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High-pressure crystal structure and phase transitions in B₂O₃

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A high-pressure polymorph of boron oxide, B₂O₃-P2₁2₁2₁, has been obtained in a laser-heated diamond anvil cell at 50(3) GPa after heating boron trioxide to a temperature of $T_{\max} \leq 2500(300)$ K. The crystal structure was determined from synchrotron single crystal X-ray diffraction and was confirmed by a combination of density functional theory (DFT) calculations and experimental Raman spectroscopy. Experimental- as well as DFT-data confirm the non-centrosymmetric/non-polar space group P2₁2₁2₁. The structural model of B₂O₃-P2₁2₁2₁ is in agreement with an earlier DFT-based crystal structure prediction. The crystal structure is characterized by corner-sharing [BO₄] tetrahedra with covalent B–O bonds. Our experimental Raman data show that B₂O₃-P2₁2₁2₁ can be recovered under ambient conditions.

In the context of studies aimed at rationalizing the formation of chemically simple carbonates of small cations (*e.g.* Be²⁺, Al³⁺, and Fe³⁺),^{1–4} we attempted to synthesize a borocarbonate by reacting B₂O₃ with CO₂ at moderate pressures in a laser heated diamond anvil cell (LH-DAC).⁵ Due to co-condensation of H₂O in the sample chamber of the DAC, the reaction product was a hydrous borocarbonate B[μ-H(CO₃)₂], obtained at ≈20 GPa and ≈1500(200) K.⁵ Here, we therefore repeated the experiment, aiming at the synthesis of an anhydrous borocarbonate. Employing an improved cryogenic loading system, which reduces the H₂O contamination,⁶ we searched for reactions in the B₂O₃–CO₂ system between 20 GPa and 50 GPa. This search was motivated by the fact that compounds containing boron oxoanions are a rich class of optical materials, which are employed in numerous applications.^{7–11} Although no reaction between B₂O₃ and CO₂ was detected, we observed the formation of a new high pressure polymorph of B₂O₃.

The present study therefore complements and significantly extends the numerous previous high-pressure studies of B₂O₃. B₂O₃ is a rare example where the structure of a high-pressure polymorph (B₂O₃-Ccm2₁)¹² was determined before the structure of the likely ground state structure (B₂O₃-P3₁21) had been correctly determined.^{13,14} The high-pressure B₂O₃ polymorph crystallizes in the non-centrosymmetric space group Ccm2₁ and was described in the non-default representations of space group Cmc21 (No. 36).¹² The experimentally challenging determination of the ambient pressure phase of B₂O₃-P3₁21 is due to the extreme difficulties encountered when attempting to crystallize samples from melts, as B₂O₃ is an outstanding glass former, and is also hygroscopic. Hence, B₂O₃ glasses have been studied in detail.¹⁵ While the earlier diffraction studies^{16–19} were therefore revised later, it was, correctly, inferred at an early stage that B₂O₃-P3₁21 transformed into a new polymorph at pressures above 2.5 GPa.²⁰ The stability field of the high pressure polymorph B₂O₃-Ccm2₁ has been discussed in several studies and is now well established up to 8 GPa and 1800 K.^{20–23} An equation of state based on compression data up to 42 GPa was determined by Nieto-Sanz *et al.*²⁴ Refitting their data to a third-order Birch–Murnaghan equation of state^{25–27} gives a bulk modulus of 160(17) GPa (with $K_p = 3.1(7)$ GPa).

There have been several atomistic modeling and crystal structure prediction studies. Li *et al.*²⁸ carried out DFT-LDA calculations to understand the band gaps and some physical properties of B₂O₃-P3₁21 and B₂O₃-Ccm2₁, while Takeda *et al.*²⁹ studied the structures of the two polymorphs with a Hartree–Fock-based approach. Dong *et al.*³⁰ used a crystal structure prediction approach to search for hard oxides and predicted a phase transition from B₂O₃-Ccm2₁ to B₂O₃-P2₁2₁2₁ at 46 GPa in the athermal limit. In contrast, another recent structure prediction study³¹ predicted B₂O₃-structures with space group symmetries of *Pbcn* at 15 GPa, *P1* at 25 GPa, and *C2/c* at 50 GPa.

