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CONFORMATIONAL ANALYSIS OF UREA-SUBSTITUTED CYANURIC ACID PRODUCTS

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ABSTRACT

The paper shows how, using the software of the ChemOffice package, you can successfully solve a number of problematic issues of student education, in in particular concerning the study of conformations heterocyclic compounds. The article deals with the conformational analysis of cyanuric acid derivatives - obtained by the condensation of urea with cyanuric acid. Thus, successfully implement one of the methodological methods of education - learning through science for students and undergraduates of the university.

When studying the conformational analysis of cyanuric acid derivatives, we studied several articles and books by foreign scientists [1-5].

Previously, we published a synthesis technique, quantum chemical calculations, molecular docking, PASS analysis and IR spectroscopy of a urea-substituted cyanuric acid product [6-14].

ChemDraw Professional software easily makes chemistry stand out with unique atom, bond, and ring coloring options. ChemDraw Professional includes ^{1}H and ^{13}C-NMR predictions, Name-to-Structure and Structure-to-Name functions, and integrations to SciFinder, Reaxys, and SciFinder-n, for quick and seamless access to important scientific literature databases. Peptide and nucleic acid chemists can also take advantage of the HELM Toolbar to easily represent biomolecules.

Moreover, the Chem3D program contains great opportunities for studying the conformations of molecules - geometric shapes resulting from rotation (rotation) around single bonds by an angle φ (torsion). Newman projections are often used to depict conformations. Usually, anti (inhibited) - and gosh (beveled) - conformations are more stable. Van der Waals and torsional stresses are minimal in them. A number of factors (intramolecular hydrogen bonds, ionic interactions) can additionally stabilize the gauche conformation and make it the most stable. Long carbon chains can take irregular, claw-shaped, zig-zag conformations.

Let us study the dependence of the potential energy of the conformations of urea-substituted cyanuric acid products resulting from the rotation of some CN-CN or CN bonds and the unpaired electron of nitrogen and oxygen around the triazine heterocycle on the angle φ.

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To do this, in the working window of ChemDraw, we will use the context menu of blanks called by the "Templates" button of the main panel. You can also draw by hand. Copy the conformation and paste it into the Chem3D working window. For greater clarity, the spatial model generated in this way will be presented in the form of "Sticks" (rods) (menu item View/Model Display/Display Mode/). Let us optimize the geometry using the molecular mechanics method (MM2 function, Calculations/MM2/Minimize Energy menu item). For conformational analysis, we select the C2–C3 bond and run the program for calculating the dependence of the conformation energy on the angle φ (Calculations/Dihedral Driver menu item).

