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Lattice dynamics of $HoGa_3(BO_3)_4$ and $HoFe_3(BO_3)_4$ crystals

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The crystals of the huntite family with the general formula $RX_3(BO_3)_4$ (R = lanthanide ions, X = Al, Ga, Fe, Cr) attract the special interest of the investigators. The stability of the huntite crystal structure due to rigidity of the BO_3 polyhedron. The optical nonliner and multiferroic properties lead to different practical applications of these materials [1-3]. The $HoFe_3(BO_3)_4$ crystal undergoes the phase transition at $T_C \approx 366$ K [4]. The low-temperature structure of the $HoFe_3(BO_3)_4$ crystal is presented in Fig. 1. The structure of two magnetic ions of different types (3d and 4f) gives rise to magnetic order at low temperatures [5]. Coexistence of structural and magnetic order parameters can open new opportunities to control their physical characteristics. The $HoGa_3(BO_3)_4$ crystal exhibits a strong magnetoelectric effect [6]. To interpret mechanisms and value of magnetoelectric relations it is necessary to know the structure of crystal vibrational spectra and mechanisms of them formation.

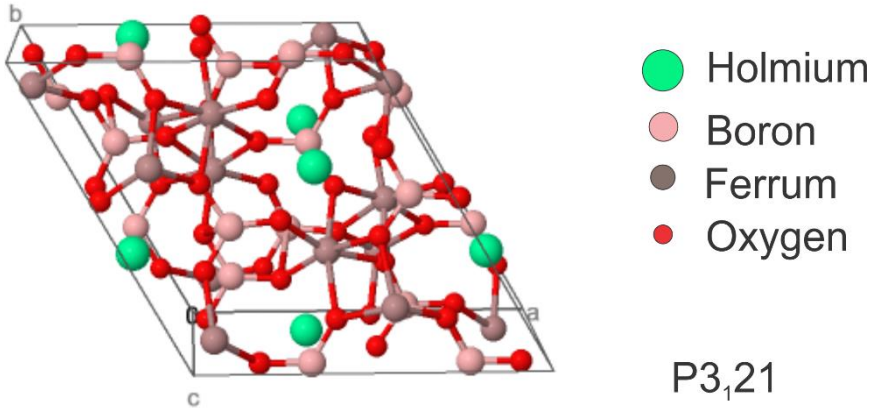

Figure 1. The structure $HoFe_3(BO_3)_4$ crystal in the low-temperature phase.

The present work devoted to ab-initio theoretical study of the lattice dynamics of $HoGa_3(BO_3)_4$ and $HoFe_3(BO_3)_4$ crystals. The calculation is based on the Density Functional Theory (DFT) approach with a plane-wave (PW) basis set using the generalized gradient approximation parameterized by Perdew, Burk and Emzerhop Perdew (GGA-PBE) [7].

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