Novel magnesium borides and their superconductivity

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(Dated: May 18, 2017)

With the motivation of searching for new superconductors in the Mg-B system, we performed ab initio evolutionary searches for all the stable compounds in this binary system in the pressure range of 0-200 GPa. We found previously unknown, yet thermodynamically stable, compositions MgB12 and MgB10. Experimentally known MgB2 is stable in the entire pressure range 0-200 GPa, while MgB17 and MgB12 are stable at pressures below 90 GPa and 35 GPa, respectively. We predict a reentrant behavior for MgB4, which becomes unstable against decomposition into MgB2 and MgB7 at 4 GPa and then becomes stable above 61 GPa. We find ubiquity of phases with boron sandwich structures analogous to the AlB2-type structure. However, with the exception of MgB2, all other magnesium borides have low electron-phonon coupling constants λ of 0.32 to 0.39 and are predicted to have Tc below 3 K.

INTRODUCTION

Tremendous efforts have been put to design conventional superconductors with higher and higher critical temperatures1–5. It is also the main focus of theoretical and experimental studies to determine how high the superconducting transition temperature Tc can be pushed in binary and ternary boron-compounds. For instance, theoretical works predicted thermodynamically unstable CaB2 to be superconducting at ~50 K1 and hole-doped LiBC to have Tc of 65 K2. Ternary Mo2Re3B with Tc= 8.5 K3, CuB2–xCx (Tc ~ 50 K)4 and multiple-phase bulk sample of yttrium-palladium-boron-carbon (Tc= 23 K5) are important boron-based superconductors.

The unexpected discovery of superconductivity in MgB2 with high Tc= 39 K6 has triggered a flurry of publications. In previous studies, superconductivity in MgB2 has been thoroughly investigated7–11. The isotope effect demonstrated the phonon-mediated nature of superconductivity in this compound10. Although doping is usually expressed as a hope to enhance the desired properties, carbon-doped MgB2 (Mg(B0.8C0.2)2) has a lower Tc = 21.9 K11. Aluminum, with one more electron than magnesium, was reported to be an unfit candidate for partial substitution for magnesium (Mg1−xAlxB2)12. This shows that increasing electron concentration suppresses superconductivity of magnesium diboride.

Elemental magnesium13 and boron14 have been shown to exhibit unexpected chemistry under high pressure, raising the motivation of studying their compounds. Moreover, materials composed of light atoms could make good conventional superconductors. The Mg-B system was subject to some explorations of superconductivity15–19. Stability of boron-rich magnesium borides, e.g., MgB17, MgB12 and MgB6B4 has been extensively studied by experiment at ambient pressure20. Borides of similar metals, e.g., Ca-B21 and Li-B22 and stability of 41 metal borides23 were studied and new compounds were shown to appear at high pressure. High-pressure phase of MgB2 (KHg2-type structure) was reported to be a poor metal with no superconductivity, highlighting the main role of delocalized bonding of the boron honeycomb layers in the superconducting properties of MgB2 with AlB2-type structure18.

To date, there is no comprehensive and systematic theoretical research into the stability and properties of magnesium borides at high pressure. Here, with the knowledge of the important role of magnesium13, crucial existence of honeycomb boron layers18, and substantial effect of electron concentration14, we present results of extensive computational searches for stable magnesium borides MgxBy and their superconductivity.

METHODS

Ab initio variable-composition evolutionary method USPEX24–27 was applied to the Mg-B system at 0, 30, 50, 75, 100, 150 and 200 GPa. This method has the capability of finding possible compositions and the corresponding stable and metastable structures at given pressures, and successfully predicted new phases of MgB2 at high pressure18 and new stable phases of different systems like Na-Cl, boron and Na-He16,28,29. High-temperature superconductivity in hydrogen-rich compounds, e.g., Sn-H30 and Ge-H31 were also studied. In this method, we created initial generation of structures and compositions randomly with up to 28 atoms in the primitive cell. Subsequent generations were obtained using heredity, transmutation, selfmutation, and random symmetric generator32.

