QUANTUM CHEMICAL CALCULATIONS OF TELLURATES WITH D-ELEMENTS

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One of the most main problems of modern chemistry is to establish the relationships between the composition, structure and properties of the substances[1]. Investigation of the dynamics of chemical bond formation in the tellurium compounds and the material feature all-up optimization are actual [2]. According to thisquantum chemical calculation ofsome undefined physico-chemical properties of tellurates with d – elements is carried out.

Three dimensional spatial structures of telluratemolecules were built with ChemBioOffice and GaussViewprograms. Quantum chemical calculation of $ZnTeO_4$,$Zn_2Te_2O_8$,$Zn_3Te_4O_{15}$molecules was calculated by restricted Hartree-Fock (RHF) method with the3-21G basis. The full energy, kinetic energy of electrons, the dipole moment and atom charges by Mulliken etc.are calculated.

Because of the different electronegativity of atoms a dipole momentum appears and these molecules are strong polar.

Additionally, the nuclear repulsion and nuclear-electron attraction energies are determined.

The valence angle, bond length, internal rotation angles between some atoms of zinc tellurate are relevant to the standard value, but some aredeviated. The charges on the atoms of zinc tellurates are compared. Spreadingthe electron density between similar atoms are not the same because one defends on the closest atomic environment.

References:

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