Quantitative analysis of aromaticity in azines by means of dissected descriptors based on the magnetic criteria

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Abstract

The effect of the systematic replacement of a CH group by an N atom in the aromaticity and stability of a benzene is a question in chemistry that has several answers. In this article we will re-examine the aromaticity using the magnetic criteria through ring current strength (RCS) and $NICS_{zz}$ descriptors dissected in their σ and π contributions at DFT level and the relative stability and ΔE_{gap} of azines at the CCSD(T) level. The results are pragmatic and show that, in effect, the replacement of a CH unit by N atom produces a reduction in aromaticity of azines being less aromatic those with more C-N units. This reduction is small so that systems still present large aromatic behaviour. Additionally, it is shown that there is an influence of the local diatropic currents located in the nitrogen atoms therefore the dissected indicators such as RCS_{π} and $NICS_{\pi,zz}(1)$ are those that best describe the aromaticity in azines. Finally, it is observed a trend between RCS values and ΔE_{gap} at the CCSD(T) level which could be explained using the maximum hardness principle. The systemic replacement causes a reduction in the relative stability of azines, and however, there is no direct relationship with aromaticity since it is necessary to take into account the σ effects. © 2021