Full Paper _____ *Thematic Section:* Physico-Chemical Research.
Registration Code of Publication: 13-35-8-126 *Subsection:* Physical Chemistry.
The article is published on the materials of speech at the XX All-Russian Conference
"The structure and dynamics of molecular systems." Yalchik 2013.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: July 31, 2013.

Evaluation of the hyperfine interaction constants and the spin density distribution in the region of copper nuclei in cubanite

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Keywords: *resonance spectroscopy, NMR in the internal magnetic field, electric field gradient, the quadrupole parameters, ab initio electronic structure calculations, electron density distribution, hyperfine interactions, spin density distribution*

Abstract

The resonance NMR spectra of ^{63,65}Cu have been studied experimentally in a local field. Using cluster approach, ab initio evaluation of the electric field gradient at the nuclei of copper in cubanite $CuFe_2S_3$ have been made. Calculations have been carried out in the framework of the self-consistent restricted method of Hartree-Fock with open shells (SCF-LCAO-ROHF). The largest cluster for which the calculations have been carried out has a formula $Cu_7Fe_{14}S_{29}^n$ (R ~ 6Å, 50 atoms), where *n* is a cluster charge. The best fitting of values of the quadrupole parameters (quadrupole frequency ν_Q and the asymmetry parameter of the electric field gradient tensor η), determined experimentally ($\nu_Q \approx 7.3$ MHz and $\eta \approx 0.82$) and by calculation ($\nu_Q \sim 7.38$ MHz and $\eta \sim 0.87$), has been obtained for a cluster $Cu_7Fe_{14}S_{29}^{10}$. For the cluster $Cu_7Fe_{14}S_{29}^{10}$, maps of the electron density distribution in the neighborhood of quadrupole nucleus of copper have been built. Based on the analysis of the resulting electron density distribution, it is suggested that the bond in cubanite is not covalent. Evaluations of the hyperfine interaction constants have been made and maps of spin density distribution in the neighborhood of quadrupole nucleus of copper have been built. Energy level diagram calculated in the high-spin approximation ROHF, defines cubanite as semiconductor with a very narrow gap LUMO-HOMO rather well and is consistent with the notion of cubanite as semiconductor.