Data Article

Data on vibrational spectra of the langasites \( \text{Ln}_3\text{CrGe}_3\text{Be}_2\text{O}_{14} \) (\( \text{Ln} = \text{La}, \text{Pr}, \text{Nd} \)) and \emph{ab initio} calculations

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\textbf{Abstract}

In “Lattice dynamics and structure of the new langasites \( \text{Ln}_3\text{CrGe}_3\text{Be}_2\text{O}_{14} \) (\( \text{Ln} = \text{La}, \text{Pr}, \text{Nd} \)): vibrational spectra and \emph{ab initio} calculations” [1], experimental and calculated results on lattice dynamics of the recently discovered new compounds \( \text{La}_3\text{CrGe}_3\text{Be}_2\text{O}_{14}, \text{Pr}_3\text{CrGe}_3\text{Be}_2\text{O}_{14}, \text{and Nd}_3\text{CrGe}_3\text{Be}_2\text{O}_{14} \) are reported. These compounds belong to the langasite series and constitute a new class of low-dimensional antiferromagnets. The data presented in this article includes IR diffuse transmission spectra of powder samples of \( \text{Ln}_3\text{CrGe}_3\text{Be}_2\text{O}_{14} \) (\( \text{Ln} = \text{La}, \text{Pr}, \text{Nd} \)) registered at room temperature with a Bruker 125HR Fourier spectrometer, Raman spectra taken in the backscattering geometry (also at room temperature) with a triple monochromator using the line 514.5 nm of an argon laser as an excitation, results of the DFT calculations with the B3LYP and PBE0 hybrid functionals on the optimized crystal structures, eigenfrequencies and eigenvectors of the normal vibrational modes. These data can be used to analyse electron-phonon interaction and multiferroic properties of the new langasites and to compare the lattice dynamics of different langasites.
The dataset is available on the Mendeley Data public repository at https://doi.org/10.17632/32grbb4p82.1. © 2019 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

1. Data description

The dataset includes 6 text files for our measured infrared (IR) and Raman spectra of Ln3CrGe3Be2O14 (Ln = La, Pr, Nd, raw data) [1]. These text files are named by rare-earth (RE) element symbol plus the method used to take the spectrum, e.g., Pr_IR.txt means an IR spectrum of Pr3CrGe3Be2O14. Each
The data file has two columns which correspond to wave number (unit: cm\(^{-1}\)) and IR absorbance or Raman intensity (in arbitrary units). The same data are presented also as Excel files, e.g., Pr\_IR.xlsx.

The data of \textit{ab initio} calculations of optimized crystal structures is provided in 5 Excel tables. Table 1 provides the coordinates of atoms in the unit cell for the optimized structures of Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) (Ln = La, Pr, Nd), calculated with the B3LYP hybrid functional. Table 2 provides the interatomic distances for the optimized structures of Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) (Ln = La, Pr, Nd), calculated with the B3LYP hybrid functional. Table 3 provides the lattice constants for the optimized structures of Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\)

### Table 1
Calculated (B3LYP) coordinates of atoms in the unit cell of Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) (Ln = La, Pr, Nd). The experimental data for Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) [14] are shown in square brackets.

| Ion site | Ln = La | Ln = Pr | Ln = Nd |
|----------|---------|---------|---------|
| x/a      | y/b     | z/c     | x/a     | y/b     | z/c     |
| Ln 3e    | 0.42858 | 0.0000  | 0.42797 | 0.0000  | 0.42776 |
| Cr 1a    | 0.0000  | 0.0000  | 0.0000  | 0.0000  | 0.0000  |
| Ge 3f    | 0.74264 | 0.0000  | 0.74243 | 0.0000  | 0.74235 |
| Be 2d    | 1/3     | 2/3     | 1/3     | 2/3     | 1/3     |
| O1 2d    | 1/3     | 2/3     | 1/3     | 2/3     | 1/3     |
| O2 6g    | 0.46708 | 0.30292 | 0.46748 | 0.30543 | 0.46770 |
| O3 6g    | 0.22247 | 0.09505 | 0.22352 | 0.09250 | 0.22402 |

### Table 2
Calculated (B3LYP) and experimentally determined [14] (in square brackets) M – O distances (Å) in the structure of Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) (Ln = La, Pr, Nd).