Structure relaxations were carried out using VASP package33 in the framework of density functional theory (DFT) adopting PBE-GGA (Perdew-Burke-Ernzerhof gener-
alized gradient approximation. The projector augmented-wave (PAW) with [He] core for both Mg and B atoms was used to describe the core electrons and their effects on valence orbitals. A plane-wave kinetic energy cutoff of 600 eV and dense Monkhorst-Pack k-points grids with reciprocal space resolution 2π × 0.03 Å−1 was used. Phonon frequencies and electron-phonon coupling (EPC) were calculated using QUANTUM ESPRESSO. PBE-GGA functional is used for this part. A plane-wave basis set with a cutoff of 60 Ry gave a convergence in energy with a precision of 1 meV/atom. For electron-phonon coupling, a 6×6×2, 6×6×4 and a 4×4×4 q-point meshes were used for C2/m-MgB3, Ammm2-Mg3B10 and C2/m-MgB4, respectively. Denser k-point meshes, 12×12×4, 12×12×8 and 8×8×8 were used for the convergence checks of the EPC parameter λ.

RESULTS

Search for stable compounds

Pressure can stabilize new or destabilize the known compounds, and a proper sampling of all promising compositions is needed. In Fig. 1(a), the enthalpies of formation ΔHf per atom (with respect to the stable structures of elemental magnesium and boron) are shown in the convex hull form as obtained from all possible compounds. Convex hull gives all thermodynamically stable compositions of a multicomponent system, and their enthalpies of formation (per atom). The convex hull (see Fig. 1(a)) includes all thermodynamically stable compositions of the MgB system, and their enthalpies of formation (per atom). The convex hull construction shows that boron-rich compounds are stabilized at high pressure.

Taking our predicted structures/comounds and experimentally known large-cell structures of MgB2, MgB6, MgB12 (all three compounds feature B12-icosahedra, and for the latter two, we constructed ordered approximants of disordered experimental structures - for MgB12 containing 388 atoms in the unit cell), we computed the phase diagram of the Mg-B system. At pressures studied here, MgB2, MgB3, Mg3B10, Mg4B5, Mg7B12 and MgB12 have stability fields, making the phase diagram (Fig. 1(b)) very rich. A recent list of 41 metal borides presented in Ref. at 0 and 30 GPa, clearly demonstrates metal borides often have a variety of stable phases at high pressure.

On increasing pressures metastable compounds, MgB3 and MgB6, get closer to the tieline. Our calculations indicate that at 54 GPa, MgB3 reaches stability and forms the C2/m structure. Unlike MgB6, MgB4 cannot compete with other compounds and remains metastable throughout the entire pressure range (0 to 200 GPa).

Although MgB6 emerges as a metastable compound from our calculations, we still studied it, keeping in mind recent observation of superconductivity in YB6. Moreover, there is experimental evidence for MgB6 as a non-equilibrium phase.

MgB2

Some of us studied high-pressure phases of MgB2 using the evolutionary algorithm USPEX. Our results accord well with that study, as the phase transition happens at 190 GPa. The transition from AlB2-type structure (Fig. 2) with space group P6/mmm to KHg2-type structure with space group Inma, completely destroys superconductivity. The role of B-B π-bonded network and charge transfer from Mg to B atoms are explained as having major role in superconducting properties.

MgB3

MgB3, one of the new high-pressure compounds, lies 5 meV/atom above the MgB2-MgB7 tieline at 50 GPa. It becomes stable at 54 GPa and remains stable until 130 GPa in the C2/m phase. Finally Cmcn structure becomes more favorable than all other possible structures up to 200 GPa. AB3 is interestingly a common stoichiometry for metal borides as reported for WB4, MnB3, and NaB3; however, MgB3 has not been studied yet, neither computationally nor experimentally.

MgB4 stabilizes at high pressure, while CaB3 and LiB3 are not stable even at high pressure. Structural information for the predicted stable MgB3 phases is provided in Table II and in Fig. 3. The metastable layered C2/m phase at pressures below 43 GPa is important, since it has graphene-like hexagonal boron pattern, which may be a hint of a potentially superconducting phase.

MgB4

MgB4 has a remarkable reentrant behavior: this compound is thermodynamically stable in the pressure range 0-4 GPa, then becomes unstable to decomposition into other borides, and then is again thermodynamically stable at pressures >61 GPa (Fig. 1(b)). Below we consider lowest-enthalpy phases corresponding to this composition (see Fig. 4).

The Pnma phase of MgB4 is stable at ambient pressure in accord with theoretical and experimental results and remains the most favorable phase up to 31 GPa. Unlike all the other MgB4 phases and most of magnesium borides at different pressure conditions, which are metallic, Pnma-MgB4 is a semiconductor. The predicted phase diagram shows that at 31 GPa the semiconducting state breaks down, and MgB4 transforms into a metallic C2/m (similar to AlB2-type) structure. C2/m has the lowest enthalpy in a narrow pressure range from 31 to 36 GPa. From 36 to 60 GPa, the P1 phase becomes more favorable, and at very high pressures (60 - 200 GPa), high symmetry structure, 14/mmm, becomes stable.

