Revisiting (anti)aromaticity and chemical bond in planar BXNX clusters (x = 2-11)

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As Nucleus-Independent Chemical Shift (NICS) measurements have shown inconsistent results with other traditional methodologies in the assignment of aromaticity for inorganic compounds, leading to a possible erroneous interpretation, a complete analysis of the (anti)aromatic character of some BxNx (x = 2-11) according to the magnetic criteria of aromaticity has been performed in order to evaluate the response of these indices in the assignment of this property. Vector mapping of the magnetically induced current density; ring current strength analysis; one- (FiPC and scans), two- (isolines), and three-dimensional (isosurfaces) NICSzz-based descriptors; and adaptive natural density partitioning analysis were performed at the PBE0/def2-TZVP level of theory. The values obtained determined the weak aromatic character for B3N3 and B5N5, antiaromatic character for B4N4, doubly antiaromatic character for B2N2, and nonaromatic character for the remaining clusters. The results show some discrepancies with the ones based on the classical NICS, which can be attributed to in-plane and core electron contributions. Finally, the presented results reveal the importance of being careful regarding the interpretations given by this index and the need to use one-, two-, or three-dimensional derived methodologies for a complete and correct analysis of (anti)aromaticity.

aromaticity

atomic clusters

boron nitride materials

NICS

ring current strength

Aromatic compounds

Aromatization

Chemical shift

Current density

Inorganic compounds

Antiaromatic character

Aromaticities

Core electrons

Magnetically induced currents

Natural density

Nucleus independent chemical shifts

Ring currents

Vector mapping

Chemical analysis