

Simplified models for fullerenes and PAHs stability

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Fullerenes and Polycyclic Aromatic Hydrocarbons (PAHs) are large carbonaceous molecules that play an important role in energetic processes that occur in space. In other fields such as materials science or biomedicine, fullerenes are also relevant. The theoretical prediction of the most stable structures is a very challenging task due to the large number of possible isomeric forms. This number is even higher when addition of external addends (e.g. hydrogenation) is considered (e.g., more than 20 billion isomers for C₆₀H₈).

In this talk, we present a simple model, based only on topological arguments, that allows us to predict the relative stability of fullerene and PAHs species. The model was first proposed to describe the stability of positively and negatively charged fullerenes [1] and it was further extended to predict the relative stability of exohedral fullerenes [2]. More recently, it was successfully applied to reproduce the regioselectivity of Diels-Alder cycloadditions to empty fullerenes [3]. The subtle interplay between π delocalization, cage strain, and steric hindrance is responsible for the stability of these compounds. The predicted most stable structures are in good agreement with those found in experiments. The model has been implemented in the **FullFun**  code for a widespread use by the fullerene community [4,5].

Very recently, we have extended the model to analyze the most stable isomeric forms of hydrogenated PAHs. Results show that addition occurs preferentially at the border of PAHs independently of the cage size and that the aromaticity of the remaining substructure after hydrogenation is the main responsible of its stability [6].

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