Supporting Information

Raman Spectroscopy Signatures of Boron-Rich Superhard Materials from Density Functional Theory

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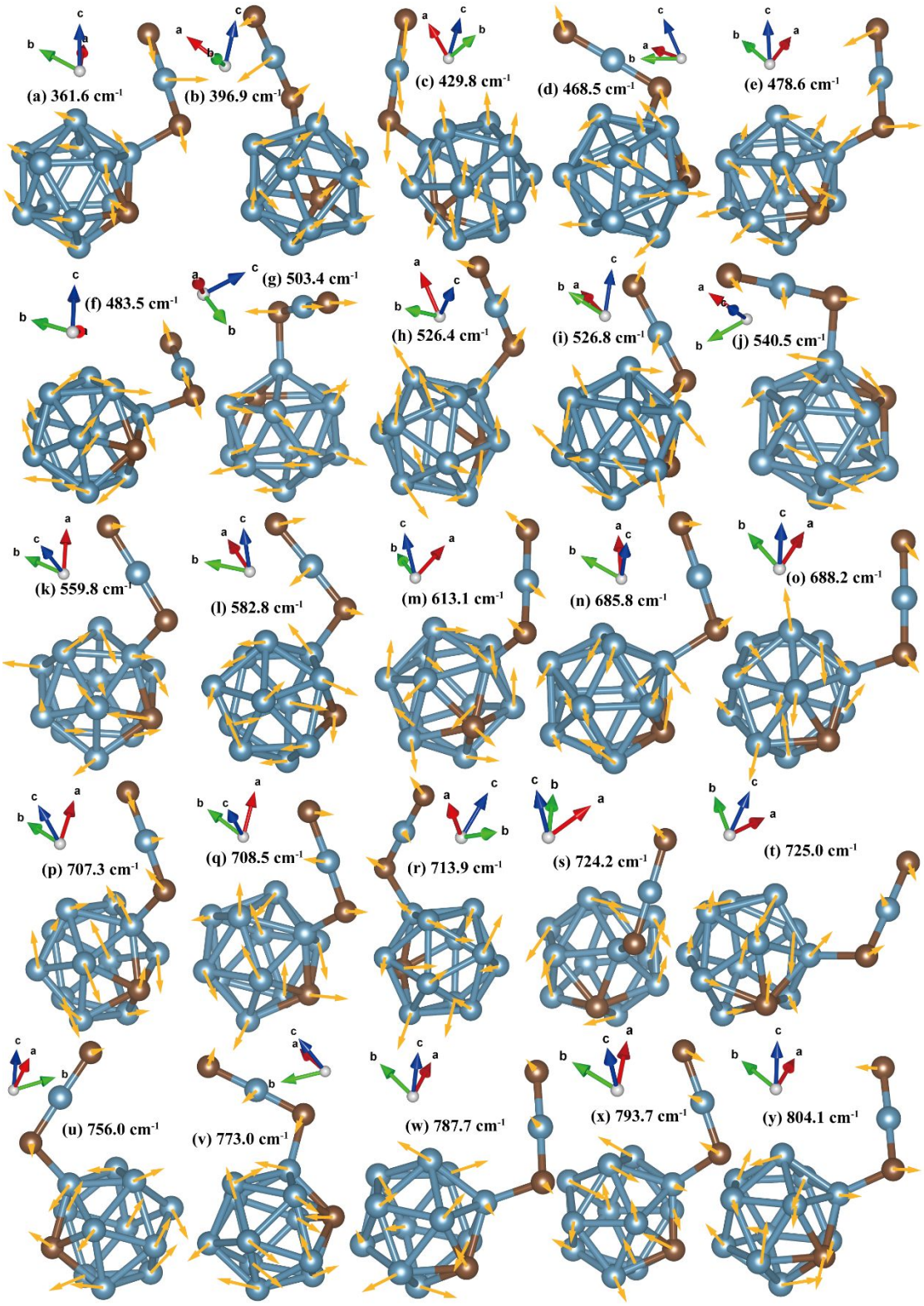

Figure S1. Calculated Raman modes and frequencies (range from 361.6 cm^{-1} to 804.1 cm^{-1}) of B_4C crystal. Atom color scheme: B: blue, C: sienna.