In our experiments, the B₂O₃ powder was first dried in an oven at ≈580 K and then placed in the sample chamber of the DAC. Afterwards, CO₂-I (dry ice) was added by cryogenic loading into the sample chamber (see the SI). In the last step, the DAC

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was closed and compressed to the target pressure of the experiment. Using Raman spectroscopy, we excluded any contamination with H₂O, due to the absence of characteristic Raman modes of H₂O-VII after the cryogenic loading at high wave numbers ($\approx 3000\text{--}3400\text{ cm}^{-1}$).^{32,33} In addition, we confirmed by Raman spectroscopy that CO₂-I (*Pa* $\bar{3}$) is present in the sample chamber.^{34,35} During cold compression, CO₂-I undergoes a phase transition to phase III (*Cmca*) in a broad ($\approx 5\text{ GPa}$) pressure range around $\approx 12\text{ GPa}$ and persists in a meta-stable state up to high pressures.^{34–36} Heating CO₂-III at pressures above $\approx 25\text{ GPa}$ causes another phase transformation to phase V (*I4* $\bar{2}d$), which is the stable CO₂-polymorph up to pressures $> 100\text{ GPa}$.^{36,37} In B₂O₃, a phase transition from B₂O₃-P3₁21 to B₂O₃-Ccm2₁ was observed in earlier studies above 2–6 GPa, depending on temperature.^{20–23}

Heating B₂O₃ in the CO₂ environment between 20 GPa and 40 GPa up to maximum temperatures of $T_{\text{max}} \leq 2500(300)\text{ K}$ did not result in the formation of a new carbonate, which can typically be identified by Raman bands due to the C–O stretching vibration. However, after laser heating ($T_{\text{max}} \leq 2500(300)\text{ K}$)

B₂O₃ at 50(3) GPa for 30 minutes (Fig. 1a), we observed, in addition to the characteristic Raman modes of B₂O₃-Ccm2₁, the appearance of new Raman modes. The experimental Raman spectrum of B₂O₃-Ccm2₁ is accurately reproduced by our DFT-based calculations (Fig. 2b), and hence the Raman bands belonging to the new phase can clearly be identified. Employing spatially resolved Raman spectroscopy we found that the unknown phase with a strong Raman mode at $\approx 280\text{ cm}^{-1}$ (Fig. 2c) is present on one side of the heated B₂O₃ grain (Fig. 1b and f). The other part of the sample shows the Raman signal of B₂O₃-Ccm2₁ (Fig. 1b and e) with a dominant Raman mode at $\approx 470\text{ cm}^{-1}$. Around the heated B₂O₃ sample, we could only detect the Raman signature of CO₂-V, which can be identified in a straightforward fashion as the experimental Raman spectrum of CO₂-V is in good agreement with our DFT-based calculations (Fig. 2a). In the unheated areas of the DAC, metastable CO₂-III is still present (Fig. 1b).

We solved the crystal structure of the unknown phase, using synchrotron-based single crystal X-ray diffraction, in the orthorhombic acentric space group *P*2₁2₁2₁ with $Z = 4$ and B₂O₃ composition (Fig. 3a). The lattice parameters at 50(3) GPa are $a = 4.1372(4)\text{ \AA}$, $b = 7.351(1)\text{ \AA}$ and $c = 3.9417(6)\text{ \AA}$ ($V = 119.88(3)\text{ \AA}^3$). The very low R_1 -value (3.7%), in combination with a reasonable reflection-to-parameter-ratio (6.9:1) for a DAC-experiment, is indicative of a good structure refinement. The displacement parameters of all atoms were refined anisotropically and no constraints or restraints were introduced. This structural model had been predicted by an evolutionary algorithm in the B–O binary system, with a proposed stability field of 46–133 GPa in the athermal limit.³⁰ Our DFT-based full geometry optimizations on B₂O₃-P2₁2₁2₁ accurately reproduce our experimental