| Ln = La | Ln = Pr | Ln = Nd |
|---------|---------|---------|
| R–polyhedron | | |
| R–O1 \times 2 | 2.637 [2.577(2)] | 2.621 | 2.613 |
| R–O2 \times 2 | 2.520 [2.457(4)] | 2.473 | 2.451 |
| R–O'2 \times 2 | 2.850 [2.816(3)] | 2.827 | 2.818 |
| R–O3 \times 2 | 2.488 [2.450(3)] | 2.449 | 2.431 |
| (R–O)_{av} | 2.624 [2.575] | 2.593 | 2.578 |
| Cr–octahedron | | |
| Cr–O3 \times 6 | 1.987 [1.979(2)] | 1.984 | 1.983 |
| Ge–tetrahedron | | |
| Ge–O2 \times 2 | 1.784 [1.760(4)] | 1.781 | 1.780 |
| Ge–O3 \times 2 | 1.774 [1.733(3)] | 1.775 | 1.775 |
| (Ge–O)_{av} | 1.779 [1.747] | 1.778 | 1.778 |
| Be–tetrahedron | | |
| Be–O1 | 1.586 [1.622(6)] | 1.589 | 1.590 |
| Be–O2 \times 3 | 1.698 [1.672(3)] | 1.694 | 1.692 |
| (Be–O)_{av} | 1.670 [1.660] | 1.668 | 1.667 |

### Table 3
Experimentally determined [14] and calculated (PBE0) lattice constants (Å) of Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\).

| Ln\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) | a   | c   |
|-----------------------------------|-----|-----|
| La\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) | 8.033(2) | 4.934(2) |
| Pr\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) | 7.957(2) | 4.904(2) |
| Nd\(_3\)CrGe\(_3\)Be\(_2\)O\(_{14}\) | 7.931(2) | 4.894(2) |
(Ln = La, Pr, Nd), calculated with the PBE0 hybrid functional. Table 4 provides the coordinates of atoms in the unit cell for the optimized structures of Ln$_3$CrGe$_3$Be$_2$O$_{14}$ (Ln = La, Pr, Nd), calculated with the PBE0 hybrid functional. Table 5 provides the interatomic distances for the optimized structures of Ln$_3$CrGe$_3$Be$_2$O$_{14}$ (Ln = La, Pr, Nd), calculated with the PBE0 hybrid functional. In Tables 1–5, available experimental data are in square brackets.

The dataset includes 3 text files for the calculated with the B3LYP hybrid functional frequencies of normal modes and their intensities in the IR and Raman spectra. These text files are named by RE element symbol plus the method to get the data, e.g., Pr_abinit.txt means the calculated data for Pr$_3$CrGe$_3$Be$_2$O$_{14}$. Each text file has four columns which correspond to the symmetry of the mode (irreducible representation), wave number (unit: cm$^{-1}$), IR intensity, Raman intensity (arb. units). First, all A$_1$ modes are listed, they are followed by the A$_2$ and, then, E modes. The same data are presented also as Excel files, e.g., Pr_abinit.xlsx. Three Excel Tables, Table 6, Table 7, and Table 8, provide all calculated modes compared with those found from the measured spectra (analyzed data), in increasing order of their frequency for La$_3$CrGe$_3$Be$_2$O$_{14}$, Pr$_3$CrGe$_3$Be$_2$O$_{14}$, and Nd$_3$CrGe$_3$Be$_2$O$_{14}$, respectively. Mode symmetries are indicated.

The data on calculated displacements of different atoms in normal crystal modes of different frequencies for Ln$_3$CrGe$_3$Be$_2$O$_{14}$ (Ln = La, Pr, Nd) is provided in 3 text files named, e.g., Pr_displ.txt. Each

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### Table 4

Calculated (PBE0) and experimentally determined [14] (in square brackets) coordinates of atoms in the unit cell of Ln$_3$CrGe$_3$Be$_2$O$_{14}$. (Ln = La, Pr, Nd).

