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A Topological Approach to the Stabilities of Isomeric Hückel and Mobius Type Cyclacenes

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Abstract: Within the constraints of Hückel molecular orbital theory, Hückel and Mobius type cyclacenes were investigated in terms of their angle of total π -electron energy, O_π , and $\cos O_\pi$ to find out how structural changes affect the stabilities. It has been theoretically deduced that as the number of benzenoid rings (R) increases the isomeric Hückel and Möbius type cyclacenes should have comparable stabilities, although for low values of R odd-Hückel type and even-Mobius type are predicted to be more stable.

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