

On the fused-to-single ring transition in 10^e structures. Insights from naphthalene to [10]annulene series

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The fused-to-single-ring transition is studied through a 10^e series given the series from naphthalene to [10]annulene. Our results suggest that change occurs at certain structure instead of a gradual transition. In the transition point, given by bicyclo[7.1.0]decapentaene, similar magnetic behavior in comparison to the single ring counterpart is found. The systems can be considered to behave as a whole single aromatic structure where the fused counterparts can be treated as a modification in the aromatic path of a single ring aromatic motif, which can be viewed as a useful approach to evaluate the formation of defects or larger-rings in graphene motifs. © 2016 Elsevier B.V. All rights reserved.