The main feature of H4/mmm and P1 phases is prisms of boron that hold one or two magnesium atoms. Having boron...
double-layers (in comparison with $\text{P6/mmm-MgB}_2$), the $\text{C2/m}$ structure can be described as boron sandwich of this composition. Boron sandwiches have graphene-like layer(s) of boron, intercalated by magnesium atoms. Phonon calculations were performed to check the dynamical stability throughout the Brillouin zone. We did not find any dynamical instability (see Fig. 10 and Fig. S9, ESI). Due to high density of states (DOS) at the Fermi level ($N(E_F)$), high-pressure phases of MgB$_6$ can be potential candidates for superconductivity. Electron-phonon coupling (EPC) calculations revealed that among MgB$_4$ phases, only layered $\text{C2/m-MgB}_4$ is a superconductor.

MgB$_4$ has analogous stoichiometry to many AB$_2$ systems, e.g. MnB$_4$, CrB$_4$, CaB$_4$ and so forth. AB$_2$ structures are mostly orthorhombic or tetragonal with 20 atoms per cell. Some of these structures are in BaAl$_2$-type structure with space group I4/mmm$^{47}$. By removing Mg from the prisms, one observes a pattern similar to the $\alpha$-Ga structure of boron$^{16}$.

Increasing pressure, we see emergence of a graphene-like boron double-layered phase (MgB$_2$) with a simple hexagonal AB$_2$-type structure, which is a single-layered phase of this type. The extra layer is located 1.7 Å from the first layer and displaced by 0.8 Å ($\alpha\alpha\beta\alpha\beta\beta$...), A represents Mg and $\alpha\beta$ are B layers. At 36 GPa, some boron blocks were formed with a pattern of 1 and 2 magnesium atoms per block. Finally, at a higher pressure 60 GPa, the body-centered tetragonal BaAl$_2$-type structure (space group I4/mmm), which is widely adopted among AB$_2$ intermetallic compounds, forms. In I4/mmm structure, magnesium is located in the center of the truncated rectangular prisms made of boron atoms. This structure is similar to $\text{Cmcm-MgB}_3$, in which, there are two magnesium atoms located in each of the truncated rectangular prisms (see Fig. 3(b), and Fig. 5(a)).

**MgB$_6$**

Although MgB$_6$ is predicted to be stable with respect to decomposition to the elements (Mg and B)$^{48}$, it is not stable against decomposition into elemental boron and MgB$_4$ (see Fig. 1(a) and (b)). Furthermore, in an experimental study at ambient pressure, MgB$_6$ was not found as an individual phase$^{49}$.

Since intercalated graphite AC$_6$ (A = Mg, Ca, Sr, Ba)$^{50-52}$ is superconductor, we searched for the lowest enthalpy MgB$_6$ phases. We observed a hexagonal distorted triple-layered phase, which is the lowest in enthalpy, in the pressure range 15-28 GPa that intrigued us. MgB$_6$ forms a recently predicted phase at ambient pressure and remains in this $\text{Cmcm}$ structure until 15 GPa$^{48}$, above which a triple-layered structure has lowest enthalpy until 28 GPa (Fig. 6(c) and (d)). Between 28 GPa and 88 GPa, the $\text{R}-3m$ structure becomes more favorable, and eventually, very high pressure imposes a pattern similar to $\text{I4/mmm-MgB}_4$ into $\text{P2}_1/m$-MgB$_6$ (see Fig. 6(a)); This pattern emerges in the pressures greater than 90 GPa in both MgB$_2$ and MgB$_4$. We found the $\text{Cmcm}$ structure to be a semiconductor in agreement with the previous report$^{48}$, whereas the rest of the phases are metallic. The semiconductor-metal transition $\text{Cmcm} \rightarrow \text{P2}_1/c$ happens at 15 GPa.

**Mg$_3$B$_{10}$**

Mg$_3$B$_{10}$, a boron-rich compound, stable above 55 GPa, has a monoclinic (space group $\text{C2/m}$) phase. Above 83 GPa this phase transforms into the $\text{P2}/m$ phase (Fig. 1(b)). Metastable $\text{Amn2-Mg$_3$B$_{10}$}$, which we predict to have the lowest enthalpy among Mg$_3$B$_{10}$ phases in the pressure range 30-42 GPa, has a layered sandwich structure and is superconducting (Fig. 7(c) and (d)).