| Ion site | Ln = La | Ln = Pr | Ln = Nd |
|----------|---------|---------|---------|
|          | x/a     | y/b     | z/c     | x/a     | y/b     | z/c     | x/a     | y/b     | z/c     |
| Ln 3e    | 0.43071 | 0       | 0       | 0.43021 | 0       | 0       | 0.42976 | 0       | 0       |
| Cr 1a    | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0       |
| Ge 3f    | 0.74464 | 0       | 0.5     | 0.74435 | 0       | 0.5     | 0.74428 | 0       | 0.5     |
| Be 2d    | 1/3     | 2/3     | 0.52203 | 1/3     | 2/3     | 0.52539 | 1/3     | 2/3     | 0.52713 |
| O1 2d    | 1/3     | 2/3     | 0.20488 | 1/3     | 2/3     | 0.20613 | 1/3     | 2/3     | 0.20711 |
| O2 6g    | 0.46553 | 0.30026 | 0.32701 | 0.46600 | 0.30279 | 0.32134 | 0.46618 | 0.30408 | 0.31883 |
| O3 6g    | 0.22215 | 0.09317 | 0.75867 | 0.22329 | 0.09093 | 0.75757 | 0.22364 | 0.08958 | 0.75679 |

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### Table 5

Calculated (PBE0) and experimentally determined [14] (in square brackets) M–O distances (Å) in the structure of Ln$_3$CrGe$_3$Be$_2$O$_{14}$. (Ln = La, Pr, Nd).

|               | Ln = La | Ln = Pr | Ln = Nd |
|---------------|---------|---------|---------|
| R–polyhedron  |         |         |         |
| R–O1 × 2      | 2.601   | 2.584   | 2.578   |
| R–O2 × 2      | 2.496   | 2.449   | 2.429   |
| R–O2’ × 2     | 2.811   | 2.788   | 2.779   |
| R–O3 × 2      | 2.468   | 2.430   | 2.412   |
| (R–O)$_{\text{e}}$ | 2.594 | 2.563   | 2.550   |
| Cr–octahedron |         |         |         |
| Cr–O3 × 6     | 1.966   | 1.963   | 1.963   |
| Ge–tetrahedron|         |         |         |
| Ge–O2 × 2     | 1.769   | 1.766   | 1.764   |
| Ge–O3 × 2     | 1.756   | 1.756   | 1.756   |
| (Ge–O)$_{\text{e}}$ | 1.762 | 1.761   | 1.760   |
| Be–tetrahedron|         |         |         |
| Be–O1         | 1.576   | 1.578   | 1.579   |
| Be–O2 × 3     | 1.683   | 1.678   | 1.677   |
| (Be–O)$_{\text{e}}$ | 1.656 | 1.653   | 1.653   |
Table 6
Experimentally determined [1] and calculated (B3LYP) frequencies in the Raman (R) and infrared (IR) spectra of La₃CrGe₃Be₂O₁₄.

| Exp, R | Calculated | Exp, IR | Exp, R | Calculated | Exp, IR |
|--------|------------|---------|--------|------------|---------|
|        | Raman      |         |        | IR         |         |
| A₁ E   | A₂         |         | A₁ E   | A₂         |         |
| 88     | 105        | 100     | 406    | 396        | 400     |
| 108    | 109        | 433     | 425    | 424        |         |
| 122    | 127        | 462     | 456    | 456        |         |
| 143    | 141        | 488     | 482    |            | 506     |
| 159    | 164        | 544     | 532    | 551        |         |
| 190    | 193        | 580     |        |            |         |
| 212    | 213        | 625     | 624    | 625        |         |
| 233    | 235        | 661     |        |            |         |
| 259    | 269        | 730     | 728    | 722        |         |
| 284    | 287        | 783     | 781    | 789        |         |
| 292    | 290        | 783     | 785    |            |         |
| 326    | 328        | 809     |        |            |         |
| 351    | 343        | 818     |        |            |         |
| 378    | 376        | 836     |        |            |         |

Table 7
Experimentally determined [1] and calculated (B3LYP) frequencies in the Raman (R) and infrared (IR) spectra of Pr₃CrGe₃Be₂O₁₄.

| Exp, R | Calculated | Exp, IR | Exp, R | Calculated | Exp, IR |
|--------|------------|---------|--------|------------|---------|
|        | Raman      |         |        | IR         |         |
| A₁ E   | A₂         |         | A₁ E   | A₂         |         |
| 83     | 96         | 89      | 409    | 401        |         |
| 108    | 108        | 435     | 431    | 430        |         |
| 123    | 127        | 462     | 459    | 462        |         |
| 145    | 141        | 548     | 538    | 556        |         |
| 161    | 164        | 575     | 565    |            |         |
| 193    | 194        | 583     |        |            |         |
| 215    | 216        | 587     | 631    | 632        | 633     |
| 235    | 235        | 668     | 721    | 728        |         |
| 260    | 265        | 732     | 734,5  | 743        |         |
| 284    | 286        | 783     | 785,6  | 794        |         |
| 295    | 294        | 785,7   | 813    |            |         |
| 295    | 297        |         | 818    |            |         |
| 355    | 348        | 352     | 821    | 823        |         |
| 382    | 378        | 836     | 843    |            |         |
The file has eight columns. The first column corresponds to the mode frequency (unit: cm$^{-1}$), the columns 2–8 correspond to the displacements (unit: Å) of the following atoms: Ln, Cr, Ge, Be, O1, O2, O3. The same data are presented also as Excel tables with 8 columns, named, e.g., Pr_displ.xlsx.

