I. INTRODUCTION

Natural stillwellite \cite{1,2} is a rare earth mineral, which accepts a very wide range of substitutions, described by the general formula \((Ln^{+3},M^{+2})B(Si,Ge,Al,P)(O,OH,F)\_5.0\) where \(Ln=La, Ce, Pr\), or \(Nd\). Among these, \(LaBGeO_5\) (LBG) can be taken as a prototype to represent the series of the larger rare-earth borogermanate stillwellite compounds. LBG is well-known for its fascinating ferroelectric and nonlinear optical properties. \cite{3,4}

LBG is characterized by its low ferroelectric transition temperature, \(T_c = 530^\circ C\). It exhibits a significant pyroelectric coefficient \(\sim 5-10 \, nC \, cm^{-2} \, K^{-1}\), a low dielectric constant \((\sim 11)\), a dielectric loss of \((\tan \delta \sim 0.001)\) at room temperature, a second harmonic generation efficiency \((SHG)\) of \(\sim 30\) units of a quartz. It also maintains a high electric resistance up to \(\sim 500^\circ C\). \cite{5,6} Due to these appealing interesting properties, LBG has drawn considerable interest in recent years. Some of its applications are a self-doubling laser \cite{7,8} and more recently a substrate for growing high-quality crystalline \(InN\) thin films. \cite{11}

The LBG crystal has a trigonal stillwellite \((CeBSiO_3)\)-type structure, with a \(P3_1\) space group symmetry and three formula units \((Z=3)\) per unit cell. The principal structural units of stillwellite consist of infinite helical chains of \(BO_4\) tetrahedra running parallel to the threefold screw axis, with each three tetrahedra forming a ring. Meanwhile, the \(GeO_4\) tetrahedra were found to be connected to the remaining free vertices of one adjacent boron tetrahedron and to the lanthanide polyhedra.

Several groups have studied the polarized and unpolarized infrared (IR) and Raman spectra of LBG. \cite{12,13} Hrubá et al., \cite{15} carried out an investigation of the Infrared (IR) and Raman inelastic scattering in the temperature range of 300 to 870 K. They reported the vibrational frequencies and the frequency-dependent dielectric function. On the other hand, based on a short-range potential functional calculation model, Smirnov et al. \cite{16} reported the IR and Raman spectral active modes of LBG.

In the present study, we extend such previous results, and present detailed calculations of the vibrational and dielectric properties of LBG using the state of the art \(ab\) \(initio\) density functional theory with the existing experimental data with a deviation of less than 0.2\%. Both the density of states and the electronic band structure are calculated, showing five distinct groups of valence bands. Furthermore, the Born effective charge, the dielectric permittivity tensors, and the vibrational frequencies at the center of the Brillouin zone are all obtained. Compared to existing model calculations, the vibrational frequencies are found in much better agreement with the published experimental infrared and Raman data, with absolute and relative rms values of 6.04 cm\(^{-1}\), and 1.81\%, respectively. Consequently, numerical values for both the parallel and perpendicular components of the permittivity tensor are established as 3.55 and 3.71 (10.34 and 12.28), respectively, for the high-(low-)frequency limit.

II. METHOD OF CALCULATIONS

The calculations have been performed using the state of the art \(ab\) \(initio\) plane-wave density functional method, as implemented in the ABINIT code. \cite{17} The all-electron potential is approximated by norm-conserving pseudopotentials generated within the Troullier-Martins \cite{18} and
extended Teter schemes. The pseudopotentials are constructed considering the following states as valence states: La$(5s^2, 5p^6, 6s^2, 5d)$, Ge$(3s^2, 3p^6)$, B$(3s^2, 3p^1)$ and O$(2s^2, 2p^4)$. The wave functions are expanded into a plane-wave basis set up to a kinetic energy cutoff of 40 Ha. The Brillouin zone integration is performed using a special $4 \times 4 \times 4$ grid of $k$-points generated with the Monkhorst-Pack scheme. We have checked that the computations are well converged with these numerical parameters. The density of states calculations are carried out using the tetrahedron method using a $16 \times 16 \times 16$ grid of $k$-points. The electron-electron interaction is approximated within local-density approximation (LDA).

