BOWL SHAPED PRECURSORS OF FULLERENES. I

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Optimized structures of neutral and triplet graphite sheets are obtained using density functional theory (B3LYP/6-31G*). The most stable aromatic polycyclic structures are presented between 14 and 35 carbon atoms. The stability of these polycyclic aromatic structures refers not only to low energy structures but also takes into account their low reactivity with simple carbon molecules.

Experimental results have shown a direct correlation between carbon ring consumption and fullerene formation in high temperature carbon vapors [1]. The evolution of carbon ring structures towards the formation of fullerenes, with the actual knowledge of carbon kinetics, necessarily involves intermediate structures of graphite sheet shape.

Since a general classification of graphite sheets or aromatic polycycles as a function of carbon atoms readily becomes extremely large, it is needed to put some restrictions for the analysis of the more probable polycycles present in the fullerenes reaction pathway in high temperature carbon vapors. The basic assumptions for this classification take into account that two dimensional carbon aromatic polycycles, for a given number of carbon atoms, have the maximum number of bonds, the minimum number of dangling bonds and minimum strain energy. These conditions can be accomplished by the hypothesis that polycyclic structures have arm chair like borders, similar quantity of peripherical and interior carbon atoms and minimum bidimensional strain energy.

Dangling bonds at an arm chair like border can easily absorb energy by a transformation to a zigzag boundary and usually will not react with smaller species. When more than one structure is possible for an initial number of atoms, energy calculations with ab-initio theoretical models are performed, and the more stable structure is identified.

The resulting classification of bidimensional carbon polycycles show that they have a bowl shape appearance and supports the experimental evidence [2] that in many cases fullerenes are formed by the addition of two of these structures.

References

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