

A new isomer of C₂₀ and a way to a new C₂₄₀

Cárdenas, Carlos

Muñoz, Francisco

Muñoz, MacArená

Bernardín, Alejandro

Fuentealba, Patricio

Here we show that the dynamic simulation of a molecular collision can give insight into new molecular species. In this way, a new stable isomer of C₂₀ (IV) has been found. It is planar with pentagonal form. This isomer is high in energy compared to the three most stable previously known isomers of C₂₀: cage (I), bowl (II) and ring (III). Most interestingly, we show that using this new isomer it is possible to construct a macrobucky C₂₄₀ (V) that is also stable. The electronic structure of this new isomer of C₂₄₀ is very different from properties of the C₂₄₀ fullerene. Contrary to the C₂₄₀ fullerene, in the new isomer the π electrons are localized. This journal is © 2012 the Owner Societies.