III. RESULTS

A. Structural properties

The calculated atomic positions (this work) of the non-equivalent atoms (one unit) are shown in Table I along with the existing experimental results. The structural parameters of the other atoms in the unit cell can still be calculated by invoking symmetry operations. The calculated lattice parameters gave values of $a=6.957$ Å and $c=6.742$ Å. These results are in good agreement compared with the reported experimental X-ray single-crystal diffraction values of $a=7.002$ Å and $c=6.860$ Å. The theoretical results that have been predicted by this investigation underestimate the experimental lattice parameters by less than 2%, which is a typical LDA error. Table III shows the inter-atomic distances of anion-oxygen for B and Ge tetrahedra as well as La Polyhedra. Both B and Ge tetrahedra are connected to O1 and O2. The Ge-O1(O2) are almost the same. A similar behavior is found in the case of B-O1(O2). The atoms O3 and O4 represent free vertex of the Ge tetrahedra with distances slightly smaller than those of Ge-O1(O2). The atom O5 is a bridge connecting adjacent B tetrahedra. Similar to the case of Ge, the B-O5s distances are found slightly smaller than those of B-O1(O2). The result makes it easier to distinguish between three different classes of oxygen atoms according to their environment. The first class consists of O1 and O2, the second consists of O3 and O4, and the last class is represented by O5 atoms. The relaxed ionic structure at fixed lattice parameters was also calculated and the results are presented in Tables I and II. In this investigation, it was found that relaxing the ionic position at fixed experimental lattice parameter is a better choice than considering the shorter LDA lattice parameters to obtain a vibrational structure in agreement with experimental data.

B. Electronic properties

The electronic density of states accompanied by the electronic band structure along the high symmetry lines have been computed as shown in Figure 2. We found that the minimum gap is indirect at Γ-K with a value of 4.54 eV. The minimum direct gap has almost the same value and exist at Γ. However, it is a well-known fact that the DFT predictions underestimate the value of the electronic gap. For similar materials, an underestimation by 2 eV is not uncommon. A more pre-
TABLE I: Comparison of the calculated internal atomic parameters with the experimental results from Ref. [24]. The results in italic are theoretical results obtained when fixing the lattice constants at their experimental values.

|       | Theory |          |          | Experiment |          |          |
|-------|--------|----------|----------|------------|----------|----------|
|       | x/a    | y/a      | z/c      | x/a        | y/a      | z/c      |
| La    | 0.4127 | 0.4120   | -0.0009  | 0.3346     | 0.3378   | 0.4107   |
|       | -0.1613 | -0.1145 | -0.0158  | 0.3069     | 0.3111   | -0.114   |
| Ge    | 0.4191 | 0.4171   | 0.0064   | 0.8362     | 0.8384   | 0.4200   |
|       | 0.1545 | 0.1538   | 0.3495   | 0.1719     | 0.0201   | 0.1538   |
| O1    | 0.3275 | 0.3279   | 0.1415   | 0.9924     | 0.9923   | 0.3320   |
|       | 0.1347 | 0.1337   | 0.6101   | 0.3835     | 0.3402   | 0.1440   |
| O2    | 0.6063 | 0.6062   | 0.1570   | 0.3380     | 0.3320   | 0.6081   |
|       | 0.0153 | 0.0119   | 0.0625   | 0.7731     | 0.7807   | 0.0131   |

TABLE II: Anion-oxygen interatomic distances (in Å). Prime indices refer to equivalent atoms in the same or adjacent unit cells.

