

How to make boron harder than diamond?

M M BALAKRISHNARAJAN and ELUVATHINGAL D JEMMIS
School of Chemistry, University of Hyderabad, Central Univ. P.O.,
Hyderabad 500 046, India

With its electron-precise covalent bonding, the extreme hardness of diamond is not surprising. On a scale of 1–15 (the modified Mohr's Scale of Hardness), diamond is at the top. Despite its widely discussed electron deficiency, the beta-rhombohedral polymorph of elemental boron has a hardness value of 11. This is to be compared to the hardness parameter of metal aluminum which stands at 3. While it is difficult to increase the hardness of diamond, it may be possible to do so for boron. We have analysed the structure of elemental boron with respect to its electron deficiency. Though the beta-rhombohedral boron is electron deficient, the extent of electron deficiency is not nearly as much as is anticipated. The schematic decomposition of the distinct structural fragments from the unit cell of elemental boron, the comparison of their electronic structures with molecules that can be constructed from these fragments, and the translation of the individual electronic structure requirements to the elemental boron polymorph are presented in detail. These studies have led, among others, to the formulation of a series of electron counting rules for polycondensed boranes and to encapsulated polyhedral structures. We also predict the precise number of electrons required per unit cell to make the beta-rhombohedral boron electron sufficient without changing its structure.