Fig. 1 depicts these displacements for all three title compounds, namely, La$_3$CrGe$_3$Be$_2$O$_{14}$, Pr$_3$CrGe$_3$Be$_2$O$_{14}$, and Nd$_3$CrGe$_3$Be$_2$O$_{14}$. It is given as the eps and opj files, Figure 1.eps and Figure 1.opj, respectively. The table in text (and Excel) format Figure 1_table.txt (and Figure 1_table.xls) provides the data necessary to create Figure 1.

### 2. Experimental design, materials, and methods

The main information on the samples and experimental equipment used to take the spectra, as well as on the calculation methods is presented in Ref. [1]. Powder samples of the studied compounds La$_3$CrGe$_3$Be$_2$O$_{14}$, Pr$_3$CrGe$_3$Be$_2$O$_{14}$, and Nd$_3$CrGe$_3$Be$_2$O$_{14}$ were synthesized by a high-temperature solid-state reaction from high-purity La$_2$O$_3$, Pr$_2$O$_3$, Nd$_2$O$_3$, and GeO$_2$, Cr$_2$O$_3$ (reagent grade), and BeO (99.5%). Stoichiometric amounts of oxides were thoroughly ground together, pressed into pellets, placed on a Pt substrate and sintered in air for 5 h at 1350°C (the Nd and Pr compounds) and at 1325°C (the La compound). To reduce the loss of GeO$_2$ due to evaporation, the pressed samples were encapsulated in the original powdered charges. The phase composition of sintering products was studied by X-ray diffraction using a diffractometer STOE STADI_MP in a transmission mode (CuK$_{a1}$ radiation). The space group P321 was confirmed for all samples.

The infrared diffuse transmission and Raman scattering spectra of Ln$_3$CrGe$_3$Be$_2$O$_{14}$ (Ln = La, Pr, Nd) powder samples were measured at room temperature. Powders of Ln$_3$CrGe$_3$Be$_2$O$_{14}$ were mixed with optical-grade KBr powder and pressed into pellets. Far-infrared diffuse transmission spectra were registered in the spectral region 50–1200 cm$^{-1}$ at a resolution 2 cm$^{-1}$ using a Fourier spectrometer Bruker IFS 125HR and a DTGS and a liquid-nitrogen-cooled MCT detectors. Raman spectra were taken in the backscattering geometry at a resolution 3 cm$^{-1}$ with a home-made triple monochromator using the line 514, 5 nm of an argon laser as an excitation.
Fig. 1. Displacements of different atoms of La$_3$CrGe$_3$Be$_2$O$_{14}$ in normal crystal modes of different frequencies.
Ab initio calculations of phonon frequencies and intensities of the infrared- and Raman-active modes of La₃CrGe₃Be₂O₁₄, Pr₃CrGe₃Be₂O₁₄, and Nd₃CrGe₃Be₂O₁₄ were performed in a framework of the density functional theory (DFT) with the hybrid functional B3LYP [2], which takes into account both local and nonlocal (in the Hartree-Fock formalism) exchange. The sequence of calculations was as follows. The optimization of the crystal structure was carried out first. After that, the phonon spectrum was calculated for the crystal structure corresponding to the minimum energy. The CRYSTAL14 program [3] designed for simulating periodic structures in the MO LCAO approximation was used for calculations. Quasi-relativistic pseudopotentials ECP₄₆MWB, ECP₅₉MWB, and ECP₆₀MWB [4,5] with corresponding valence basis sets ECPₙMWB [6] were taken for La, Pr, and Nd. All-electron basis sets of TZVP type were used for Cr, Ge, Be, and O [7]. All-electron basis sets of TZVP type were used for Cr, Ge, Be, and O [7]. These basis sets are available at the CRYSTAL website. The reciprocal space sampling was performed by Monkhorst-Pack mesh. The algorithm of calculation of the two-electron Coulomb and exchange integrals is given in Ref. [8]. The tolerance of self-consistently solving of the system of Kohn-Sham equations was \( 10^{-9} \). The phonon spectrum was calculated in the harmonic approximation. In the Hessian matrix, the first (second) derivatives were calculated analytically (numerically). To perform numerical calculations of the second derivatives, the atom was displaced from the equilibrium position by 0.003 Å [8].