|       | La polyhedra | Ge tetrahedra | B tetrahedra |
|-------|--------------|---------------|--------------|
| Theory @ V_{Th.} |              |               |              |
| O1    | 2.719        | O1': 2.606    | O1: 1.730    |
| O2    | 2.692        | O2': 2.699    | O2: 1.732    |
| O3    | 2.415        | O3': 2.530    | O3: 1.673    |
| O4    | 2.414        | O4': 2.530    | O4: 1.678    |
| O5    | 2.594        |               |              |
| Theory @ V_{Expt.} |              |               |              |
| O1    | 2.753        | O1': 2.634    | O1: 1.739    |
| O2    | 2.747        | O2': 2.721    | O2: 1.740    |
| O3    | 2.435        | O3': 2.574    | O3: 1.682    |
| O4    | 2.435        | O4': 2.575    | O4: 1.686    |
| O5    | 2.635        |               |              |
| Experiment |              |               |              |
| O1    | 2.772        | O1': 2.651    | O1: 1.782    |
| O2    | 2.680        | O2': 2.684    | O2: 1.772    |
| O3    | 2.433        | O3': 2.566    | O3: 1.625    |
| O4    | 2.412        | O4': 2.589    | O4: 1.761    |
| O5    | 2.672        |               |              |

cise value of the gap can be obtained usually by employing many-body perturbation theory (the GW approximation), which is however beyond the scope of this study. However, although the DFT value of the electronic band gap is known to differ from the experimental one, the characteristics of the valence band are usually believed faithful. As seen in Figure 2, five groups of bands are identified. The lowest set (not shown, consisting of 3 bands) is located at -28 eV, characterized by a sharp DOS peak, and attributed to La s-states. The second set (consisting of 15 bands), located between -20 and -16.5 and related to O s-bands, is slightly hybridized with Ge, B and La orbitals. The third set (consisting of 9 bands) which is located between -13.5 and -12.5 eV, corresponds to La p-orbitals. The fourth bands (consisting of 3 bands) is located between -8.6 and -8.1 eV and attributed to B s-orbitals. This set is slightly hybridized with O p-orbitals. The last set, which has the largest dispersion (∼7 eV), is composed of a mix of O p-, La d-, and Ge p- and B p-orbitals. The conduction band edge consists of a mix of La-s, La-d and Ge-s with a slight hybridization of O orbitals. Analysis of the energy bands indicate a mixed ionic-covalent behavior, as will be confirmed in the following section.

C. Born effective charge

The Born effective charge tensor $Z_{\alpha\beta,j}^n$ is defined as the induced polarization of the solid along the Cartesian direction $\alpha$ by a unit displacement in the direction $\beta$ of the sublattice generated by atom $j$. Equivalently, it is the force along the direction $\alpha$ on the atom $j$ due to
a homogeneous electric field in the direction $\beta$. The effective charge tensors have been calculated for the eight non-equivalent atoms in the unit cell. The results are shown in Table [III]. The charge tensors for the remaining atoms of the unit cell can be still be obtained by invoking the symmetry operations. The charge neutrality sum rule ($\sum_j Z^*_{\alpha\beta,j} = 0$) is almost perfectly verified (with a total value lower than 0.05) suggesting that our results are well converged.

Since the local site symmetry of each ion in this structure can be completely represented by $C_1$, the charge tensors of all ions are anisotropic, with non-zero off-diagonal elements. Thus it might be more convenient to analyze the charge tensor elements along the ion principal axis (the principal values).

The effective charge of each La-ion, between 3.73 and 4.61, is anomalously large compared to its nominal ionic charges (La: +3). This agrees well with what have been obtained in case of La$_2$O$_3$. The anomalously large $Z^*$ values indicate a strong dynamic charge transfer along the LaO bond, confirming the above-mentioned a mixed ionic-covalent bond.

