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 σ and π electron delocalization throughout the molecular plane, giving rise to concepts of σ and π 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 \bigcirc 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:

[1] "Aromatic Metal-Centered Monocyclic Boron Rings: $Co@B_9^-$ and $Ru@B_9^-$ " (Constantin Romanescu, Timur R. Galeev, Wei-Li Li, A. I. Boldyrev, and L. S. Wang), Angew. Chem. Int. Ed. **50**, 9334-9337 (2011).

[2] "Transition-Metal-Centered Nine-Membered Boron Rings: $M \odot B_9$ and $M \odot B_9^-$ (M = Rh, Ir)" (Wei-Li Li, Constantin Romanescu, Timur R. Galeev, Zachary Piazza, A. I. Boldyrev, and L. S. Wang), J. Am. Chem. Soc. **134**, 165-168 (2012).

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