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Diamondlike carbo-boride C5B compound? Testing crystal structures and stability with Global Space Group Optimization (GSGO)[1] ARKADIY MIKHAYLUSHKIN, National Renewable Energy Laboratory, USA, XIUWEN ZHANG, Colorado School of Mines, Golden, USA, ALEX ZUNGER, University of Colorado, Boulder, USA — Diamond-like C5B has been alleged to be a new exciting material discovered at high pressures and temperatures. Using density-functional based evolutionary Global Space Group Optimization (GSGO) we established the likely structures of BC3 and BC5 phases and the known B4C compound. Examining the ground state line between solid Carbon and solid Boron we find only B4C is a ground state structure. C5B and C3B are high energy structure at high pressure. The reaction between BC3 and solid carbon producing C5B is found to have a positive reaction enthalpy that depends only weakly on pressure. In contrast to the previous reports, we argue that at 0 T the BC5 is less stable than BC3 in access of carbon. However, a small positive enthalpy of the reaction BC5 $\rightarrow$ BC3 +2C cannot rule out formation of the BC5 from the BC3 precursor material as thermally stabilized due to vibrational entropy or/and disorder effects.

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