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SURPRISES IN NICS STUDIES AND A NEW NICS-BASED CRITERION FOR AROMATICITY

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All the different NICS methods (for example, NICS(r), $NICS(r)_{zz}$, etc., where r is the distance from the molecular plane) are calculated at and above the geometric center of the molecule. The rational behind this is that the induced magnetic field by the π electrons induced current (under an external magnetic field) is the strongest along the line that originates at the center and perpendicular to the molecular plane. However, a careful study, using a two-dimensional grid of BQs, suggests that at (relatively) short distances from the molecular plane the maximal induced magnetic field is off-center. Only at larger distances (1.4–2.2 Å, depending on the specific system), the maximal induced field is above the geometrical center of the system.

The paper discusses the possible reasons for these findings and suggests a new aromaticity criterion - $\int NICS_{\pi,zz}$, which is based on the pure π-induced ring current.