**Superconductivity**

Kolmogorov et al., proposed metal sandwiches consisting of one or more layers of metal and a graphene-like layer of boron i.e., MS-2 and MS-4 with single hexagonal layer of B$^{43}$. In our study we found, boron sandwiches, new structures with one layer of metal atoms alternating with multiple boron layers. Interestingly, boron sandwich structures are ubiquitous here. For example, in MgB$_3$, there is a layered structure with space group $\text{C2/m}$ below 43 GPa (see Fig. 9.) featuring $\alpha A\beta\beta B\gamma\pi$... stacking of B-Mg layers (A and B denotes Mg and $\alpha\beta\gamma$ are B layers). $\text{C2/m}$ structure of MgB$_4$ in 31-36 GPa, $\text{Amn2}$ structure of MgB$_{10}$ in 30-42 GPa and $\text{P2}/c$ structure of MgB$_6$ in 15-28 GPa (see colored areas in Fig. 1(b).) also feature boron sandwiches.

Boron sandwiches are layered structures with stackings of [MgB$_2$] and/or [MgB$_4$] blocks (see Fig. 9.). For example, Mg$_3$B$_{10}$ can be represented as a [MgB$_2$][MgB$_4$]... sequence of layers, and MgB$_3$ can be represented as a [MgB$_2$][MgB$_4$]... Superconductivity in Mg$_3$B$_{10}$ is mostly related to the boron layers, i.e. B-B $\sigma$ and $\pi$-bonded network, therefore, sandwich borides with hexagonal boron layers might have superconducting properties. We checked this by electron-phonon coupling calculations. Eliashberg spectral function ($\alpha^2 F$) calculations lead to the results depicted in Fig. 10. and listed in Table I. The electron-phonon coupling constants ($\lambda$) for different structures at given pressures, logarithmic averaged phonon frequencies ($\omega_{log}$) and superconducting transition temperatures ($T_c$) are also provided (for more information, see the ESI). Density of states at $E_F$ listed in Table I shows $T_c$ is higher for boron sandwiches with higher $N(E_F)$ per electron. One can see from the projected density of states that 2$p$ states of B atoms, located in planar nets, dominate the DOS at the Fermi level (see Fig. 8). Bands structures and total DOS of other sandwich borides are also provided in the ESI, Fig. S3, S6 and S10.

The critical temperature of superconductivity is estimated from the Allen-Dynes modified McMillan equation$^{54}$:

$$T_c = \frac{(\omega_{log})}{1.2} \exp \left( -\frac{-1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right),$$

where $\omega_{log}$ is the logarithmic average phonon frequency and $\mu^*$ is the Coulomb pseudopotential.
\[ \omega_{\text{log}} = \exp \left[ \frac{2}{\lambda} \int \frac{d\omega}{\omega} \alpha^2 F(\omega) \ln(\omega) \right] \] (2)

The EPC parameter \( \lambda \) is defined as integral involving the spectral function \( \alpha^2 F \):

\[ \lambda = 2 \int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega. \] (3)

Here we used \( \mu^* \) = 0.10 for Coulomb’s pseudopotential, as a reasonable value for most materials. After MgB\(_2\), \( C2/m\)-MgB\(_4\) has the highest \( T_c \) of 2.8 K at zero pressure (it is metastable at 0 GPa). In \( C2/m\)-MgB\(_4\), high-frequency phonons, mostly by boron atoms, contributes 80.5% to the total EPC parameter, and low-frequency modes are mainly from magnesium vibrations with 19.5% contribution. Sandwich borides, in general, have high phonon density between 200 to 400 cm\(^{-1}\), however, Eliashberg spectral function indicates a poor electron-phonon coupling in this range. Logarithmic average phonon frequencies \( (\omega_{\text{log}}) \) is comparable to that of \( P6/mmm\)-MgB\(_2\), however, much weaker electron-phonon coupling and lower densities of states at the Fermi level result in very low transition temperatures 0.7-2.8 K. (For more information about phonon band structures, phonon density of states, Eliashberg spectral function and electronic band structures of these phases, see the ESI)

Directly relevant to superconductivity of sandwich borides is the value of DOS at the Fermi level. For example, the DOS activity can be related to the higher density of states at the \( E_F \) when we have higher DOS (values are listed in Table I). However, other parameters are essential as well. Since logarithmic average phonon frequencies are almost equal, outstanding MgB\(_2\) superconductivity can be related to the higher density of states at the \( E_F \) mainly from boron \( p \)-states and stronger electron-phonon coupling parameter \( \lambda \) = 0.73 mainly affected by lower frequency modes. \( \lambda \) of other boron sandwiches is about half of the value of MgB\(_2\) (see values listed in Table I), which due to exponential dependence of \( T_c \) on \( \lambda \), the \( T_c \) value of MgB\(_2\) is about 10 times higher than other magnesium borides.

