

Quantum-chemical modeling of process iron and zinc sulfides synthesis from their chlorides

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Abstract

Quantum-chemical calculations are executed with use of the *Priroda 6* program by means of a hybrid method of functionality of density of DFT functional = PBE, basis of basis 4.in. High temperature of sulfides synthesis is a condition of chemical interactions between components as steady cyclic sulfuric molecules pass into radicals. However also other way of radical transformations of sulfur is known and it is connected with activation of sulfur under elektrophilic components. Calculations proved formation of difficult sulfides, the containing S_n (n = 1, 2, 4, 6, 8) in process iron and zinc sulfides synthesis from their chlorides. The activating effect of chlorides on sulfur consisting in destabilization and disclosure of cyclic molecules is established.