

BOOK OF ABSTRACTS

XIV International School on Organometallic Chemistry “Marcial Moreno Mañas”



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Thermal vs Metal-catalyzed trimerization of COTynes: A direct entry to Dewar benzenes vs curved benzotri[8]annulenes

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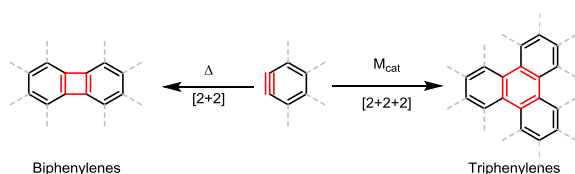
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The immense interest in planar carbon nanostructures (graphenes, PAHs) is driven by the extraordinary properties displayed by molecular nanocarbons themselves.¹ Distorted polycyclic aromatic hydrocarbons (PAHs) have recently emerged as intriguing units due to their ability to modify and improve the electronic and optical properties of their planar analogous.² The non-planarity is typically originated by the installation of non-hexagonal rings into the framework to induce negatively (saddle-shaped structure)³ or positively curvature (bowl-shaped structure).

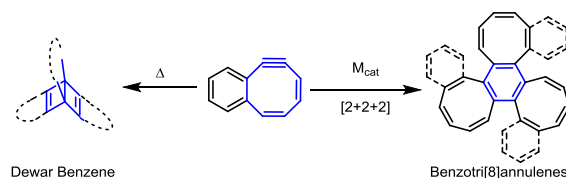
The synthesis of planar or distorted PAHs, usually requires regioselective fusions of many rings, where the use of metal-catalyzed [2+2+2] cycloadditions and thermal [2+2] cycloadditions involving arynes/alkynes became one of the most engaging synthetic strategies.⁴ While the metal-catalyzed trimerization of planar arynes is well established,⁵ the trimerization of cyclooctatrienynes and their benzofused derivatives (COTynes and benzoCOTynes) under TM catalysis has been scarcely studied.⁶

We herein report the novel metal-catalyzed trimerization of COTynes and benzoCOTynes to benzotri[8]annulenes (tub-shaped PAHs). The structure-dependent reactivity of dibenzo-, benzo- and COTynes under thermal and metal-catalyzed conditions will also be described.

a) Well established benzyne reactivity



b) Unknown COTyne reactivity. This work



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