Boron: do we know the ground state structure?[1]

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Boron is only the fifth element in the periodic table, having a simple electronic configuration, yet, it is known to form one of the most complicated crystal structures, β-rhombohedral structure. Up to date, the best estimate on the number of atoms in its hexagonal unit cell is 320.1, not even an integer number. The key concept to understand its complexity is covalency and electron deficiency: It does not have enough valence electrons to form a simple covalent crystal, like carbon or silicon. Instead it forms a complicated packing of icosahedrons. The structural model of β-boron was developed in the 1960s based on X-ray experiment. Although this model structure captures the most of the structural characteristics of β-boron, it has a crucial pitfall; the number of atoms per cell estimated by X-ray experiment does not agree with the number of atoms estimated by the pycnometric density. In 1988, Slack et al. discovered four more POS, by which the discrepancy in the number of atoms is reconciled [J. of Solid State Chem. 76, 52 (1988)]. There still remains an unanswered question; how are these POS atoms configured? Is it completely random? Or there is some kind of order as it has been suggested in Slacks paper? A major challenge here is the astronomical number of possible configurations, roughly 150 million even for the irreducible cell. We tackle this problem using *ab-initio* simulated annealing coupled with a Lattice Model Monte Carlo simulated annealing. Our results reveal that the stable structure, indeed, has a certain type of correlation in its POS configuration. More detail on the structural property and its impact on electronic property of β-boron will be discussed at the presentation. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/ LLNL under contract no. W-7405-Eng-48.