The Frozen Cage Model: a computationally low-cost tool for predicting the exohedral regioselectivity of cycloaddition reactions involving endohedral metallofullerene derivatives

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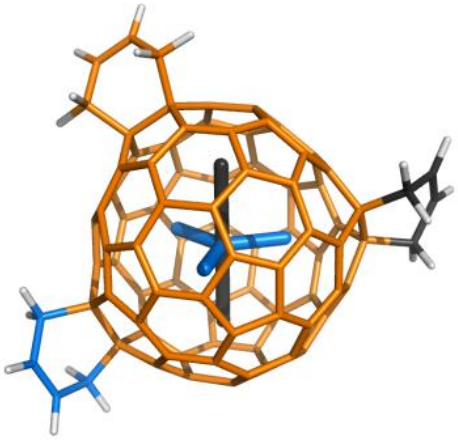
Since their discovery, interest in fullerenes has only grown because of their potential applications in medicine (as a drug transporter, for example) and technological (interesting electronic properties) fields. But until now, reactivity of fullerene compounds and their behavior are still largely unknown. The aim of the present study is to advance in the comprehension of the behavior in cycloaddition reactions of the endohedral metallofullerenes (EMFs) derivatives. In that sense, we have studied the [2+4] Diels-Alder cycloaddition between D_{3h}-C_{78},[1] and its endohedral metalloderivatives X@D_{3h}-C_{78} (X = Ti_2C_2,[2] Sc_3N,[3] and Y_3N[3]). In this work, we have applied different analyzing tools,[4] such are the Distortion/Interaction Model or the Non-Cluster Model (NCM),[2] among others.

From the results obtained we propose a new method for predicting, at very low computational cost, the cycloaddition regioselectivity of EMF derivatives based on the structures of free fullerene, the Frozen Cage Model (FCM). This new model allows us to find the EMFs most reactive positions predicting which will be the major (most stable) product of the cycloaddition reaction. These studies represent an advance in the knowledge of the fullerene compounds chemistry. Only when we understand fullerene species behavior, we will be able to convert the potential applications of this family of compounds into real ones.



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