STUDY OF MAGNESIUM SELENATE USING COMPUTATIONAL CHEMISTRY METHODS

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In recent years, study of the selenium physicochemical property and structure is rapidly developed. It should be noted that the selenates of the alkaline-earth elements are still not enough investigated.

In addition, the methods of quantum chemistry are among the most important tools for the theoretical study of physical and chemical properties. In connection with this, the physicochemical properties of some compounds of alkaline-earth selenates were carried out by quantum-chemical methods [1].

In order to obtain electronic and geometric structures of magnesium selenates, using ChemBio3D Ultra program to create three-dimensional models of molecules $MgSeO_4$, $MgSe_2O_7$. In quantum-chemical calculations of the structure of the investigated compounds the 3-21G basis and ab initio Hartree-Fock method were used.

$MgSeO_4$molecule is a chemical compound in which the selenium atom has a structure of six valence and hexagonal structure. The molecule $MgSe_2O_7$ is a part of polymer, and here selenium atom has the same valence and structure. The several variants of molecule structure were constructed. Among them, the most stable structure was chose. At the same time, the molecular kinetic energy of electrons, nuclear repulsion and the nuclei-electron attraction energies as a result of quantum-chemical calculations are determined [2].

In the course of the study, there was a dissimilar distribution of the electron density in molecules. In addition, the different value of atomic charges of compounds means that they have electrical properties. In other words, these molecules have electric dipole moments, being the polar ones.

References:

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2. WELLS, A. 1987. *Structural inorganic chemistry*. V.2. Moscow: Mir