

PHOTOELECTRON SPECTROSCOPY OF ALUMINUM DOPED BORON CLUSTERS

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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 σ - and π -electron delocalizations throughout the molecular plane, giving rise to concepts of σ - and π -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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