

Journal of Low Temperature Physics 2015, pages 1-6

---

# Phonon Spectrum in Hydroxyapatite: Calculations and EPR Study at Low Temperatures

Biktagirov T., Gafurov M., Iskhakova K., Mamin G., Orlinskii S.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

---

## Abstract

© 2015 Springer Science+Business Media New York Density functional theory-based calculations within the framework of the plane-wave pseudopotential approach are carried out to define the phonon spectrum of hydroxyapatite (Formula presented.) (HAp). It allows to describe the temperature dependence of the electronic spin-lattice relaxation time (Formula presented.) of the radiation-induced stable radical (Formula presented.) in HAp, which was measured in X-band (9 GHz, magnetic field strength of 0.34 T) in the temperature range  $T = (10-300)$  K. It is shown that the temperature behavior of (Formula presented.) at (Formula presented.) 20 K can be fitted via two-phonon Raman type processes with the Debye temperature (Formula presented.) evaluated from the phonon spectrum.

<http://dx.doi.org/10.1007/s10909-015-1419-2>

---

## Keywords

Debye model, DFT, Phonons, Spin-lattice relaxation