

Local and global aromaticity in a molecular carbon nanobelt: Insights from magnetic response properties in neutral and charged species

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The formation of carbon nanobelt made exclusively from fused benzene rings has recently been achieved. Our results reveal an interesting shift from a local aromatic character constrained in each of the six aromatic Clar sextets (6 π -electron circuit) to a global aromatic character in charged species (+2 and -2) involving the overall π -circuit from the molecular nanobelt. This demonstrates the suppression of the local aromatic character in favor of a global aromaticity by selecting the oxidation state of the carbon nanobelt, giving rise to a shielding cone extended within the structure.

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