

STUDY OF STRUCTURE AND PHYSICOCHEMICAL PROPERTIES OF ACIDIC SODIUM SELENITES BY COMPUTATIONAL CHEMISTRY

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Study of the physical and chemical properties of substances and determining the relationship between the structure and properties are of theoretical and practical interest.

According to the modern requirements quantum chemistry methods systemize chemical phenomena and objects and also allows predicting a geometric structure, energy and other properties of polymolecules. All of these are realized in the GAUSSIAN program. Above mentioned properties for the sodium selenites were investigated.

Three-dimensional models of molecules of the compounds with formulas of NaHSeO_3 , $\text{NaH}_3\text{Se}_2\text{O}_6$, $\text{Na}_4\text{H}_6(\text{SeO}_3)_5$ are built by GAUSSIAN 2009 and ChemBio3D Ultra programs. Their geometric and *physicochemical* parameters are individually identified. Also comparative analysis of the properties is carried out.

Selenium atoms in NaHSeO_3 , $\text{NaH}_3\text{Se}_2\text{O}_6$, $\text{Na}_4\text{H}_6(\text{SeO}_3)_5$ sodium selenites has tetrahedral and flat structure.

The full energy of these molecules, the kinetic energy of electrons, the dipole moment and Mulliken charges are determined.

Furthermore, nuclear repulsion energy, electron-nucleus attraction energy, high occupied molecular orbital and low unoccupied molecular orbital energies and energy difference are calculated.

References:

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