Which NICS method is most consistent with ring current analysis? Assessment in simple monocycles

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The aromaticity of benzene, Al42- cluster, cyclopropane, borazine and planar cyclooctatetraene (COT) was analyzed according to different strategies based on nucleus-independent chemical shift (NICS) computations. The analysis of NICS-components evolution along the main molecular axis seems to be the most adequate and simplest strategy to predict the aromatic or antiaromatic character of the studied systems. Moreover, the analysis of the ?- and ?-electron contributions to the out-of-plane component of NICS (NICSzz) leads to the same qualitative and quantitative conclusions previously obtained by the analysis of the magnetically induced ring current densities.