For Ge and B ions, the effective charges are noticeably smaller than their nominal ionic charges (Ge: +4, B: +3). The presence of five non-equivalent oxygen atoms is reflected in differences between their Born effective charge tensors. Hence, 3 different types of Oxygen atoms are recognized. Where O1 and O2 is each connected to Ge and B tetrahedra simultaneously. O5 is a bridge between two B tetrahedra. O3 and O4 are each connected to a single Ge atom.

The anisotropy of the effective charge tensor is measured by considering the deviation of each principal value from the isotropic value. The anisotropy of La-ion charge tensor is found to be (11, -1, and -10%). In case of Ge (13, -2, -11%), and (11, -4, -7%) for B. The weak anisotropy of La-, Ge-, B-ions can be understood in terms of the bonding environment. Each La-ion is surrounded by 9 O-ions with close bonding lengths.

Similar arguments can be drawn for Ge and B where both are connected by tetrahedral bonds to O-ions. Despite the small differences in bond lengths, still the isotropic environment remains a valid scenario.

### D. Vibrational and Dielectric properties

Group theory analysis, for space group $C_3$, indicates that the irreducible representations of phonon modes at $\Gamma$ are

$$\Gamma_{vib} = 24 E \oplus 24 A,$$

where $E$ and $A$ modes are doubly and singly degenerate modes, respectively, and generate together a total of 72 modes. The $E$ modes are marked by collective displacement patterns in the $x-y$ plane, while the $A$ modes has collective displacements along the $z$ direction. Due to absence of the center of inversion, all modes allow simultaneous IR and Raman activities. The contribution of these modes to the frequency dependent dielectric permittivity is calculated via

$$\varepsilon_{\alpha\beta}^0(\omega) = \varepsilon_{\alpha\beta}^{\infty} + \sum_m \Delta \varepsilon_{\alpha\beta,m}(\omega)$$

where $\Delta \varepsilon_{\alpha\beta,m}(\omega)$ is the contribution of the vibrational mode $m$ to the dielectric tensor along the Cartesian coordinates $\alpha$ and $\beta$ and given as

$$\Delta \varepsilon_{\alpha\beta,m}(\omega) = \frac{4\pi}{V} S_{\alpha\beta,m} \frac{\omega^2}{\omega^2 - \omega^2 - i\Omega}$$

$S_{\alpha\beta,m}$ is the $m$th mode oscillator strength along both $\alpha$ and $\beta$ direction. The damping frequency $\Omega$ is taken to be identical for all modes with a value 7 cm$^{-1}$.

The infrared reflectivity is related to the frequency dependent dielectric permittivity as

$$R(\omega) = \left| \frac{\sqrt{\varepsilon_{\alpha\beta}^0(\omega)} - 1}{\sqrt{\varepsilon_{\alpha\beta}^0(\omega)} + 1} \right|^2$$

The calculated phonon frequencies at the center of the Brillouin zone $\Gamma$, computed in this work, are compared with measured values and presented in Table [IV]. For comparison reasons, phonon frequencies from theoretical model calculations are also cited. For each mode, longitudinal and transverse optical (LO) and (TO) frequencies are being shown. Such splitting is normally attributed to the long range dipole-dipole interaction. Results from this investigation demonstrate good agreement with existing experimental data with absolute and relative rms values of 6.04 cm$^{-1}$, and 1.81%, respectively.

Two additional $A$ modes are found at 184 cm$^{-1}$ and 301 cm$^{-1}$, respectively. They are marked by their low oscillator strengths and as such introduce a negligible contributions to the dielectric permittivity, which explains why they were not detected experimentally.
TABLE III: Calculated Born effective charge tensors $Z^*$ along with their principal values $\lambda$. The percentages indicate the relative deviations of the principal values from the isotropic values.

