The induced magnetic field in the study of the aromaticity

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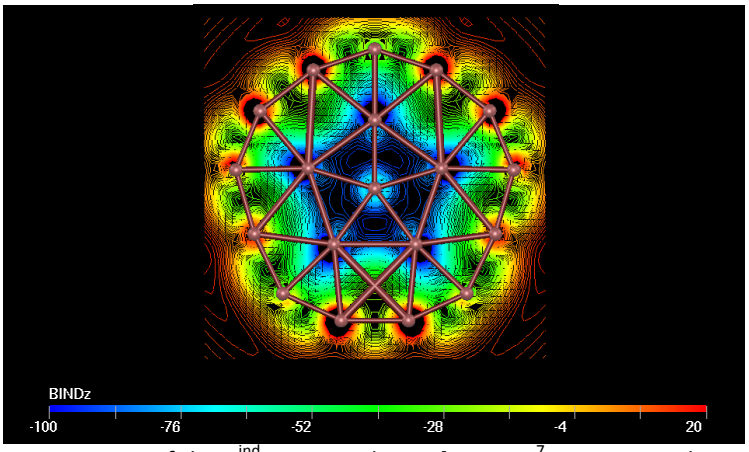
Aromaticity is a concept widely used in the chemical literature, but does not have an absolute scale. There are different techniques to try to quantify –or qualify- this property. Some are based in the geometry of the molecule (bond length), other in their reactivity (chemical behavior), other based in the highlighted stability and other in the magnetic properties. In this last group we found the induced magnetic field ($\mathbf{B}^{ind}$). When one molecule is exposed to an external magnetic field the valence electrons generate a ring current, which produces a second magnetic field, the $\mathbf{B}^{ind}$. This new magnetic field is characteristic of the electronic system of the molecule. The induced magnetic field is computed by the next equation

$$\mathbf{B}^{ind} = - \sigma_{\alpha\beta} \mathbf{B}^{ext}$$

where σ is the shielding tensor and $\mathbf{B}^{ext}$ is the vector that represents the external magnetic field.[1] This equation allows compute the induced magnetic field in any point in the space. The magnetic response can be separated in its molecular orbital contributions.[2] This technique has been employed in several chemical systems like organic compounds including molecules with planar tetracoordinated carbons,[3] all-metal salts,[4] boron wheels,[5] molecular stars.[6]



Isolines of the z component of the $\mathbf{B}^{ind}$ computed in B_{19}^- system.[7] Negative and positive values are related with shielding and deshielding regions, respectively. The scale is in ppm.

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