Disk aromaticity in singlet and triplet boron clusters. A current density point of view

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Abstract

The disk-like boron clusters are among the most captivating boron cluster forms. It has been proposed that molecular orbital distribution in these clusters can be predicted based on the simple particle-on-a-disk model. In this model, the molecular orbitals come by pairs except for m = 0 (no angular nodes). Within the CTOCD-DZ (continuous transformation of origin of current density method - diamagnetic zero) method the induced current density of the particle-on-a-disk-based model can be rationalized by applying simple symmetry- and energy-based selection rules on the virtual orbital transitions. The particle-on-a-disk model predicts that if the number of valence electrons is increased or reduced by two electrons, the disk-like boron clusters that are aromatic (sustain diatropic currents) in their ground states remain aromatic in their lowest-lying triplet states. In this study we employed the magnetically induced current densities to test the performance and limits of the particle-on-a-disk model in description of the electronic structure of the disk-like boron clusters. It was found that Hückel and Baird's rules can be successfully applied to predict aromatic character of the studied disk-like boron clusters in their lowest-lying singlet and triplet states, with the exception of triplet $^3B_{19}^-$.