| Ion | $Z^*$ | $\lambda$ | Ion | $Z^*$ | $\lambda$ |
|-----|-------|-----------|-----|-------|-----------|
|     |       |           | La  | 3.82  | 4.61      | 11%          | 3.18  | 3.66      | 13%          |
|     | 0.06  | -0.15    |      | 4.09  | 3.73      | -10%         | -0.04 | 2.15      | -2.57        |
|     | 0.14  | 4.08     |      | 2.83  | 2.44      | 11%          | 0.33  | 0.37      | 2.53         |
| B   |       |           |      | -0.13 | 0.17      | -0.14        | -1.21 | -0.15     | 2.53         |
|     | 2.59  | 0.12     |      | 2.38  | 3.38      | -4%          | 0.21  | -0.17     | 2.69         |
| O2  |       |           |      | 1.55  | 1.78      | -11%         | 0.37  | -0.18     | 2.76         |
|     | -0.53 | 0.01     |      | -2.77 | -2.19     | 32%          | -0.08 | -0.14     | 7.36         |
| O4  |       |           |      | 0.37  | -0.74     | -0.10        | 1.55  | -0.17     | 1.55         |
|     | -2.63 | -2.23    |      | -1.19 | -1.19     | 7%           | 0.35  | 0.35      | 1.78         |
|     | 0.07  | -0.17    |      | 1.06  | -1.06     | 42%          | 0.21  | -0.02     | -1.16        |

Due to the trigonal symmetry of the crystal, the electronic $\varepsilon_\infty$ and static dielectric tensors $\varepsilon_0$ possess two independent components $\varepsilon_{||}$ and $\varepsilon_{\perp}$, along and perpendicular to the $c$ axis, respectively.

These values of $\varepsilon_\infty$ and $\varepsilon_0$ are presented in Table VI. It has been noticed that the major mode contribution to $\varepsilon_\perp$ comes from $E_4$ mode (experimentally observed at 163 cm$^{-1}$), with $\Delta\varepsilon=2.77$, that is nearly 40% of the overall lattice contribution. This outcome agrees reasonably well with the experimental findings that $\Delta\varepsilon$ of the equivalent mode is found to be the largest among other modes, with a value around 2.99. Similar agreement has been found in the case of $\varepsilon_{||}$, the largest ionic contribution coming from the A$^3_5$ mode (experimentally observed at 173 cm$^{-1}$), with $\Delta\varepsilon=4.33$ in reasonable agreement with the experimental value of 4.28. The large contribution from these modes, found experimentally, had not been reproduced by the model calculations of Ref. 10.

Analyzing the eigendisplacement of the modes with the highest $\Delta\varepsilon$, namely, $E_4$ and $A_5$, we found that these modes are characterized by rigid unit translations of Ge and B tetrahedra opposite to La ions.

In general we found that the low-frequency modes have significant contributions to the dielectric tensor due to the large displacement of the La ions (for which the Born effective charge is anomalously large, as mentioned in the previous section). This is in contrast with high-frequency modes which have less contribution to the dielectric tensor, due to negligible displacements of the La ions.

The calculated IR reflectivity and dielectric loss are presented in Figs. 3 and 4 respectively, along with the correspondent measured data. The overall agreement between both calculated and experimental results is rather good as all the major features of the experimental infrared spectra are already obtained.

For comparison reasons, it is noted that $\varepsilon_\infty$ can be estimated from the refraction index $n$, which has been reported experimentally to be about 1.88, 12 $\varepsilon_\infty=n^2=3.53$. The calculated values of $\varepsilon_\infty$ are 3.55 and 3.71 for the perpendicular and parallel components, respectively. The anisotropy is weak, although non-negligible. They are in excellent agreement with experimental measurements. In fact, the reported value of $\varepsilon_0=11$ falls nicely between the presently calculated values of 10.34 and 12.28 for the perpendicular and parallel components, respectively. The ionic contribution to $\varepsilon_0$ is much more anisotropic than the electronic contribution.

**IV. CONCLUSION**

A comprehensive study of the structural, electronic, vibrational and dielectric properties of the LaBGeO$_5$ compound with the stilwellite structure has been presented.
### TABLE IV: Calculated and experimental TO and LO frequencies (in cm$^{-1}$).