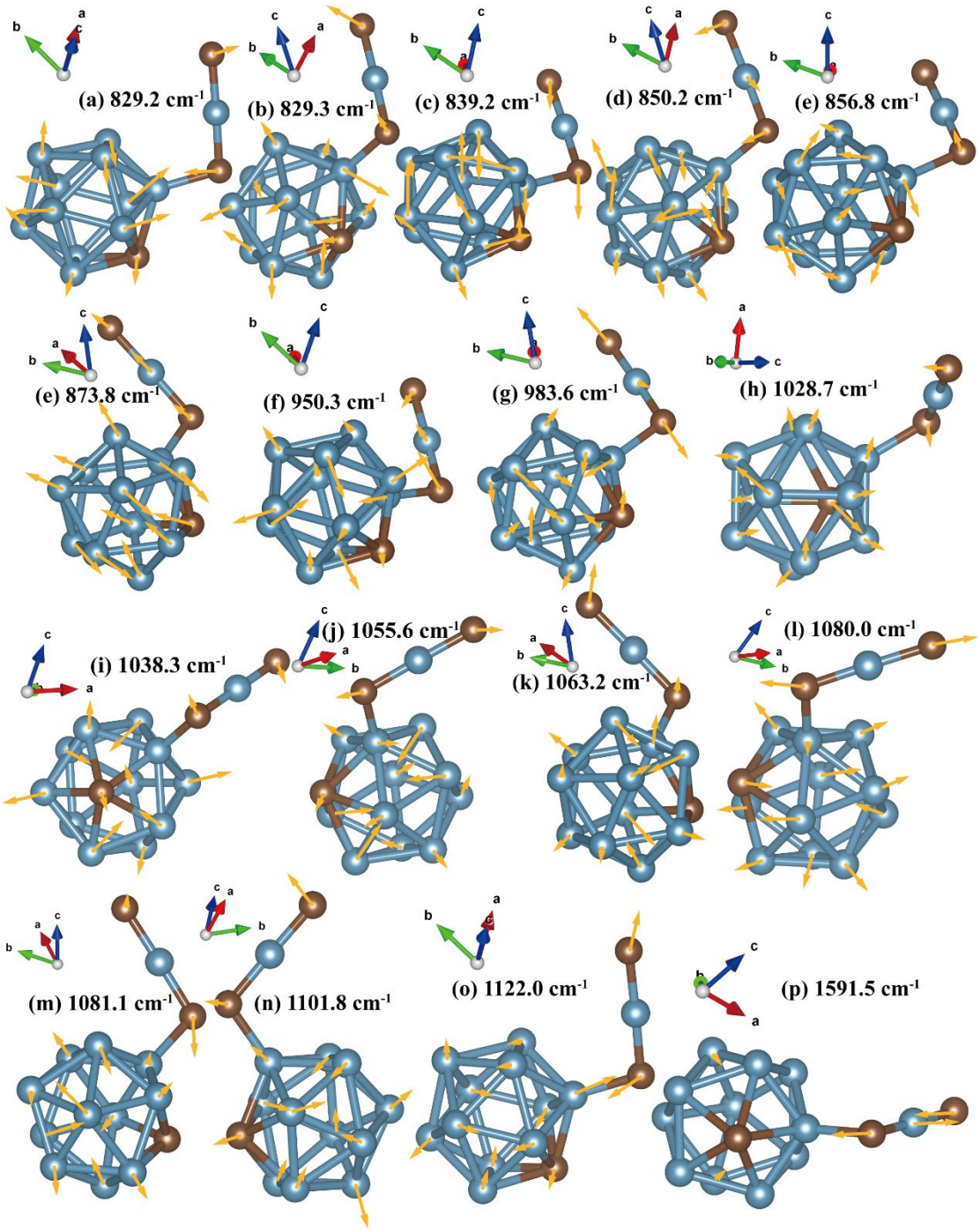

Figure S2. Calculated Raman modes and frequencies (range from 829.2 cm^{-1} to 1591.5 cm^{-1}) of B_4C crystal. Atom color scheme: B: blue, C: sienna.

