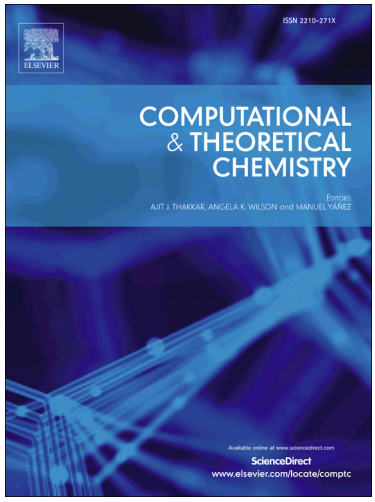

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Chemical bonding in the pentagonal-pyramidal benzene dication and analogous isoelectronic hexa-coordinate species

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Abstract

The nature of the chemical bond in the pentagonal-pyramidal benzene dication and related species was described by Modern Valence Bond calculations and the Generalized Product Function Energy Partitioning method. The results suggest that the π space of $C_6H_6^{2+}$ is composed of a donor-acceptor bond from a cyclopentadienyl anion moiety, described as a 5c-6e π bonding, to a triply charged Lewis acid CH structure. Similar results were found for isoelectronic species, such as $C_5H_5BH^+$, C_5H_5BeH, and $C_5H_5LiH^-$, leading to different main-group hexa-coordinate atom-bearing structures. A pictorial mechanism for the bonding of the studied molecules was constructed, and different geometrical and electronic features could be explained by this straightforward model. Finally, the results suggest that several poly-coordinate atom-containing molecules, sandwich-type compounds, oligomers, and polymers could be formed by the interaction of a π system and Lewis acid moieties.

Keywords: Valence Bond Theory; Spin-Coupled Theory; Generalized Valence Bond; Chemical Bond Theory; Benzene Dication; Hexa-coordinate Carbon

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