The aromaticity in bowl-shaped polycyclic aromatic hydrocarbons

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The aromaticity in a series of bowl-shaped polycyclic aromatic hydrocarbons (PAH) and several fullerenes has been studied by means of *ab initio* methods. NICS and delocalization indices have been used to quantify the aromaticity in PAHs and fullerenes. The series of PAHs selected includes $C_{14}H_8$, $C_{26}H_{12}$, and $C_{30}H_{12}$, with benzene and naphthalene ($C_{10}H_8$) taken as planar references and C_{60} as a curved reference. The change in the aromaticity of the six-membered rings when going from benzene to C_{60} has been analyzed. We have discussed also the relationship between the aromaticity of the studied PAHs and their reactivity in Diels-Alder cycloadditions of 1,3-butadiene to their [6,6]-bonds. Finally, we have also compared the aromaticity of C_{60}^{+10}, C_{70}, and open [5,6]- and closed [6,6]-$C_{59}NH$ with that of C_{60}.