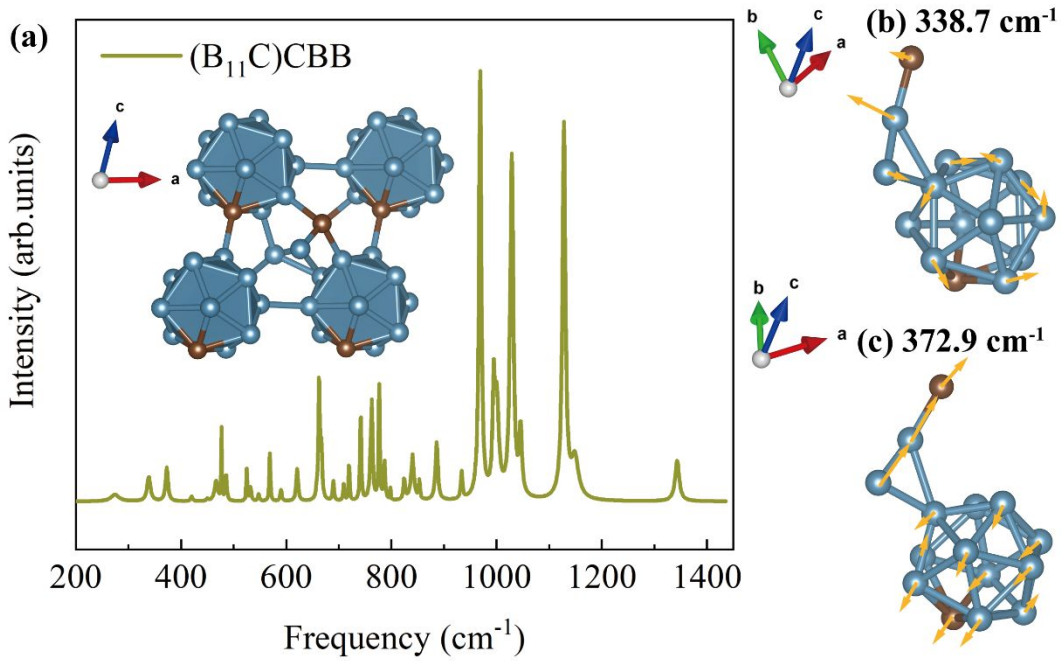

Figure S3. (a) The Raman spectrum and the crystal structure of $(B_{11}C)C$-B-B; (b) Calculated Raman modes at 338.7 cm^{-1} and 372.9 cm^{-1} of $(B_{11}C)C$-B-B crystal. Atom color scheme: B: blue, C: sienna.

