Structural Properties and Lattice Dynamics of $HoFe_3(BO_3)_4$, $HoGa_3(BO_3)_4$ crystals: ab initio calculation

S. N. Krylova,[1,*] A. S. Krylov,[1] E. M. Roginskii,[2,3]

[1] Kirensky Institute of Physics FRC KSC SB RAS, Academgorodok 50/38, Krasnoyarsk, Russia
[2] Ioffe Institute, Polytekhnicheskaya 26, 194021, Sankt-Peterburg, Russia
[3] Faculty of Physics, St Petersburg State University, Petrodvoretz, 194508 St. Petersburg, Russia

[*]Corresponding Author: slanky@iph.krasn.ru

$HoFe_3(BO_3)_4$ and $HoGa_3(BO_3)_4$ crystals belong to huntite family with general formula $RM_3(BO_3)_4$ (R = Rare Earth, M = Al, Ga, Sc, Cr, Fe) and crystallize in a trigonal structure (space group R32, no. 155) with three formula units in the unit cell, Z = 3 [1]. The structure of the $HoGa_3(BO_3)_4$ crystal is presented in Fig.1. The $HoGa_3(BO_3)_4$ crystal exhibits a strong magnetoelectric effect, which is lower only than that in $HoAl_3(BO_3)_4$ among $RM_3(BO_3)_4$ [2]. The $HoFe_3(BO_3)_4$ crystal exhibits a phase transition at T c ≈ 366 K [3]. Temperature changing can induce structural and magnetic phase transitions in the borates, but their character is not clear at present in most cases. Magnetic ordering can, in principle, occur both in the iron (gallium) and holmium sublattices, and these sublattices also determine the optical properties. To interpret mechanisms and value of magnetoelectric relations it is necessary to know the structure of crystal vibrational spectra and mechanisms of them formation.

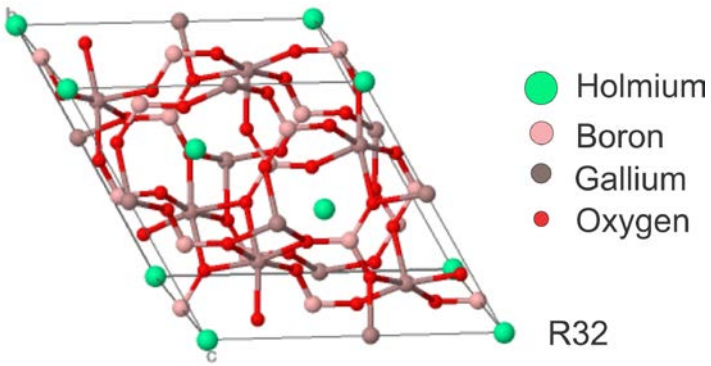

Figure 1. The structure of the $HoGa_3(BO_3)_4$ crystal

To calculate the equilibrium lattice parameters, optimization of $HoGa_3(BO_3)_4$ and $HoFe_3(BO_3)_4$ structures were performed. The structural optimization, energy and Raman calculation were carried out by the CASTEP code [4] using the density-functional theory (DFT). Analysis of the computational results allowed us to assignment of peaks in the Raman and infrared spectra.

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References

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