On the Relationship between π-Electron Energy and Topological Resonance Energy

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Within series of isomeric benzenoid hydrocarbons there is a very good linear correlation between the topological resonance energy (TRE) and the total π-electron energy (E_π). Furthermore, the slope of the TRE vs. E_π regression line is almost independent of the benzenoid isomers considered, and (for all sets of isomers) is nearly equal to 0.5. This implies that comparison of benzenoid isomers with regard to their aromaticity can be made, with equal success, by using both TRE and E_π. However, E_π is computed significantly simpler than TRE, and thus advantage should be given to the former. Correlations between TRE and E_π exist also in the case of non-benzenoid isomers (both alternant and non-alternant), but are of much inferior quality.

Key words: Total π-Electron Energy; Topological Resonance Energy; Aromaticity; Benzenoid Hydrocarbons.