

Effect of benzo-annulation on local aromaticity: to what extent do different aspects of aromaticity agree?

Slavko Radenković, Slađana Đorđević

*Faculty of Science, University of Kragujevac, Radoja Domanovica 12, 34000
Kragujevac, Serbia*

Recent systematic studies demonstrated that the intensity of cyclic electron delocalization in the six membered rings of benzenoid hydrocarbons can be significantly altered by means of benzoannulation. In particular, linear (resp. angular) benzo-annulation was found to decrease (resp. increase) the intensity of cyclic electron delocalization. These regularities were initially observed using the energy effect (ef) which is a graph-theory-based quantity calculated at the level of the simple HMO theory. Eventually, the ef-based results were corroborated at higher levels of calculations by means of the multi centre delocalization index (MCI) and harmonic oscillator model of aromaticity (HOMA) index. On the other hand, the nucleus independent chemical shifts (NICS) index does not support the results obtained by the other employed aromaticity indices. Our aim is to provide a better understanding of the found disagreement between the NICS, as a magnetic index, and the electronic-, energy- and geometry-based aromaticity indices. Here we employed the integrated current strength (current strength susceptibility) to quantify the local aromaticity of individual rings in anthracene and acridine benzo-annulated derivatives. The magnetic aspect of the local aromaticity in the studied molecules was found to be not related to the electronic, geometric and energetic aspects, findings that underline earlier observations on differences between the various aspects of the aromaticity phenomenon.