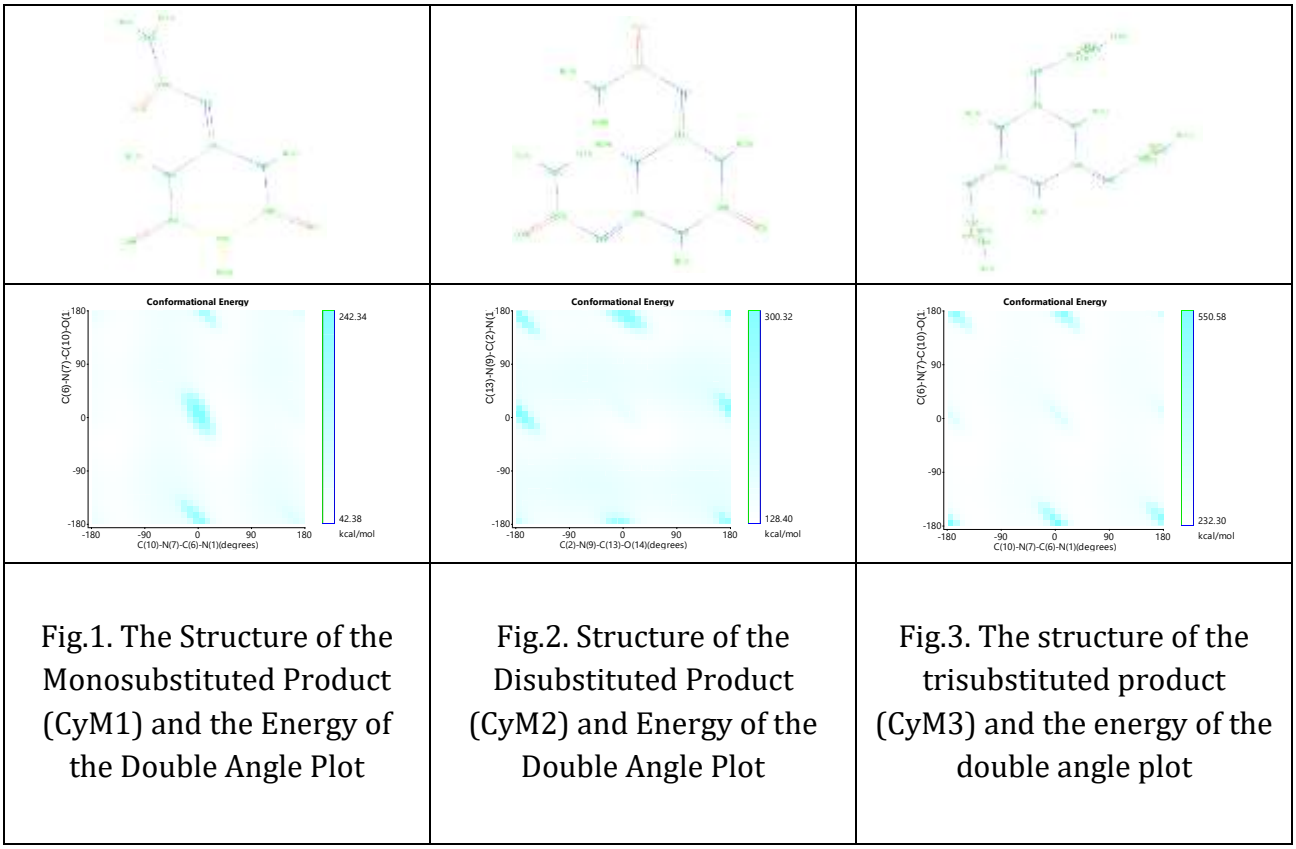

Fig.1. The Structure of the Monosubstituted Product (CyM1) and the Energy of the Double Angle Plot

Fig.2. Structure of the Disubstituted Product (CyM2) and Energy of the Double Angle Plot

Fig.3. The structure of the trisubstituted product (CyM3) and the energy of the double angle plot

Found from the graph (Fig. 1-3), the minimum and energy maxima of the plot with a double angle for urea-substituted products are as presented in tables 1.

Double Angle Plot Energy for a Monosubstituted Product	Double angle plot energy for a disubstituted product	Double angle plot energy for a trisubstituted product
242.34 max	300.38 max	550.58 max
42.38 min	128.40 min	232.30 min

Figures 4-5 below show the conformational analysis of cyanuric acid derivatives conformingaround the triazine heterocycle of some CN-CN or CN bonds and an unpaired electron of nitrogen and oxygen and dependence of energy on the internal angle.

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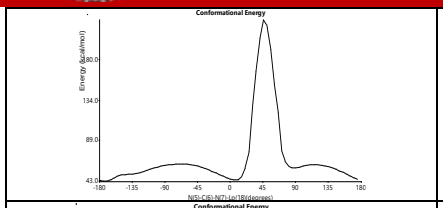


Fig.4.Energy dependencymonosubstituted product (CyM1)

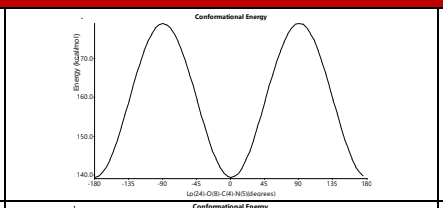


Fig.5.Energy dependencydisubstituted product (CyM2)

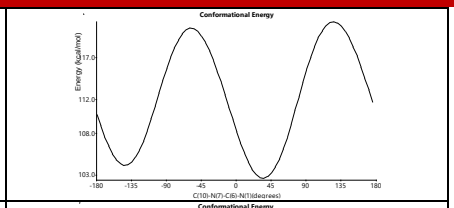
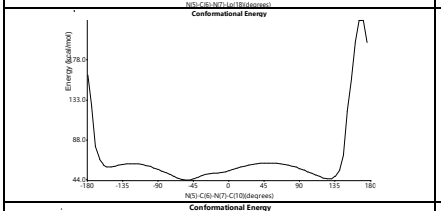
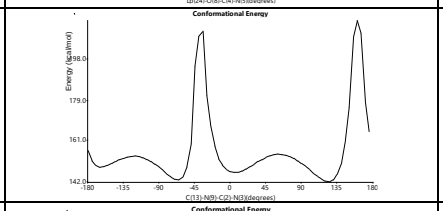
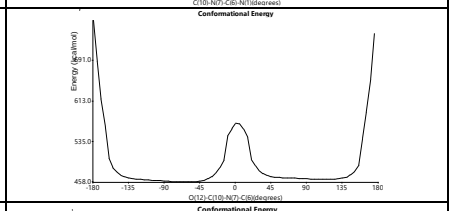
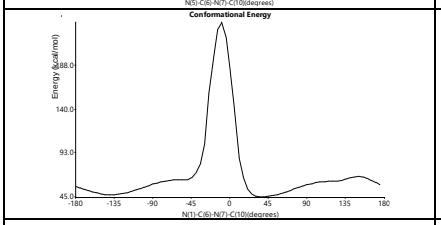


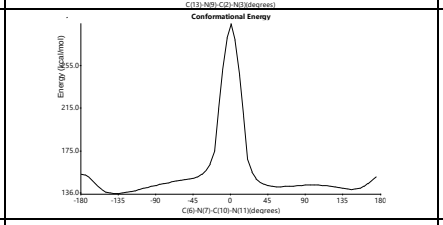
Fig.6.Energy dependencytrisubstituted product (CyM3)

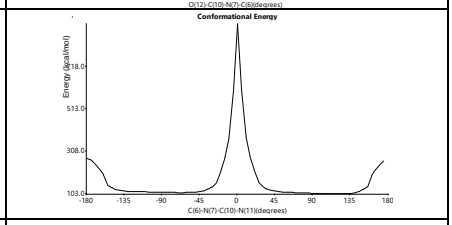












In conclusion, conformational analyzes of urea-substituted derivatives of cyanuric acid were studied and results were obtained using ChemDraw software.

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