Planar ten-membered 10-?-electron aromatic (CH)5(XH)5 {X = Ge, Sn} systems

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Being monocyclic planar, benzene retains 6? Hückel aromatic backbone. However, for larger analogues, the repulsion between vicinal C-H bonds makes them nonplanar, as for [10]-annulene. Thus, on this basis, a planar 10-?-aromatic C10H10 is unreachable. A detailed structural comparison among the C3H3 +, C4H4 2+, C5H5 ?, C6H6, C7H7 +, C8H8 2+, C9H9 ?, and C10H10 systems supports that the repulsion between vicinal C-H bonds is the primary reason for the loss of planarity, despite the favorable aromatic electron count. In this respect, here we have discussed ten-membered monocyclic planar 10-?-aromatic, (CH)5(XH)5 {X = Si, Ge, Sn} systems, modeled by using DFT. From NBO analysis and the overall magnetic behavior it is shown that (CH)5(GeH)5, (CH)5(SnH)5 molecules are promising planar 10-?-aromatic system. Thus, such species represent plausible Hückel aromatic rings retaining a ten-membered backbone as discussed here, which may lead to the characterization of novel species expanding the chemistry of larger aromatic rings. We believe that the present study may open new avenues in the formation of 10-?-aromatic species. [Figure not available: see fulltext.].

10-?-electron

Density functional theory

Hückel aromaticity

Magnetic shielding region

Planar system

aromatic compound

benzene

germanium

silicon

tin

Article

comparative study

conformation

electron

hybridization

natural population

nuclear magnetic resonance

priority journal