We used the Born charges when calculating Raman and infrared intensities in the CRYSTAL code [9]. Electric dipole properties were calculated using the periodic coupled-perturbed Hartree-Fock (CPHF) or Kohn-Sham (CPKS) approach [10–12].

The Placzek approximation was used to calculate the intensity of the Raman modes at a non-resonant excitation [11]. For an oriented single crystal, the intensity associated with the mode \( \omega_k \) is [3]:

\[
I_k^R = C \left( \alpha_{ij}^k \right)^2,
\]

where \( \alpha_{ij}^k \) is an element of the Raman tensor, \( i, j = x, y, z \). The value \( C \) in (1) is defined by the laser frequency \( \omega_L \) and the temperature \( T \) dependence as follows:

\[
C \sim \frac{1 + n(\omega_k)(\omega_L - \omega_k)^4}{30 \omega_k},
\]

where

\[
1 + n(\omega_k) = \left[ 1 - \exp \left( \frac{\hbar \omega_k}{K_B T} \right) \right]^{-1},
\]

\( n(\omega_k) \) being the Bose occupation factor.

The simulation of the intensity of Raman modes for powder sample has been done by computing integrals over all possible orientations of ideal bulk crystal. These integrals can be reduced to three rotational invariants [13]:

\[
C_k^{(0)} = \frac{1}{3} \left( \alpha_{xx}^k + \alpha_{yy}^k + \alpha_{zz}^k \right)^2
\]

\[
C_k^{(1)} = \frac{1}{2} \left[ \left( \alpha_{xy}^k - \alpha_{yx}^k \right)^2 + \left( \alpha_{xz}^k - \alpha_{zx}^k \right)^2 + \left( \alpha_{yz}^k - \alpha_{zy}^k \right)^2 \right]
\]

\[
C_k^{(2)} = \frac{1}{2} \left[ \left( \alpha_{xy}^k + \alpha_{yx}^k \right)^2 + \left( \alpha_{xz}^k + \alpha_{zx}^k \right)^2 + \left( \alpha_{yz}^k + \alpha_{zy}^k \right)^2 \right] + \frac{1}{3} \left[ \left( \alpha_{xx}^k - \alpha_{yy}^k \right)^2 + \left( \alpha_{zz}^k - \alpha_{zz}^k \right)^2 + \left( \alpha_{yy}^k - \alpha_{zz}^k \right)^2 \right]
\]
The intensity for the powder sample can be calculated as [14]:

\[
I_{\text{powder}}^{\text{tot},k} = I_{\parallel,k}^{\text{powder}} + I_{\perp,k}^{\text{powder}},
\]

where

\[
I_{\parallel,k}^{\text{powder}} = C \left( 10G_k^{(0)} + 4G_k^{(2)} \right)
\]

\[
I_{\perp,k}^{\text{powder}} = C \left( 5G_k^{(1)} + 3G_k^{(2)} \right)
\]

and \( C \) is given by Eq. (2).

The infrared intensity of the \( p \)-th mode can be written as [3]:

\[
I_p = \pi \frac{N_A}{c^2} d_p \left| \vec{Z}_p \right|^2,
\]

where \( N_A \) is the Avogadro’s number, \( c \) is the speed of light, \( d_p \) is the degeneracy of the mode, \( \vec{Z}_p \) is the mass-weighted Born effective charge vector of the mode. The infrared intensity was calculated assuming an isotropic response.

The high-spin (\( S = 3/2 \)) state of the \( \text{Cr}^{3+} \) ions was set in the calculations. At the simulation, magnetic moments of chromium ions were codirected (along the \( z \) axis), hereby the ferromagnetic state was simulated. In this work, we consecutively calculate the crystal structure and, then, the phonon spectrum. The initial structural data were taken from Ref. [14].

When choosing a functional, calculations with the hybrid functional PBE0 [15] were also performed.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104889.

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