The contributions of the phonon modes to the static dielectric tensor $\Delta\varepsilon$ are indicated.

| Mode | TO @ $V_{\text{Expt.}}$ | LO @ $V_{\text{Expt.}}$ | $\Delta\varepsilon$ | TO @ $V_{\text{Th}}$ | LO @ $V_{\text{Th}}$ | $\Delta\varepsilon$ | Model [16] | Experiment [15] |
|------|------------------------|-------------------------|--------------------|------------------------|------------------------|--------------------|-------------|----------------|
| $E_1$ | 90                     | 90                      | 0.05               | 91                     | 89                     | 0.04               | 101         | 1.07          |
| $E_2$ | 110                    | 111                     | 0.13               | 113                    | 114                    | 0.12               | 119         | 1.43          |
| $E_3$ | 128                    | 128                     | 0.15               | 133                    | 133                    | 0.01               | 125         | 1.85          |
| $E_4$ | 163                    | 176                     | 2.86               | 162                    | 180                    | 2.47               | 141         | 0.22          |
| $E_5$ | 183                    | 197                     | 0.56               | 196                    | 199                    | 0.42               | 187         | 0.05          |
| $E_6$ | 207                    | 211                     | 0.11               | 214                    | 214                    | 0.17               | 214         | 0.00          |
| $E_7$ | 221                    | 222                     | 0.04               | 234                    | 235                    | 0.04               | 245         | 0.01          |
| $E_8$ | 259                    | 261                     | 0.14               | 263                    | 265                    | 0.14               | 289         | 0.09          |
| $E_9$ | 307                    | 321                     | 0.90               | 310                    | 324                    | 0.81               | 319         | 0.57          |
| $E_{10}$ | 333                  | 347                     | 0.29               | 345                    | 363                    | 0.44               | 370         | 0.14          |
| $E_{11}$ | 377                 | 391                     | 0.31               | 390                    | 402                    | 0.23               | 382         | 0.21          |
| $E_{12}$ | 418                 | 431                     | 0.17               | 431                    | 446                    | 0.19               | 456         | 0.01          |
| $E_{13}$ | 446                 | 446                     | 0.00               | 458                    | 460                    | 0.01               | 518         | 0.00          |
| $E_{14}$ | 485                 | 489                     | 0.06               | 500                    | 503                    | 0.05               | 557         | 0.01          |
| $E_{15}$ | 609                 | 611                     | 0.05               | 624                    | 626                    | 0.04               | 653         | 0.00          |
| $E_{16}$ | 690                 | 690                     | 0.02               | 702                    | 703                    | 0.04               | 719         | 0.03          |
| $E_{17}$ | 723                 | 743                     | 0.32               | 737                    | 756                    | 0.33               | 717         | 0.03          |
| $E_{18}$ | 790                 | 824                     | 0.37               | 811                    | 847                    | 0.38               | 785         | 0.04          |
| $E_{19}$ | 835                 | 843                     | 0.02               | 859                    | 866                    | 0.02               | 809         | 0.02          |
| $E_{20}$ | 869                 | 872                     | 0.02               | 892                    | 895                    | 0.01               | 861         | 0.04          |
| $E_{21}$ | 912                 | 923                     | 0.10               | 930                    | 943                    | 0.10               | 936         | 0.04          |
| $E_{22}$ | 971                 | 1031                    | 0.25               | 998                    | 1056                   | 0.24               | 968         | 0.01          |
| $E_{23}$ | 1092                | 1095                    | 0.00               | 1120                   | 1124                   | 0.01               | 1043        | 0.03          |

