PHOTOELECTRON SPECTROSCOPY OF ALUMINUM DOPED BORON CLUSTERS

WEI-LI LI, CONSTANTIN ROMANESCU, LAI-SHENG WANG, *Brown University, Chemistry Department, 324 Brook Street,Providence, RI 02912, USA*.

Anionic boron clusters have been shown to be planar or quasi-planar up to $B_{21}^-$ from a series of combined photoelectron spectroscopy and theoretical studies. All these boron clusters consist of a peripheral ring characterized by strong two-center-two-electron (2c-2e) B-B bonds and one or more interior atoms. The propensity for planarity is due to $\sigma$- and $\pi$-electron delocalizations throughout the molecular plane, giving rise to concepts of $\sigma$- and $\pi$-aromaticity. The quasi-planarity, on the other hand, can be mechanical in nature - the circumference of the cluster is too small to fit the inner atoms - even for doubly aromatic clusters. Two questions arise: firstly, can isoelectronic substitution by a single aluminum atom on the outer ring enhance the planarity of quasi-planar structures, and, secondly, can the interior boron atoms be replaced by aluminum? A series of aluminum isoelectronic substitution of boron clusters have been investigated ranging from $B_7^-$ to $B_{12}^-$. Aluminum turns out to avoid the central position in the all these clusters and enhance the planarity of $AlB_6^-$ and $AlB_{11}^-$ clusters by expanding the peripheral ring.

References:

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