Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Predicted Novel Superhard B-C-O Structures under Pressure from First Principles

This file includes two tables and five figures.

Table S1. Crystal structures B-C-O compounds at ambient pressure.

B_4CO_4			
Space group: I-4, Lattice parameters: a=5.7403 Å, c=3.7171 Å			
Atom	*x*	*y*	*z*
B 8g	0.6953	0.8972	0.0000
C 2d	0.0000	0.5000	0.7500
O 8g	0.8883	0.7831	0.2100
B_2CO_2			
Space group: C2/m, Lattice parameters: a=9.7757 Å, b=2.4884 Å, c=5.3945 Å, β=90.84°			
B1 4i	0.8893	0.0000	0.2427
B2 4i	0.1297	0.5000	0.2023
C 4i	0.2496	0.0000	0.5856
O1 4i	0.1387	0.0000	0.0472
O2 4i	0.9737	0.5000	0.2752
$B_6C_2O_5$			
Space group: P1, Lattice parameters: a=4.5015Å, b=4.5381Å, c=4.5565Å, α=99.07°, β=98.20°, γ = 99.40°			
B1	0.4157	0.5975	0.0113
B2	0.6804	0.1571	0.1263
B3	0.9801	0.7208	0.2901
B4	0.5468	0.8782	0.5669
B5	0.3273	0.3492	0.4768
B6	0.1295	0.0131	0.8429
C1	0.3008	0.6218	0.3229
C2	0.4459	0.9087	0.8859
O1	0.5680	0.1822	0.4381
O2	0.8810	0.8290	0.5839
O3	0.7349	0.4836	0.0799
O4	0.9869	0.0337	0.1403
O5	0.2091	0.3321	0.7567

Table S2 Calculated elastic stiffness constants (C_{ij}) (GPa) of B-C-O compounds.

B_4CO_4					
C_{11}	C_{33}	C_{44}	C_{66}	C_{12}	C_{13}
480	449	268	259	152	131

B_2CO_2												
C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	C_{15}	C_{25}	C_{35}	C_{46}
594	774	619	242	206	257	122	72	136	-76	7	51	-13

$B_6C_2O_5$												
C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	C_{15}	C_{25}	C_{35}	C_{46}
437	578	529	164	206	230	117	99	44	29	26	70	41
C_{14}	C_{16}	C_{24}	C_{26}	C_{34}	C_{36}	C_{45}	C_{56}					
-29	27	-55	3	25	20	12	-36					

Figure captions

Fig. S1. Phonon dispersion curves of *I-4* B_4CO_4 at ambient pressure.

Fig. S2-S3. Phonon dispersion curves (S2) and electronic band structure (S3) of *C2/m* B_2CO_2 ambient pressure.

Fig. S4-S5. Phonon dispersion curves (S4) and electronic band structure (S5) of *P1* $B_6C_2O_5$ at ambient pressure.

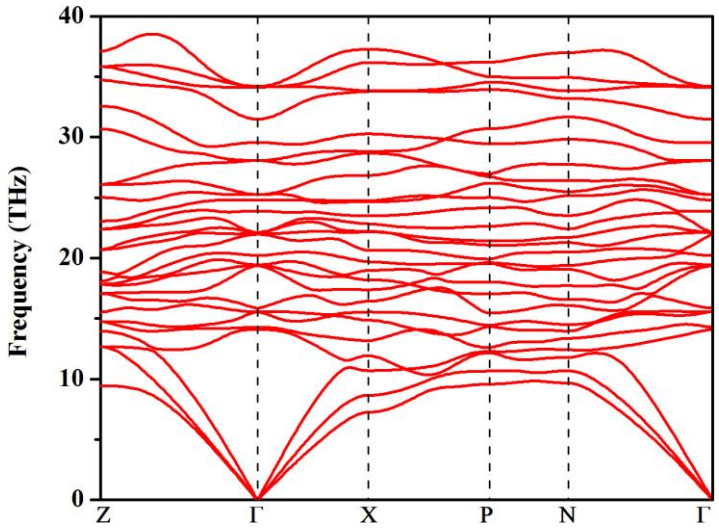

Fig. S1. Phonon dispersion curves of *I-4* B_4CO_4 at ambient pressure.

