

In table 3 represented data about adsorption energies in sphalerite cluster with molecules of some inorganic acids, water and hydrogen peroxide.

Table 3 – Adsorption energies in sphalerite cluster systems - reagent molecules

Adsorption system	ΔE_{ad} , kJ/mol
HF	-142.13
HCl	-156.24
HBr	-157.23
H ₂ O	-135.12
H ₂ O ₂	-127.26
HNO ₂	-21.14
HClO ₂	-367.19

Table 3 shows that the adsorption systems of sphalerite clusters with simple molecules have negative adsorption energies that are negative in sign and average in absolute value. By changing the absolute values of the adsorption energy in the case of molecules of mineral acids, water, and hydrogen peroxide, a series can be made:



The minima energy of adsorption has HNO₂ which equal -21.14 kJ/mol and maxima energy has HClO₂ about -367.19 kJ/mol. The calculated adsorption energy allows a preliminary conclusion about the strength of the interaction of clusters and allows you to choose substances for flotation

REFERENCES

- [1] Soloviev M.E., Soloviev M.M. Computer chemistry. M.: SOLON-Press, 2005.
- [2] Tsirelson V.G. Quantum chemistry. Molecules, Molecular systems and solids: study guide for universities. M.: BINOM. Lab Knowledge, 2010.
- [3] Butyrskaya E.V. Computer Chemistry: Fundamentals of Theory and Work with Gaussian and Gauss View Programs. M.: SOLON-Press, 2011. (Ser. "Library of students") Molecular modeling for the design of novel performance chemical s and materials, (ed.) Beena Rai, Publication Date: March, 2012.
- [4] Yekeler M., Yekeler H. Reactivities of some thiol collectors and their interactions with Ag⁺ ion by molecular modeling // Appl. Surf. Sci. 2004. Vol. 236.
- [5] Yekeler M., Yekeler H. A density functional study on the efficiencies of 2-mercaptobenzoxazole and its derivatives as chelating agents in flotation processes, Colloids Surf. A: Physicochem. Eng. Aspects. 2006. Vol. 286.