

# Revisiting Aromaticity and Chemical Bonding of Fluorinated Benzene Derivatives

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The electron delocalization of benzene (C<sub>6</sub>H<sub>6</sub>) and hexafluorobenzene (C<sub>6</sub>F<sub>6</sub>) was analyzed in terms of the induced magnetic field, nucleus-independent chemical shift (NICS), and ring current strength (RCS). The computed out-of-plane component of the induced magnetic field at a distance (*r*) greater than or equal to 1.0 Å above the ring center correlates well ( $R^2 > 0.99$ ) with the RCS value. According to these criteria, fluorination has two effects on the C<sub>6</sub> skeleton; concomitantly, the resonant effects diminish the  $\pi$  electron delocalization and the inductive effects decrease the charge density at the ring center and therefore reduce the magnitude of the paratropic current generated in this region. The equilibrium between both effects decreases aromaticity in the fluorinated benzene derivatives. These results can be extrapolated to determine the aromaticity of any derivative within the series of fluorinated benzene derivatives (C<sub>6</sub>H<sub>(6-n)</sub>F<sub>n</sub>, where *n*=1-5). © 2014 The Authors.

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adaptive natural partitioning analysis

aromaticity

fluorinated benzenes

induced magnetic fields

magnetically induced current density