| A$_1$ | 91                     | 93                      | 0.47               | 90                     | 90                     | 0.00               | 105         | 0.10          |
| A$_2$ | 97                     | 97                      | 0.02               | 95                     | 96                     | 0.31               | 110         | 0.16          |
| A$_3$ | 118                    | 122                     | 1.15               | 124                    | 126                    | 0.60               | 122         | 0.45          |
| A$_4$ | 148                    | 149                     | 0.18               | 154                    | 155                    | 0.17               | 142         | 0.07          |
| A$_5$ | 166                    | 184                     | 4.46               | 186                    | 196                    | 3.34               | 163         | 1.31          |
| A$_6$ | 184                    | 210                     | 0.00               | 199                    | 212                    | 0.07               | —           | —             |
| A$_7$ | 210                    | 217                     | 0.01               | 213                    | 230                    | 0.04               | 198         | 0.01          |
| A$_8$ | 280                    | 280                     | 0.00               | 283                    | 283                    | 0.00               | 284         | 0.00          |
| A$_9$ | 301                    | 302                     | 0.04               | 306                    | 307                    | 0.04               | 304         | 0.02          |
| A$_{10}$ | 303                 | 304                     | 0.01               | 319                    | 319                    | 0.00               | 340         | 0.25          |
| A$_{11}$ | 322                 | 327                     | 0.23               | 334                    | 334                    | 0.19               | 375         | 0.00          |
| A$_{12}$ | 372                 | 381                     | 0.68               | 381                    | 395                    | 0.82               | 401         | 0.47          |
| A$_{13}$ | 388                 | 419                     | 0.34               | 403                    | 433                    | 0.29               | 485         | 0.00          |
| A$_{14}$ | 492                 | 501                     | 0.14               | 498                    | 509                    | 0.15               | 555         | 0.00          |
| A$_{15}$ | 539                 | 544                     | 0.07               | 550                    | 556                    | 0.07               | 599         | 0.00          |
| A$_{16}$ | 624                 | 626                     | 0.03               | 637                    | 640                    | 0.03               | 697         | 0.00          |
| A$_{17}$ | 732                 | 744                     | 0.20               | 749                    | 762                    | 0.18               | 752         | 0.04          |
| A$_{18}$ | 810                 | 817                     | 0.12               | 830                    | 836                    | 0.08               | 792         | 0.00          |
| A$_{19}$ | 818                 | 819                     | 0.00               | 840                    | 840                    | 0.00               | 800         | 0.16          |
| A$_{20}$ | 850                 | 854                     | 0.09               | 870                    | 872                    | 0.08               | —           | —             |
| A$_{21}$ | 860                 | 873                     | 0.11               | 880                    | 896                    | 0.13               | 848         | 0.01          |
| A$_{22}$ | 948                 | 981                     | 0.43               | 986                    | 1005                   | 0.34               | 930         | 0.01          |
| A$_{23}$ | 990                 | 1043                    | 0.07               | 1013                   | 1074                   | 0.10               | 1034        | 0.07          |
TABLE V: The dielectric permittivity tensor components along and perpendicular to the trigonal axis. The sums of ionic contributions to static dielectric tensor $\Delta \varepsilon_{\text{tot}}$ are also indicated.

| $\varepsilon_{\parallel}$ | $\varepsilon_{\perp}$ | $\varepsilon_{\infty}$ | $\Delta \varepsilon_{\text{tot}}$ | $\varepsilon_0$ |
|-------------------------|----------------------|------------------------|-------------------------------|----------------|
| 3.55                    | 3.71                 | 10.34                  | 8.57                          | 12.28          |

FIG. 4: Calculated (black) and measured (red) dielectric loss parallel and perpendicular to the trigonal axis. The experimental results are from Ref. [15].

in this investigation using ab initio density functional theory. The structural parameters of this compound were found to agree well with the available experimental data with a negligible deviation of less than 0.2%. The DFT electronic structure, which had not yet been computed, has been presented. The calculated vibrational and dielectric properties of this representative compound of the larger rare-earth borogermanate family of the stillwellite structure are found to fit neatly and therefore consolidate the existing experimental published results. In particular, we improve the agreement significantly with respect to the previous model calculation.

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