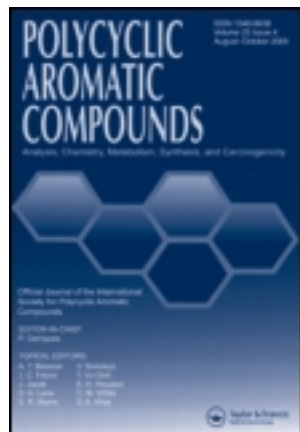


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Local Aromaticity in Benzo- and Benzocyclobutadieno-Annulated Phenanthrenes

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The effects of benzo- and benzocyclobutadieno-(BCBD-)annulation on the local aromaticity of the central ring (X) of phenanthrene were examined. The local aromaticity of the ring X was estimated using a graph-theory-based index and two geometry-based indices. DFT calculations of phenanthrene congeners showed that many of these molecules are nonplanar, with significant steric strain. All three indices indicate that the effect of benzo-annulation is opposite to that of BCBD-annulation. The deviation of some phenanthrene derivatives from planarity does not influence the effects of annulation. This finding is in accord with some previously reported studies on the dependence of the aromaticity of the ring(s) on distortion from planarity.

Key Words: phenanthrene, benzo-annulated phenanthrenes, benzocyclobutadieno-annulated phenanthrenes, aromaticity, deviation from planarity

INTRODUCTION

The effects of benzo- and benzocyclobutadieno-(BCBD-)annulation on local aromaticity of a particular six-membered ring in benzenoid hydrocarbons have been investigated in several recent papers [1–6]. In Figure 1, diagrams 2 and 3 illustrate linear and angular benzo-annulation of an arbitrary benzenoid hydrocarbon (diagram 1), whereas diagrams 4 and 5 illustrate linear and angular BCBD-annulation of the same hydrocarbon. The six-membered ring whose local aromaticity has been examined is marked by X. Note that the congeners

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