

# Aromaticity Survival in Hydrofullerenes: The Case of $C_{66}H_4$ with Its $\pi$ -Aromatic Circuits

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## Abstract

The isolated-pentagon rule (IPR) is a determining structural feature that accounts for hollow fullerene stabilization and properties related to  $C_n$  ( $n \geq 60$ ) cages. The recent characterization of an unprecedented non-IPR hydrofullerene,  $C_{2v} C_{66}H_4$ , bearing two heptagons with adjacent fused-pentagon motifs, largely dismisses this feature. Herein, employing DFT calculations, the  $^{13}C$  NMR spectroscopy and aromatic behavior of  $C_{2v} C_{66}H_4$  are explored. The results show the presence of three  $\pi$ -aromatic circuits at the bottom boat section of  $C_{66}H_4$ , indicating the unique features of this hydrofullerene in comparison to those of pristine  $C_{60}$ . In addition, under specific orientations of the external field, certain  $\pi$ -aromatic circuits are enabled, resulting in a more aromatic fullerene than that of  $C_{60}$ , but lower than that of the spherical aromatic  $C_{60}^{6-}$  fulleride. Notably, under a field aligned with the saturated carbon atoms, nonaromatic characteristics are exposed. This reveals that spherical-like cages can involve a complex magnetic response that heavily depends on the orientation of the applied field.

## Author keywords

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ring currents