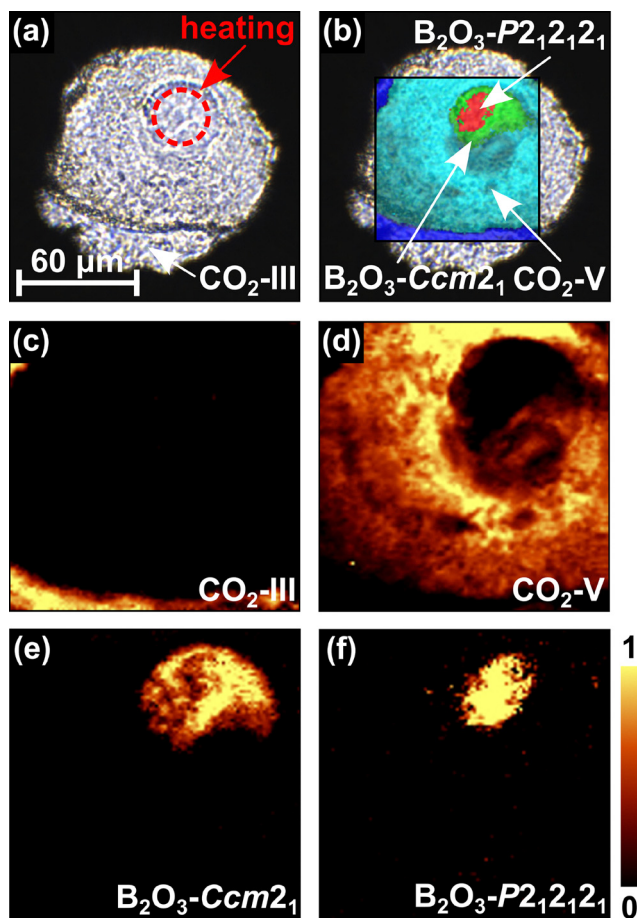


Fig. 1 (a) B₂O₃ grain in a CO₂ atmosphere at 50(3) GPa after laser heating ($T_{\text{max}} \leq 2500(300)\text{ K}$). (b) Combined Raman maps of B₂O₃-P2₁2₁2₁, B₂O₃-Ccm2₁, CO₂-V and CO₂-III after laser heating overlaid on a picture of the sample chamber. Raman maps of: (c) CO₂-III ($\approx 370\text{ cm}^{-1}$), (d) CO₂-V ($\approx 800\text{ cm}^{-1}$), (e) B₂O₃-Ccm2₁ ($\approx 470\text{ cm}^{-1}$) and (f) B₂O₃-P2₁2₁2₁ ($\approx 280\text{ cm}^{-1}$) after laser heating at 50(3) GPa.

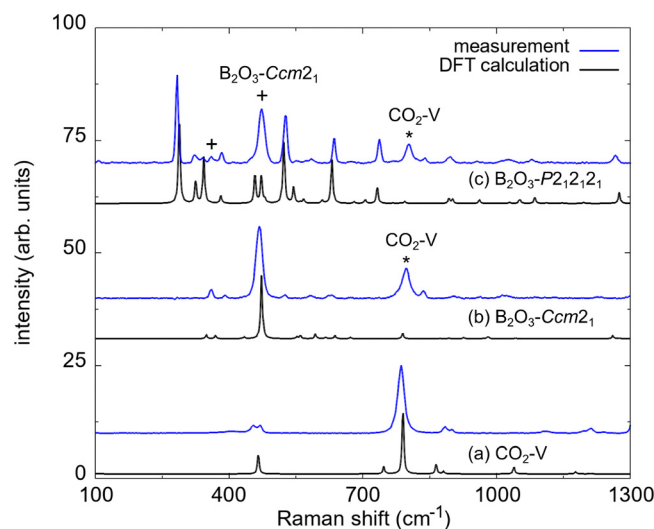


Fig. 2 Raman spectroscopy at 50(3) GPa after laser heating: (a) Raman spectra of CO₂-V. (b) Raman spectra of B₂O₃-Ccm2₁. (c) Raman spectra of B₂O₃-P2₁2₁2₁. Experimental Raman spectra are shown in blue, and DFT-based calculations are shown in black. The Raman shifts of the theoretical spectra of B₂O₃ are marked with an asterisk (*). Peaks of B₂O₃-Ccm2₁ in the Raman spectra of B₂O₃-P2₁2₁2₁ are marked with a cross (+).