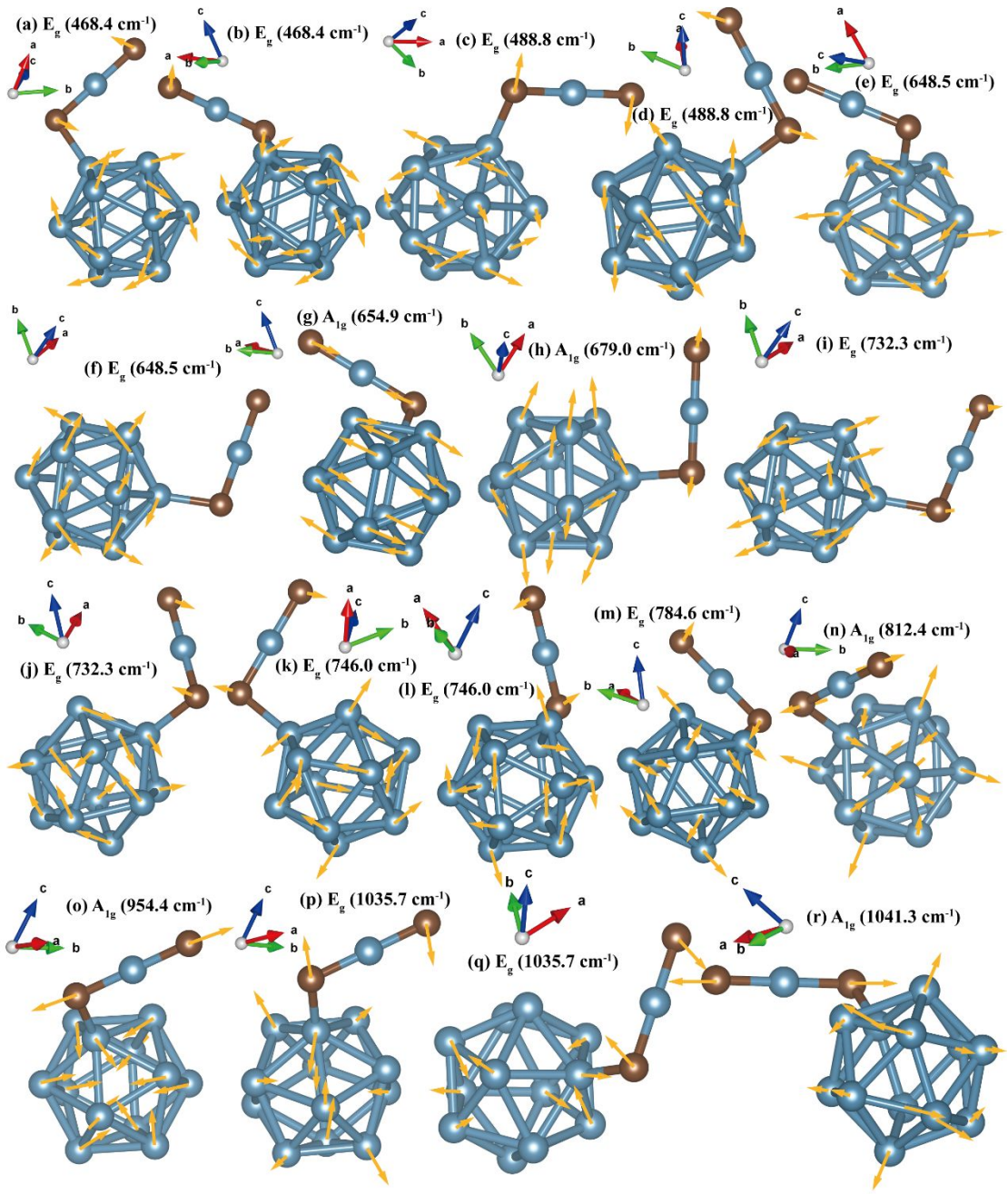

Figure S4. Calculated Raman modes and frequencies of $(B_{12})CBC$ crystal. Atom color scheme: B: blue, C: sienna.

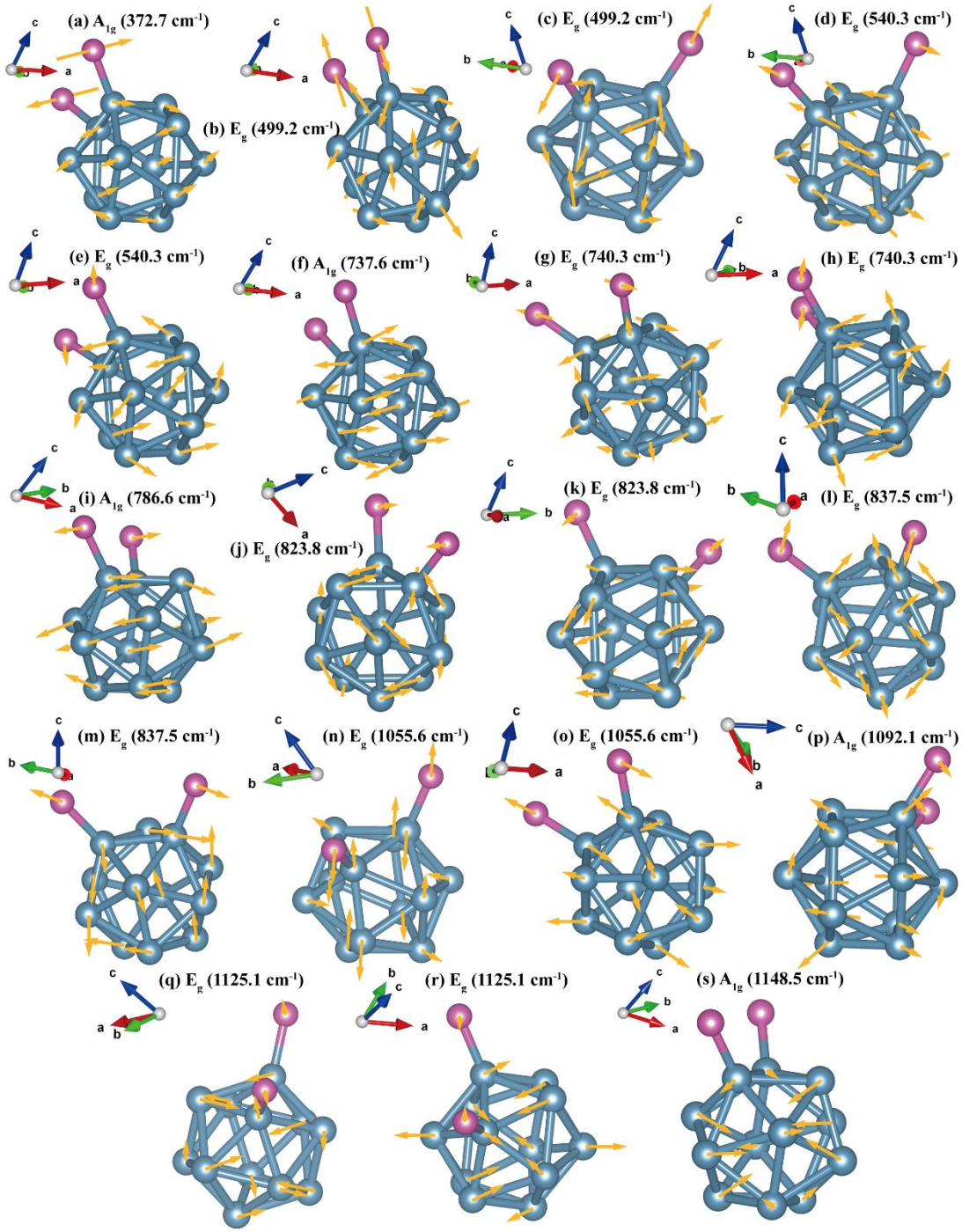

Figure S5. Calculated Raman modes and frequencies of B_6O crystal. Atom color scheme: B: blue, O: pink.

