

Cubane and Bicyclo(1.1.1)pentane – Rigid Hydrocarbon Linkers for Flexible Uses

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Small rigid hydrocarbon (RHC) scaffolds such as cubane or bicyclo(1.1.1)pentane (BCP) are used as bioisosteres in medicinal and materials chemistry and offer potential as rigid (linear) and isolating linker units in electron transfer compounds, as molecular tectons in supramolecular chemistry and as molecular scaffolds with defined geometry.¹ Despite being known for a long time, generally applicable synthetic methods for their functionalization and uses outside of medicinal chemistry are only slowly emerging. Our work in this area entailed the use of redox-active esters for the synthesis of 1,4-disubstituted aryl and heteroaryl derivatives, including porphyrins.² Additionally, bisalkynylcubanes could be used in Sonogashira-type couplings with bromoporphyrins for the construction of complex porphyrin arrays. In connection with their use as bioisosteres crystal engineering studies and analyses of solid-state interactions in cubane and BCP derivatives revealed unique bonding patterns.³ Synthetic studies targeted donor-acceptor systems, supramolecular systems, and functionalization methods for BCP.⁴ Ongoing studies focus on the use of RHCs to develop novel macrocycles⁵ and in on-surface chemistry for molecular organic electronics.⁶

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