Is Platonic Icosahedral Solid Relevant to the Digital Age? Boron-based Icosahedra, the Computational/Electron Diffraction Structural Consequences of Functionalising the Cluster Atoms, their Removal, and of Sharing Two Icosahedra. Possible Application in Materials Science and Medicine

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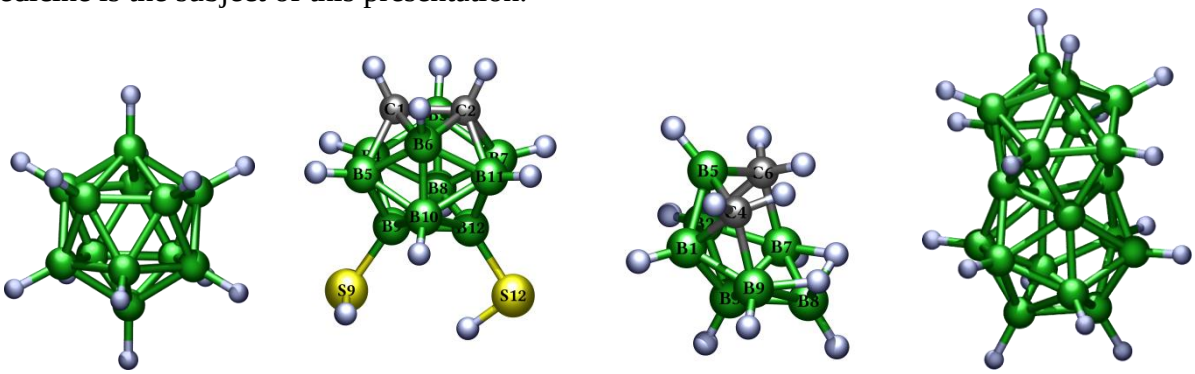
Just as carbon forms hydrocarbons, its neighbour, boron, forms boron hydrides. Due to the electron deficiency of boron, these boron hydrides do not resemble hydrocarbons in terms of molecular shapes. The geometries of boron clusters are based on various polyhedra, with the icosahedron being the most prominent. Indeed, *closo*-$B_{12}H_{12}^{2-}$ represents one of the most important building blocks in boron cluster chemistry and, moreover, is the most symmetrical geometric arrangement of boron and hydrogen atoms (I_h point-group symmetry). Departure from this symmetry may be achieved by replacing boron with heteroatoms, such as carbon, in various positions within the cage, by replacing hydrogen atoms with a variety of substituents (halogens and SH are often seen), and, finally, by removing one, two, or more vertices, resulting in further classes of boron clusters, such as *nido* or *arachno*. Boron based icosahedra also tend to be joined in various modes of sharing common vertices to get *macropolyhedral* clusters as a consequence.

Experimentally known examples derived by substituting carbon atoms into *closo*-$B_{12}H_{12}^{2-}$, by replacing hydrogen atoms with other atoms or moieties, by the removal of the aforementioned carbon atoms, and by sharing two icosahedra in different modes were studied using gas electron diffraction in conjunction with *ab initio* and DFT computational protocols of various quantities, the latter being sometimes the only possible structural tool applicable. Selection of such types clusters, their structural studies and outline of possible applications in materials science and medicine is the subject of this presentation.



Icosahedron: *its outer and inner functionalization* *its inner functionalization and removal of three vertices* *four-vertex sharing*