Understanding the aromaticity of C6X6 (X?=?H, F, Cl, Br, I). Insights from different theoretical criteria

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Different theoretical methodologies were applied to a series of substituted benzenes C6X6 (with X = H, F, Cl, Br and I) to pursue the property of aromaticity. HOMA (as structural criterion), NICS (FIPC-NICS, isotropic and ZZ employed as magnetic criteria) as well as the indexes ASE, MCI, PDI and FLU, interestingly provided controversial data respect to the magnetically induced current density plots and chemical intuition, which is extensively discussed in the herein work. Furthermore, EDA-NOCV was used to complement the rational explanation of the observed results.