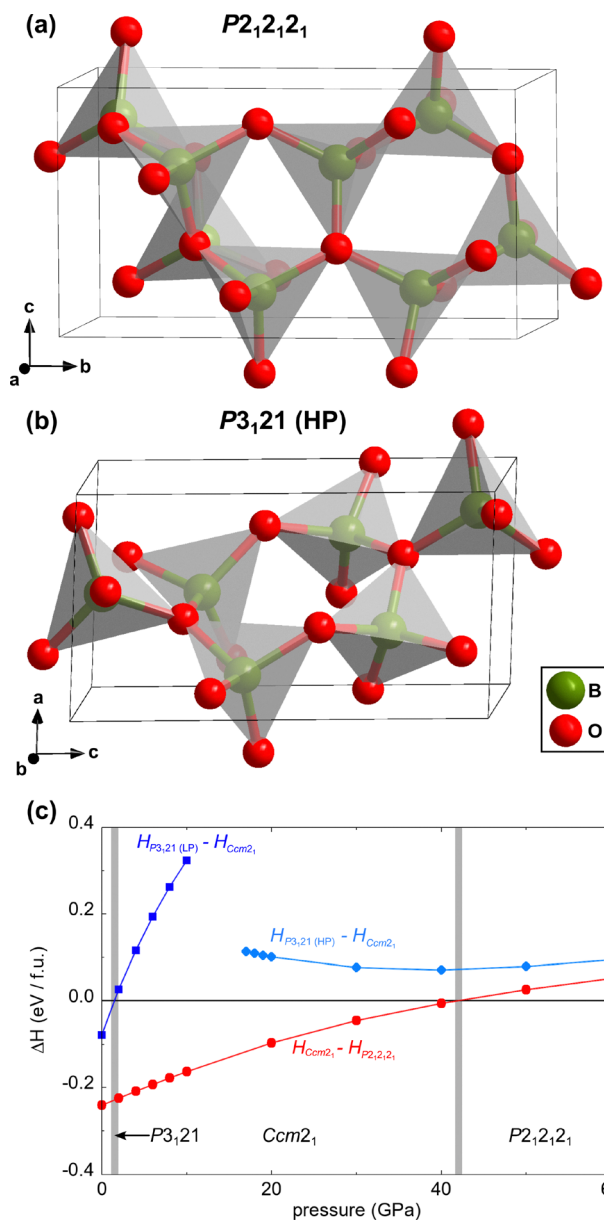


Fig. 3 (a) Crystal structure of B_2O_3 - $P2_12_12_1$ obtained from synchrotron single-crystal X-ray diffraction at 50(3) GPa. (b) Crystal structure of B_2O_3 - $P3_12_1$ (HP) obtained from DFT-based calculations at 50 GPa. (c) Enthalpy difference (ΔH) between different B_2O_3 phases for the pressure range 0–60 GPa from DFT-based calculations.^{12,13,30}

structural model and the earlier structure prediction (Table S1 in the SI).³⁰ Hence, our single crystal X-ray diffraction data clearly show that no reaction between B_2O_3 and CO_2 had occurred.

