Boron Fullerenes: A New Class of Carbon-Free Hollow Nanostructures

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The discovery of boron fullerenes introduces a unique class of hollow nanostructures that fundamentally differ from their well-known carbon counterparts. While carbon fullerenes, such as C_{60}, derive their stability from delocalized π-bonding and *sp*² hybridization, boron fullerenes rely on multicenter bonding and electron-deficient frameworks to maintain structural integrity. Early theoretical predictions suggested that boron could form fullerene-like cages, with B_{80} [1] proposed as an analog to C_{60}. The first experimentally verified boron fullerene, B_{40} [2], exhibited D_{2d} point group symmetry with a unique C_2 axis, contrasting sharply with the near-spherical icosahedral symmetry of C_{60}. More recently, advances in gas-phase synthesis enabled the realization of the long-theorized B_{80} structure [3], confirming its viability as another boron-based counterpart to carbon fullerenes. Unlike the symmetric carbon buckyball composed solely of pentagons and hexagons, boron fullerenes stabilize through a mix of triangular, pentagonal, hexagonal, and even heptagonal faces. In this work, we present a comparative analysis of the electronic and structural properties of boron fullerenes, highlighting their differences and similarities with carbon fullerenes. Figure 1 illustrates the structure of B_{12}, B_{40}, and B_{80} fullerenes, demonstrating their structural diversity. By exploring their energetic landscapes and electronic properties, we establish boron fullerenes as a new class of molecular building blocks for boron-based nanomaterials [4] with promising applications in molecular electronics, energy storage, and catalysis. Their unique bonding mechanisms and chemical versatility offer advantages beyond traditional carbon-based materials, and the successful synthesis of B_{80} represents a milestone in fullerene chemistry, opening new possibilities for boron nanotechnology and expanding the frontier of low-dimensional materials.

References

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[3] H. W. Choi et al., ChemRxiv (2024) DOI: 10.26434/chemrxiv-2024-2xnxl.
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Figures

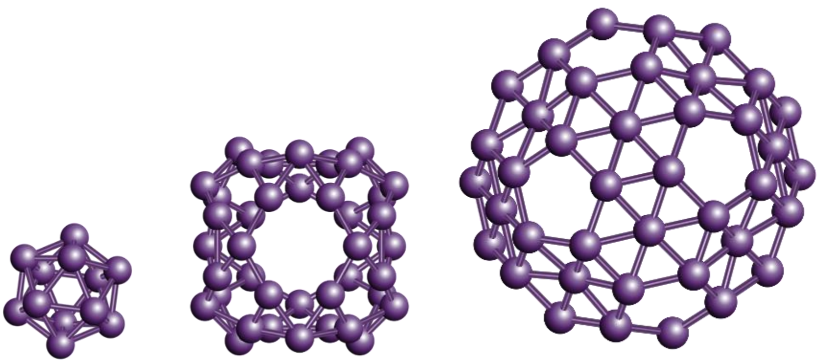

Figure 1: Atomic structures of the boron fullerenes B_{12}, B_{40}, and B_{80}, illustrating their structural diversity.