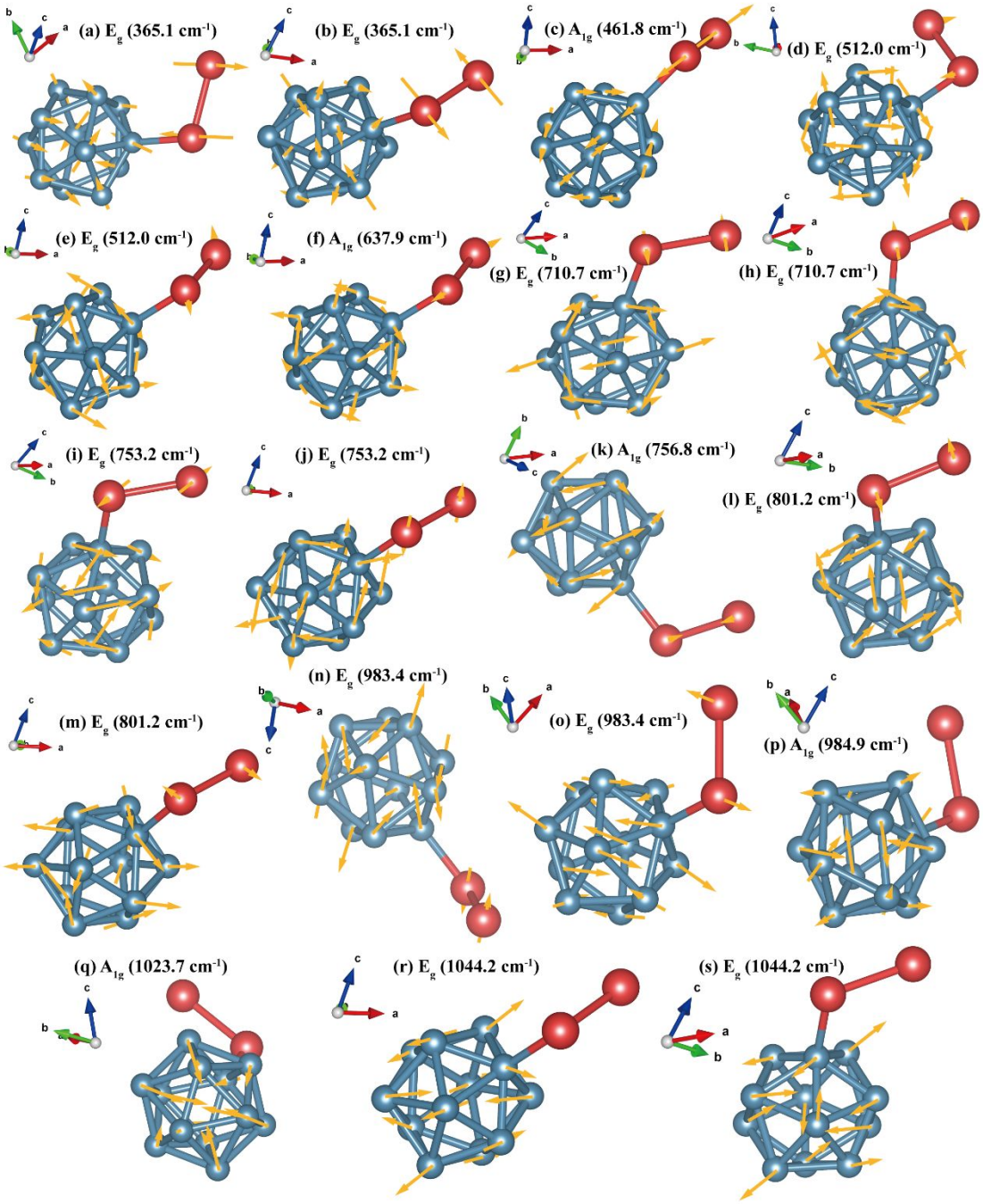

Figure S6. Calculated Raman modes and frequencies of $B_{12}P_2$ crystal. Atom color scheme: B: blue, P: red.