TRANSITION-METAL-DOPED PLANAR BORON CLUSTERS: A NEW CLASS OF AROMATIC COMPOUNDS WITH HIGH COORDINATION

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Photoelectron spectroscopy in combination with computational studies over the past decade has shown that boron clusters possess planar or quasi-planar structures, in contrast to that of bulk boron, which is dominated by three-dimensional cage-like building blocks. All planar or quasi-planar boron clusters are observed to consist of a monocyclic circumference with one or more interior atoms. The propensity for planarity has been found to be due to both \( \sigma \) and \( \pi \) electron delocalization throughout the molecular plane, giving rise to concepts of \( \sigma \) and \( \pi \) double aromaticity. We have found further that the central boron atoms can be substituted by transition metal atoms to form a new class of aromatic compounds, which consist of a central metal atom and a monocyclic boron ring (M\( \text{c} \)\( \text{⃝} \)B\(_n\)). Eight-, nine-, and ten-membered rings of boron have been observed, giving rise to octa-, ennea-, and deca-coordinated aromatic transition metal compounds [1-3].

References:
[3] “Observation of the Highest Coordination Number in Planar Species: Decacoordinated Ta\( \text{c} \)\( \text{⃝} \)B\(_{10}\) and Nb\( \text{c} \)\( \text{⃝} \)B\(_9\) Anions” (Timur R. Galeev, Constantin Romanescu, Wei-Li Li, L. S. Wang, and A. I. Boldyrev), Angew. Chem. Int. Ed. 51, 2101-2105 (2012).