The structure of B_2O_3 - $P2_12_12_1$ is characterized by interconnected $[BO_4]$ tetrahedra (Fig. 3a) with B–O bond lengths between 1.355(5) Å and 1.519(7) Å at 50(3) GPa. The experimental B–O bond lengths are in agreement with our DFT calculations (1.35–1.46 Å). In the crystal structure of B_2O_3 - $P2_12_12_1$, two symmetrically independent boron atoms are present, each within a $[BO_4]$ tetrahedron (Fig. 4a). Each of the $[BO_4]$ tetrahedra is connected by corner-sharing to the neighboring

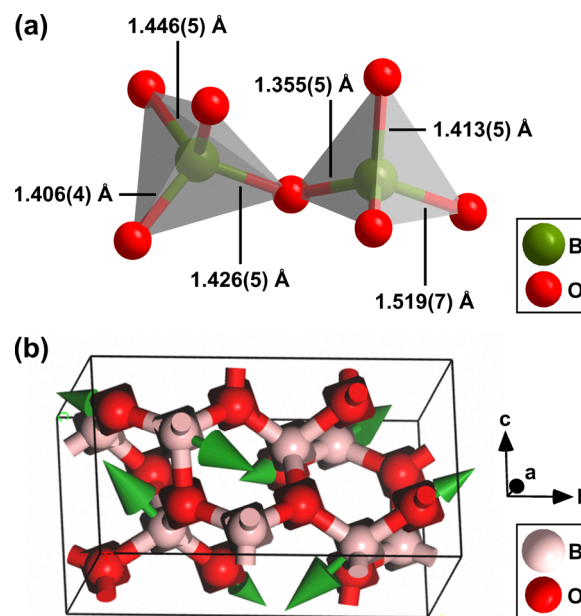


Fig. 4 (a) Geometry of two $[BO_4]$ tetrahedra in the crystal structure of B_2O_3 - $P2_12_12_1$ from single crystal structure refinement at 50(3) GPa. (b) Eigenvector of the atomic displacements in B_2O_3 - $P2_12_12_1$ for the characteristic Raman mode at ≈ 1332 cm^{-1} from DFPT calculations.

tetrahedra (Fig. 3a and 4a). Two of the symmetrically independent oxygen atoms form bonds to three boron atoms of other tetrahedra. The last independent oxygen atom forms only two B–O contacts, which are noticeably shorter than other B–O bonds in the crystal structure. A Mulliken population analysis yielded noticeably stronger bonds for the shortest B–O bonds (0.87 $e^- \text{Å}^{-3}$) than for the longest B–O bonds (0.58 $e^- \text{Å}^{-3}$). All B–O bonds show a significantly covalent character. The B–O bond length (1.35–1.48 Å) and the bond populations (0.79 – 0.57 $e^- \text{Å}^{-3}$) are in agreement with our DFT-based calculations for the $[BO_4]$ tetrahedra in B_2O_3 - $Ccm2_1$ at 50 GPa.

We employed DFPT-based calculations in order to derive a theoretical Raman spectrum of B_2O_3 - $P2_12_12_1$ at 50 GPa. Our experimental Raman spectrum is in reasonable agreement with the theoretical one. For several Raman modes, the calculated Raman intensities differ noticeably from the experimental data (Fig. 2c). This can be rationalized by noting that we computed the Raman spectrum for an ideal powder, while experimentally we record the spectrum of very few grains with unknown orientation. An analysis of the eigenvectors shows that the characteristic Raman bands are due to complex displacement patterns, which generally defy a straightforward simple classification. An exception is the mode at 1332 cm^{-1} (Fig. 4b), which is due to an asymmetric stretching vibration of the $[BO_4]$ tetrahedra.

We computed the p,V -relations for all three polymorphs and fitted the equation of states (EoS) to these data (Fig. S2 in the SI). We also computed the elastic stiffness tensors for all three polymorphs (Table S3 in the SI). As expected, the bulk modulus from the EoS calculations increases from 41.0(9) GPa for B_2O_3 - $P3_12_1$ to 145(4) GPa for B_2O_3 - $Ccm2_1$ to 157(1) GPa for B_2O_3 -