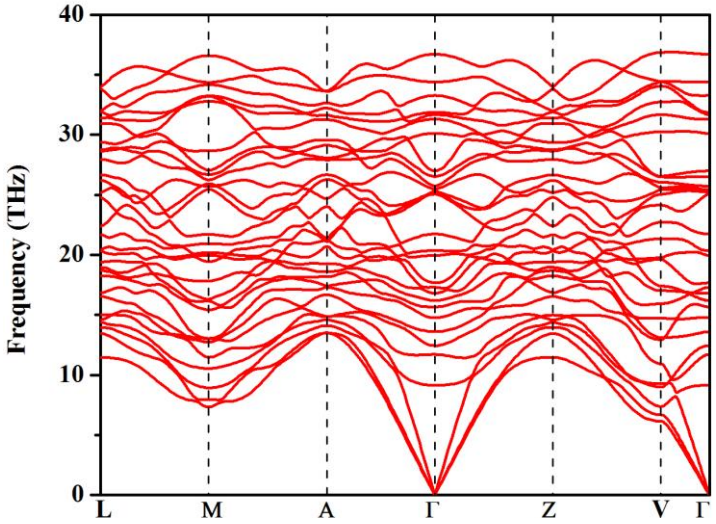

Fig. S2. Phonon dispersion curves of *C2/m* B_2CO_2 at ambient pressure.

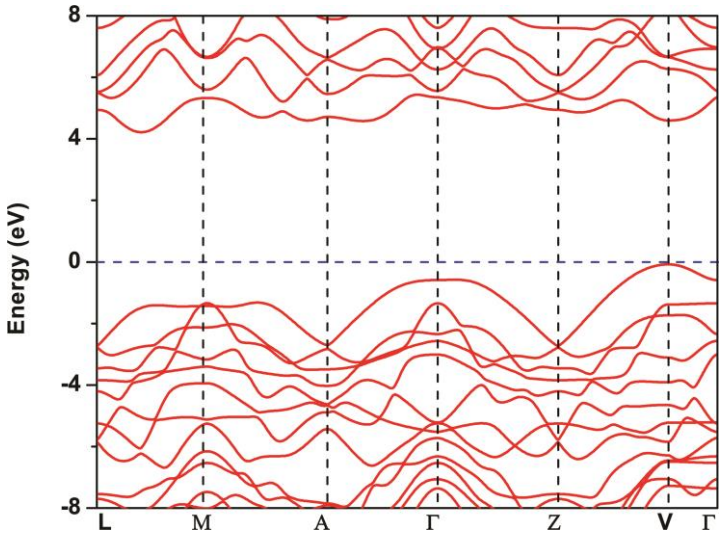

Fig. S3. Electronic band structure of C2/m B_2CO_2 at ambient pressure.

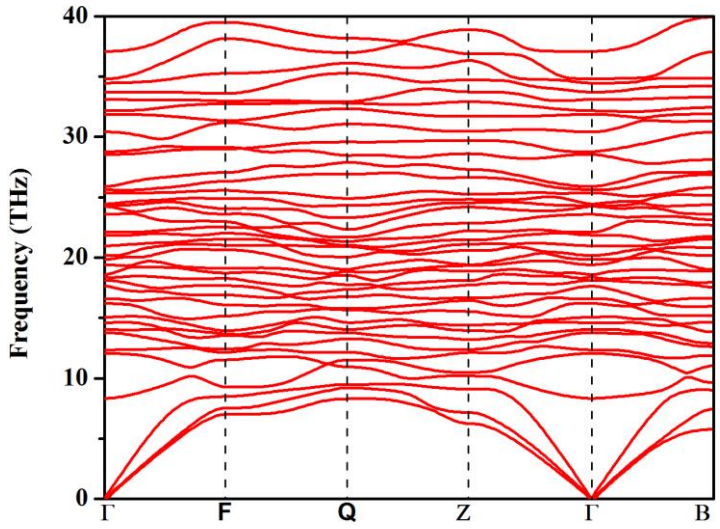

Fig. S4. Phonon dispersion curves of $B_6C_2O_5$ at ambient pressure.

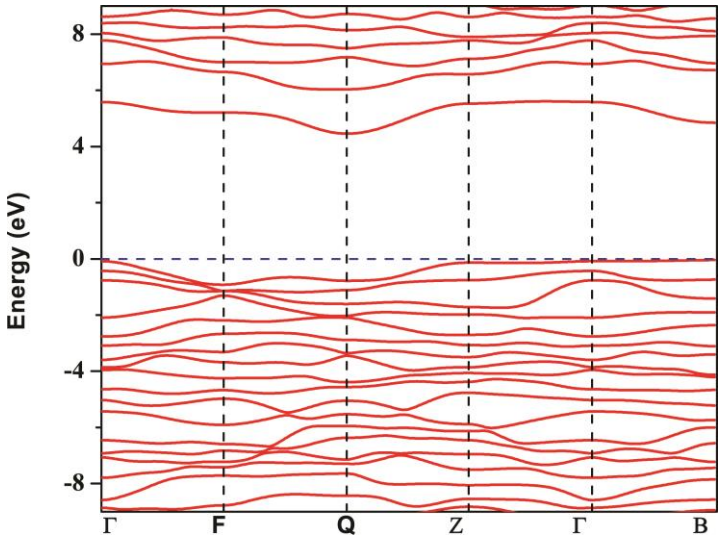

Fig. S5. Electronic band structure of $B_6C_2O_5$ at ambient pressure.