Heteroatom effects on aromaticity of five-membered rings in acenaphthylene analogs

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Abstract

The pattern of cyclic conjugation was thoroughly studied in the series of N- and P-acenaphthylene derivatives using several different aromaticity indices: the energy effect (ef), multicenter delocalization index (MCI), harmonic oscillator model of aromaticity (HOMA) index and nucleus independent chemical shifts (NICS). The Kekulé-structure-based reasoning predicts that there would be no cyclic conjugation in the "empty" five-membered heteroatom-containing rings in the studied molecules. It was found that, according to the ef, MCI and HOMA values, the extent of cyclic conjugation in the pentagonal rings is strongly influenced by the number and mutual arrangement of the hexagonal rings. In addition, it was revealed that in some of the examined molecules the intensity of cyclic conjugation in the "empty" pentagons is even stronger than that of some hexagonal rings within the same molecule. The obtained results refute what one would expect based on "chemical intuition", which is usually strongly rooted to the Kekulé structures.

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