$P2_12_12_1$. The corresponding values from the stress-strain calculations agree with these values within a few GPa (see the SI). Our results are consistent with the data reported by Dong *et al.*³⁰ From our DFT calculations, we also found that another B_2O_3 polymorph may be formed metastably at elevated pressures. The ambient pressure phase B_2O_3 - $P3_12_1$ (LP) undergoes an isostructural phase transition to B_2O_3 - $P3_12_1$ (HP) at ≈ 17 GPa (Fig. 3b). This phase transition is accompanied by a significant volume decrease of $\approx 10\%$ within 1 GPa and a change of the boron coordination from trigonal-planar $[BO_3]$ units to $[BO_4]$ tetrahedra (Table S4 in the SI). The bulk modulus of this new high-pressure phase is significantly higher ($K_0 = 202(1)$ GPa with $K_p = 3.70(4)$) than calculated for the other two high-pressure polymorphs. A comparison of the enthalpies of all four B_2O_3 phases between ambient pressure and 60 GPa (Fig. 3c) shows that B_2O_3 - $P3_12_1$ (LP) is less stable than B_2O_3 - $Ccm2_1$ at pressures > 1.5 GPa. B_2O_3 - $Ccm2_1$ remains stable up to 42 GPa and undergoes a phase transition to B_2O_3 - $P2_12_12_1$. These results are consistent with the earlier work by Dong *et al.*³⁰ predicting the phase transitions at similar pressures. The metastable polymorph B_2O_3 - $P3_12_1$ (HP) is less stable by ≈ 0.1 eV f.u.⁻¹ with respect to B_2O_3 - $Ccm2_1$ at 17 GPa. Hence, we assume that this phase may be found experimentally by careful cold-compression of B_2O_3 - $P3_12_1$ (LP) in a hydrostatic pressure transmitting medium (*e.g.* helium).

We also computed the phonon dispersion curves of B_2O_3 - $P2_12_12_1$ at 50 GPa and at ambient pressures (Fig. S4 in the SI). In agreement with the experimental observations, B_2O_3 - $P2_12_12_1$ is dynamically stable at 50 GPa in the athermal limit. Hence, we measured Raman spectroscopy during decompression in order to understand if B_2O_3 - $P2_12_12_1$ can be recovered under ambient conditions. Our experimental Raman data clearly show that the characteristic Raman modes of both B_2O_3 - $P2_12_12_1$ and B_2O_3 - $Ccm2_1$ are still present after opening the DAC (Fig. S3 in the SI). They are in agreement with our Raman spectra obtained from the DFPT-calculations, confirming that both phases can be recovered under ambient conditions. This is in agreement with our phonon dispersion curves at ambient pressures, which show that B_2O_3 - $P2_12_12_1$ is dynamically stable at the athermal limit (Fig. S4 in the SI).

In conclusion, we have obtained the boron trioxide polymorph B_2O_3 - $P2_12_12_1$ in a LH-DAC at 50(3) GPa, which crystallizes in a non-centrosymmetric/non-polar space group. B_2O_3 - $P2_12_12_1$ was obtained by heating up to a maximum temperature of $T_{max} \leq 2500(300)$ K. We determined the crystal structure by synchrotron single crystal X-ray diffraction and corroborated the structural model by a combination of experimental Raman spectroscopy and DFT-based calculations. Its acentric orthorhombic crystal structure is in agreement with the results from an earlier crystal structure prediction,³⁰ while the predicted structures in another study³¹ were not obtained. Our experimental data show that B_2O_3 - $P2_12_12_1$ can be recovered under ambient conditions next to the well-established high-pressure polymorph B_2O_3 - $Ccm2_1$.¹² Our results show that B_2O_3 does not react with CO_2 at elevated pressures and temperatures. This is in contrast to other chemically simple oxides such as Al_2O_3 ,

Fe_2O_3 , Cr_2O_3 or I_2O_5 , which readily form carbonates when heated in a CO_2 environment.^{3,4,6,38}

Conflicts of interest

There are no conflicts to declare.

Data availability

All study data are included in the article and/or in the supplementary information (SI). Supplementary information: experimental and computational details, crystallographic data, X-ray single crystal measurements, Raman spectroscopy and DFT-based calculations. See DOI: <https://doi.org/10.1039/d6cc00368k>.

CCDC 2523450 contains the supplementary crystallographic data for this paper.³⁹

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