Supplemental Material for

“Computational Discovery and Characterization of New B$_2$O Phases”

Jianyun Wang,$^a$ Quan Li,$^{a,*}$ Chris J. Pickard,$^{b,c}$ Changfeng Chen,$^d$ and Yanming Ma$^{a,*}$

$^a$State Key Laboratory of Superhard Materials, Key Laboratory of Automobile Materials of MOE, Innovation Center for Computational Physics Method and Software, and Department of Materials Science, Jilin University, Changchun 130012, China

$^b$Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

$^c$Advanced Institute for Materials Research, Tohoku University 2-1-1 Katahira, Aoba, Sendai, 980-8577, Japan

$^d$Department of Physics and Astronomy, University of Nevada, Las Vegas, Nevada 89154, USA

Fig. S1. The calculated electronic band structures for the Cmmm phase at 0 GPa (a-c) and P-3 phase at 2 GPa (d-f) using the standard PBE-GGA, vdW-DF and PBEsol functionals.
Fig. S2. The fluctuations of the total energy of the \textit{Cmmm} (left) and \textit{P}-3 (right) supercells as a function of the molecular dynamic simulation step at 300 K.

Fig. S3. The simulated X-ray diffraction with \(\lambda\) of 1.5406 Å for the \textit{Cmmm} and \textit{P}-3 phases at 0 and 2 GPa, respectively.
The structural details (in cif format) of the two newly predicted B₂O phases.

For Cmmm at 0 GPa:

```
  _pd_phase_name                         "
  _cell_length_a                         5.53300
  _cell_length_b                         10.90600
  _cell_length_c                         5.46600
  _cell_angle_alpha                      90
  _cell_angle_beta                       90
  _cell_angle_gamma                      90
  _symmetry_space_group_name_H-M         'C m m m'
  _symmetry_Int_Tables_number            65

loop_
  _symmetry_equiv_pos_as_xyz
    'x, y, z'
    '-x, -y, -z'
    '-x, -y, z'
    'x, y, -z'
    '-x, y, -z'
    'x, -y, z'
    'x, -y, -z'
    '-x, y, z'
    'x+1/2, y+1/2, z'
    '-x+1/2, -y+1/2, -z'
    '-x+1/2, -y+1/2, z'
    'x+1/2, y+1/2, -z'
    '-x+1/2, y+1/2, -z'
    'x+1/2, -y+1/2, z'
    'x+1/2, -y+1/2, -z'
    '-x+1/2, y+1/2, z'
    '-x+1/2, y+1/2, -z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  B1     1.0     0.342200    0.635700    0.500000     Uiso  1.000000 B
```
For P-3 at 2 GPa

```
_pd_phase_name                         "
_cell_length_a                         4.18900
_cell_length_b                         4.18900
_cell_length_c                         7.95600
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_symmetry_space_group_name_H-M         'P -3'
_symmetry_Int_Tables_number            147

loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
  '-x, -y, -z'
  '-y, x-y, z'
  'y, -x+y, -z'
  '-x+y, -x, z'
  'x-y, x, -z'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol
B1  1.0    0.004500    0.670200    0.775300     Uiso  1.000000 B
B2  1.0    0.097100    0.691200    0.561000     Uiso  1.000000 B
O3  1.0    0.335300    0.005000    0.846200     Uiso  1.000000 O
```