Aromaticity in heterocyclic analogues of benzene: Dissected NICS and current density analysis

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The magnetic aromaticity of 6-membered monoheterocycles containing Group 13 to 16 elements (C5H5X, where X = SiH, GeH, N, P, As, O+, S+, Se+) was assessed by using 2 magnetic descriptors: the ?-electron contribution to the out-of-plane component of the nucleus-independent chemical shifts (NICSzz,?) and ring current strength. The results show that both descriptors lead to the same conclusion regarding magnetic aromaticity. However, they do not agree with the predictions obtained by isotropic NICS, which is a most commonly used method. Ring current strength and NICS? predict that benzene is the most aromatic molecule of the series, with an only slightly less aromatic pyridine. Additionally, aromaticity decreases when going down in the same group of the periodic system. The only exception is the pyrylium cation, which is predicted as the least aromatic species of this series.

benzene analogues

current density

magnetic aromaticity

NICS

Benzene

Current density

Magnetism

Aromatic molecules

Aromatic species

Aromaticities

Magnetic aromaticity

NICS

Nucleus independent chemical shifts

Out-of-plane components

Ring currents

Aromatization