

An unprecedented π -electronic circuit involving an odd number of carbon atoms in a grossly warped non-planar nanographene

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Abstract

The formation of π -aromatic circuits along a grossly warped nanographene, C₈₀H₃₀, containing five- and seven-membered rings inserted into a six-membered mesh, reveals global π -circuits at the edge of the backbone. Based on DFT calculations, one of the two most favorable circuits for π -electron delocalization formally has 50 π -electrons abiding by Hückel's rule, whereas the second one formally has 75 π -electrons and, remarkably, it does not follow any of the known rules of aromaticity.