The ionization potentials determined for all the clusters were in the range about 12.19-10.36 eV (in absolute value). The presence of atoms identical in electronegativity in clusters of sphalerite and wurtzite leads to approximately the same ionization potentials. According to this the energies of the higher occupied molecular orbitals (HOMO) for these clusters are approximately equal. The energies of the lowest unfilled molecular orbital(LUMO) in all clusters differ more appreciably: the LUMO energy, which is the largest in absolute value, is characteristic for the wurtzite cluster, and the smallest for the sphalerite cluster.

The considered sphalerite clusters Zn_4S_4 and wurtzite Zn_6S_6 have a sufficiently large difference between the energies of the boundary orbitals, i.e. upper occupied (HOMO) and lower free (LUMO) molecular orbitals. This indicates that in the clusters studied the polar covalentbond, and the clusters of iron and lead sulfides are coordinating unsaturated, which indicates their potential to form various bonds with flotation agents.

A rather interesting picture is revealed when considering the dipole moments of the clusters studied. In particular, a comparison of this characteristic for pyrite and sphalerite clusters containing the same number of atoms in their composition shows that in the first of them the dipole moment is 0.011 D, while in the second one it is absent. The dipole cluster of a wurtzite containing the same atoms as the sphalerite cluster is insignificant and equal to 0.001 D. In general, it can be noted that the dipole moments of the sphalerite and wurtzite clusters have relatively small values, which indicates a high symmetry of both models. The sphalerite cluster is completely symmetrical. Confirmation of these conclusions is the charge characteristic in all model clusters.

Thus, as a result of approbation of the semiempirical “DFT” method, the parameters described abovefor the clusters oftwo zinc sulfides are calculated for the first time.

In the flotation pulp molecules and ions of different nature can exist, and they can participate in adsorption processes on the surfaces of sulfide minerals. Therefore, first of all we carried out a quantum chemical study of the sphalerite and wurtzite model complexes with the neutral molecules of mineral acids, water and hydrogen peroxide. The model complexes of sphalerite and wurtzite for study were Zn_4S_4·HF, Zn_4S_4·HCl, Zn_4S_4·HBr, Zn_4S_4·H_2O, Zn_4S_4·H_2O_2, Zn_4S_4·HNO_2, Zn_4S_4·$HClO_2$and Zn_6S_6·HF, Zn_6S_6·HCl, Zn_6S_6·HBr, Zn_6S_6·H_2O, Zn_6S_6·H_2O_2, Zn_6S_6·HNO_2, Zn_6S_6·$HClO_2$respectively.

The results of the calculation represented in tables 2 and 3.

The cluster systems:mineral-neutral molecules. In table 2 represented models of the adsorption complex of sphalerite cluster with various molecule of some inorganic substances. Some of the results published in [6].

The binding energy or energy of the adsorption $\Delta_{adc}E$ can be defined as

$$\Delta_{adc}E = E_{adc} - \left(E_T + \sum_l E_{a,l} \right),$$

where E_{adc}, E_T and E_a are the total energies of the adsorption complex of the sulfide mineral cluster and the adsorbate respectively [4-6].