A Negatively Curved Nanographene with four embedded Seven-membered Rings and its Supramolecular Interactions with Fullerenes

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Fully sp^2-hybridised carbon allotropes are of fundamental scientific interest due to their unique physical properties as known for 0D (fullerenes), 1D (carbon nanotubes) or 2D (e.g. graphene) materials. However, approaches to conjugated 3D allotropes, such as Mackay-Terrones Schwarzite crystals (or short: Schwarzites),[1] are rare and limited in terms of structure elucidation as well as homogeneity.[2] Thus, there is a rising urge to synthesis discrete cut-outs of Schwarzites, namely negatively curved polycyclic aromatic hydrocarbons (PAHs). Although the introduction of eight and especially seven-membered rings is a common approach to create this class of PAHs, to the best of our knowledge there is only one example each for PAHs with four,[3] five[4] or six[3] seven-membered rings reported till date.

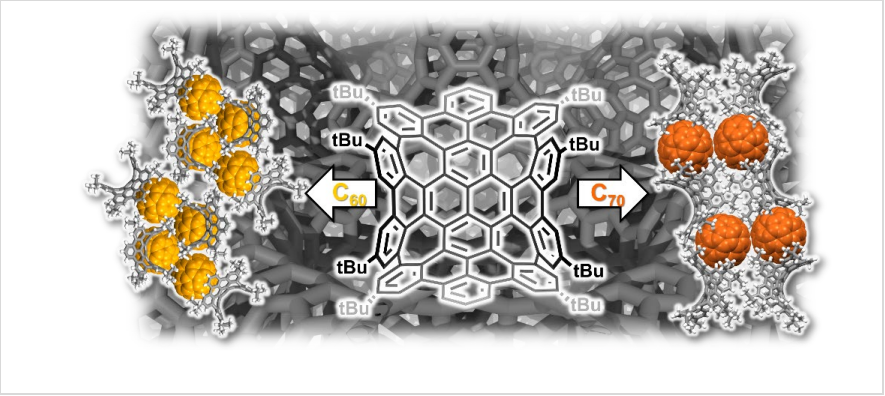

Figure 1: Schematically representation of a Negatively Curved Nanographene with four embedded Seven-membered Rings and cut-outs of single crystal X-ray structures with C_{60} (left) and C_{70} (right).

Here we present a saddle-shaped negatively curved PAH with four embedded seven-membered rings, that can be seen as a dibenzannulated cut-out of the Mackay crystal 6-1-1-p.[1] The

negative curvature of the saddle was unambiguously proven by single crystal X-ray diffraction analysis (SCXRD) and due to the concave aromatic surface, supramolecular interactions with convex molecules such as the fullerenes C_{60} and C_{70} where studied in co-crystals by SCXRD as well as spectroscopic methods in solution.[5]

References:

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