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Electronic structure and indirect spin-spin interactions in bournonite (CuPbSbS3) according to antimony nuclear quadrupole resonance

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Abstract

A complex sulfide CuPbSbS3 (bournonite) has been studied by the nuclear quadrupole resonance on 121,123Sb. The temperature dependences of the spectroscopic and relaxation parameters in the temperature range of 10-295 K have been obtained. The crystallochemical features of the environment of the two non-equivalent Sb positions in the unit cell have been revealed from the nuclear quadrupole resonance spectra. The existence of the lattice vibrations with the frequency ω = 110 cm-1 has been demonstrated on the basis of the temperature dependence of the nuclear quadrupole resonance frequencies. Slow beats have been observed on the decay curve of the spin echo signal. Experimental data have been analyzed in order to reveal the existence of the indirect spin-spin interactions involving Sb atoms. The indirect spin-spin coupling constant has been estimated as J = 2.5 ± 0.5 kHz. © 2013 Pleiades Publishing, Ltd.

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