**CONCLUSIONS**

Using ab initio evolutionary structure search, we have extended our previous study of MgB\(_2\) to other possible Mg-B compounds up to megabar pressures. A remarkable variety of candidate high-pressure ground states has been identified. In this systematic study, under pressures from 0 to 200 GPa, we have found 6 stable compounds, i.e., MgB\(_2\), MgB\(_3\), MgB\(_4\), Mg\(_3\)B\(_{10}\), MgB\(_7\) and MgB\(_{12}\). Interestingly, MgB\(_7\) and MgB\(_{12}\), which are reported to be stable at ambient pressure, are not competitive at very high (above 90 GPa) pressure. In all compounds, at sufficiently high pressures sandwich borides give way to structures with three-dimensional topology.

Most of the predicted stable phases are metallic. No magnesium-rich phases are stable. By decreasing pressure to 0 GPa, the \( T_c \) value of \( C2/m\)-MgB\(_4\) is enhanced and reaches 2.8 K. The importance of layered structures at the boron-rich end of the Mg-B phase diagram is noteworthy. The valence bands close to and below the \( E_F \) are dominated by boron \( p \)-states in layered structures. Therefore, EPC calculations are performed and revealed Mg-B sandwich borides are superconducting with \( T_c \) of 2.5, 1.0 and 0.7 K for \( C2/m\)-MgB\(_3\), \( Amm2\)-Mg\(_3\)B\(_{10}\) and \( C2/m\)-MgB\(_4\) at 31, 40 and 33 GPa, respectively.

**ACKNOWLEDGEMENTS**

We thank DARPA (grant W31P4Q1210008), the Government of Russian Federation (14.A12.31.0003) and the Foreign Talents Introduction and Academic Exchange Program (B08040). X.F.Z thanks the National Science Foundation of China (grant no. 11174152), the National 973 Program of China (grant no. 2012CB921900), and the Program for New Century Excellent Talents in University (grant no. NCET-12-0278).

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FIG. 1: Stability of magnesium borides. (a) Calculated convex hulls at different pressures. $\alpha$-phase, $\gamma$-phase and $\alpha$-Ga-type structures are used for boron$^{16}$ and for magnesium, hexagonal close-packed (hcp) and body-centered cubic (bcc) structures were used$^{15}$. (b) Pressure-composition phase diagram. Solid bars show stable phases, whereas hatched bars indicate metastability. Colored areas illustrate layered structures (boron sandwiches) analogous to AlB$_2$-type structure.

FIG. 2: Structure of thermodynamically stable MgB$_2$ phase with space group $P6/mmm$. Projections of layered structure along the (a) [001] and (b) [010] directions.

FIG. 3: Structures of thermodynamically stable/metastable phases of MgB$_3$ (a) $C2/m$ and (b) $Cmcm$ and (c) projections of layered structure with space group $C2/m$ along the [001] and (d) [100] directions.

FIG. 4: Enthalpy per formula unit relative to the $P\bar{1}$ structure as a function of pressure for the best phases with the MgB$_4$ stoichiometry.

FIG. 5: Structure of MgB$_4$ phases (a) $I4/mmm$ (b) $P\bar{1}$ and projections of $C2/m$ structure (c) along the [001] and (d) [100] directions.

FIG. 6: Structure of magnesium hexaboride phases (a) $P2_1/m$ (b) $R-3m$ and projections of $P2_1/c$ structure (c) along the [010] and (d) [001] directions. Large spheres are Mg atoms and small sphere are Boron atoms.

FIG. 7: Structure of Mg$_3$B$_{10}$ phases (a) $P2/m$, (b) $C2/m$ and projections of Amm2 structure (c) along the [001] and (d) [100] directions.

FIG. 8: Band structure and partial densities of states for the $C2/m$-MgB$_4$ structure at ambient pressure.

