

Using the software package Chembiooffice'2010 in the specialized chemical class

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Abstract

The recommendations for using the chemical applications of the ChemOffice in teaching chemistry at school and related scientific physical and chemical research are given. It was shown that this software package includes specialized applications like ChemDraw, which allows compiling and editing the structural formulas, Chem3D-program for visualization of the spatial structure of the compounds, as well as for physical and chemical calculations. On the example of n-butane we consider different conformations resulting from rotation around single sigma bonds. The visualization of the occupied and virtual molecular orbitals in ethylene, acetylene, benzene, butadiene molecules is carried out. The possibilities of the program for evaluation of the effective charges on the atoms and thermodynamic parameters are indicated.