for isoquinoline derivative. The calculated IR-spectra are presented in figures 3 and 4.

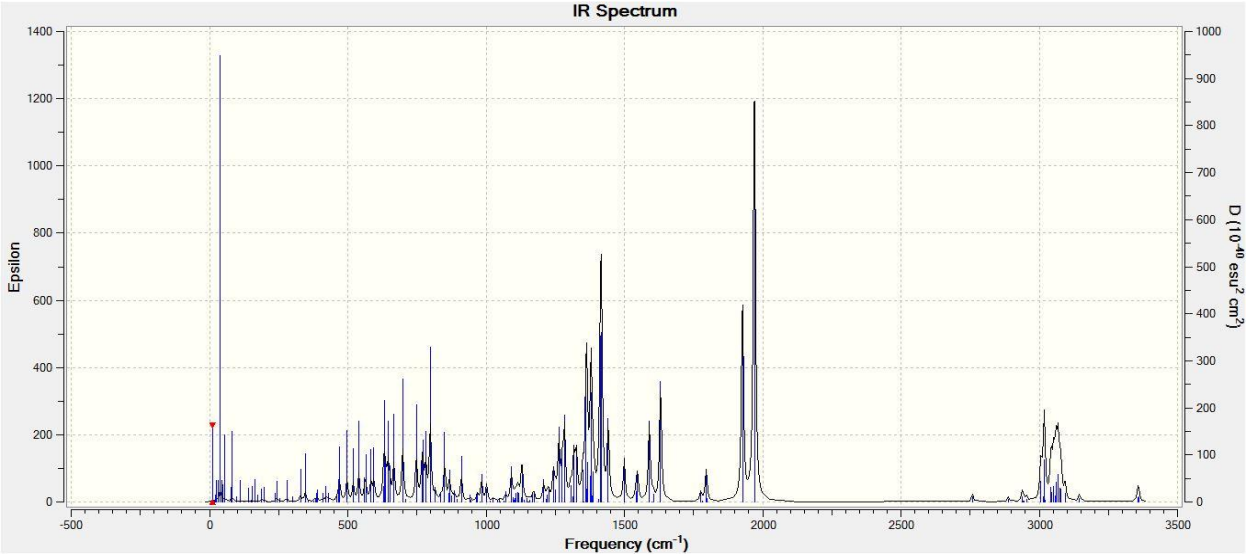

Figure 3. Calculated IR-spectrum of amide

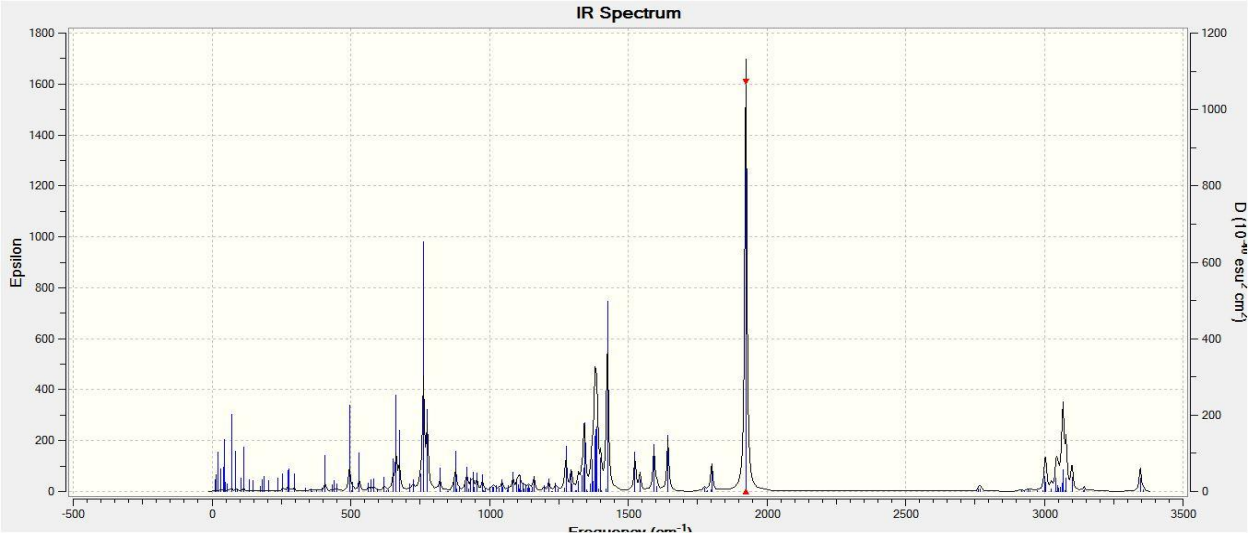

Figure 4. Calculated IR-spectrum of isoquinoline

Conclusions

1. The proceeding of the reactions of condensation and cyclization between homoveratrylamine and glycine has been studied by quantum-chemical methods and by building energetic profiles of the reaction.

2. Standard and calculated IR-spectra of the reagents were evaluated on their suitability degree determined using the least squares method.

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