FIG. 9: Boron sandwiches in Mg-B compounds. (a) $C2/m$-MgB$_3$, (b) Amm2-Mg$_3$B$_{10}$ (c) $C2/m$-MgB$_4$ and (d) $P2_1/c$-MgB$_6$

FIG. 10: Phonon band structure, Eliashberg spectral function $\alpha^2 F(\omega)$, the integrated electron-phonon coupling constant $\lambda(\omega)$ and PHDOS of $C2/m$-MgB$_4$ quenched to atmospheric pressure.
TABLE I: Computed superconducting T\textsubscript{c} of different sandwich borides

| Structure          | MgB\textsubscript{2} (P6/mmm) | MgB\textsubscript{3} (C2/m) | Mg\textsubscript{3}B\textsubscript{10} (Amm2) | MgB\textsubscript{4} (C2/m) |
|--------------------|-------------------------------|----------------------------|---------------------------------|-----------------------------|
| P (GPa)            | 0                             | 31                         | 40                              | 33                          | 0                           |
| N(E\textsubscript{f}) [states/eV per electron] | 0.084                         | 0.064                      | 0.038                           | 0.039                       | 0.044                       |
| \(\lambda\)       | 0.73*                         | 0.38                       | 0.33                            | 0.32                        | 0.39                        |
| \(\langle\omega_{\text{log}}\rangle\) (K) | 719*                          | 811                        | 843                             | 784                         | 749                         |
| T\textsubscript{c} (K) | 27.6*                        | 2.5                       | 1.0                             | 0.7                         | 2.8                         |

*\(T\textsubscript{c}\) of MgB\textsubscript{2} is calculated for comparison with other compounds. Note that \(T\textsubscript{c}\) values in this table are calculated without anharmonicity, using isotropic Eliashberg formalism. \(T\textsubscript{c}\) for MgB\textsubscript{2} is in agreement with Reference\textsuperscript{\textdegree}. Higher \(T\textsubscript{c}\) are expected if anisotropy of the electron-phonon interaction is included, e.g., account for anisotropy results in overestimation of the \(T\textsubscript{c}\) of MgB\textsubscript{2} to 55 K. On the other hand, anharmonicity of the phonons usually lowers the \(T\textsubscript{c}\) and in the MgB\textsubscript{2} case, it lowers the \(T\textsubscript{c}\) to 39 K\textsuperscript{\textdegree}. 
| Phase | Lattice parameters | Atom | x    | y    | z    |
|-------|-------------------|------|------|------|------|
| C2/m  [2 f.u.] | a = 2.998 Å, b = 5.109 Å, c = 8.852 Å, \( \beta = 115.30^\circ \) | Mg(4i) | 0.7471 | 0.0000 | 0.7982 |
|       | at 30 GPa         | B₁(4g) | 0.0000 | 0.6673 | 0.0000 |
|       |                   | B₂(8i) | 0.5210 | 0.6717 | 0.4055 |
| C2/m  [4 f.u.] | a = 7.959 Å, b = 2.850 Å, c = 10.833 Å, \( \beta = 116.98^\circ \) | Mg₁(4i) | 0.4363 | 0.0000 | 0.7000 |
|       | at 50 GPa         | Mg₂(2c) | 0.0000 | 0.0000 | 0.5000 |
|       |                   | Mg₃(2b) | 0.0000 | 0.5000 | 0.0000 |
|       |                   | B₁(4i) | 0.9041 | 0.0000 | 0.1214 |
|       |                   | B₂(4i) | 0.8063 | 0.0000 | 0.2382 |
|       |                   | B₃(4i) | 0.7390 | 0.0000 | 0.5339 |
|       |                   | B₄(4i) | 0.6943 | 0.0000 | 0.6689 |
|       |                   | B₅(4i) | 0.8529 | 0.0000 | 0.8334 |
|       |                   | B₆(4i) | 0.7445 | 0.0000 | 0.9430 |
| Cmcm  [2 f.u.] | a = 2.676 Å, b = 11.521 Å, c = 2.668 Å | Mg(4c) | 0.0000 | 0.5997 | 0.2500 |
|       | at 200 GPa        | B₁(4c) | 0.0000 | 0.2490 | 0.2500 |
|       |                   | B₂(4c) | 0.0000 | 0.8302 | 0.2500 |
|       |                   | B₃(4c) | 0.0000 | 0.9667 | 0.2500 |
