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# Interaction of BUCKYBALLS in (100) planes of FULLERITES $[C_{60}]_5$, $[C_{70}]_5$, $[C_{80}]_5$ and $[C_{96}]_5$: Analysis of the HOMO-LUMO, charges, distances, dipoles, using the MNDO, HF and DFT methods with Huzinaga 6-31G basis set

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**Abstract** – Since the discovery of fullerenes, the investigation of the electronic structure and the possible interactions between the molecules that crystallize in the cubic face centered form (fullerites) have been made. We have thus investigated in this work the (100) planes of the crystals of $C_{60}$, $C_{70}$, $C_{80}$ e $C_{90}$. It has been observed that there is a stabilization of the structures when forming a plane and that there are no variations larger than the gap when the plane is formed. Using the MNDO method the largest variation between the molecule and the plane was de 0.2 eV for $C_{80}$.

Since the discovery of the buckminsters in 1985 by KROTO et al, fullerenes of various sizes were detected. The $C_{60}$ is the most abundant followed by $C_{70}$, as well as $C_{80}$ e $C_{96}$. The crystals of these substances were detected in the cubic face centered form, called fullerites [1, 2]. In this work we investigated the interaction of $[C60]_5$, $[C70]_5$, $[C80]_5$ e $[C96]_5$ in (100) planes of fullerites using the MNDO, HF and DFT methods with 6-31G e Huzinaga basis sets. The models used in the calculations are represented in Figure 1. The energy variation for the formation of the plane was calculated following the equation given below:

$$5C_n \rightarrow [C_n]_5; \Delta E = E_{[C_n]_5} - E_{C_n}; \text{ with } n = 60,\ 70,\ 80 \text{ or } 96$$

These variations of energy are calculated by the MNDO, Hartree-Fock and DFT methods. All these planes ($[C_n]_5$) indicate stable energies in relation to the ($C_n$) fullerene molecule. For both methods the energy variation for the formation of the plane $[C_{96}]_5$ in relation to $[C_{80}]_5$ indicates a variation of less energy. Through the analysis of the energy Gap (HOMO-LUMO) indicated in Table 1, it is observed that the variation of the gap is small, when planar interactions are formed between the fullerenes, with a larger variation for the type $C_{80}$, which was 0.2 eV.

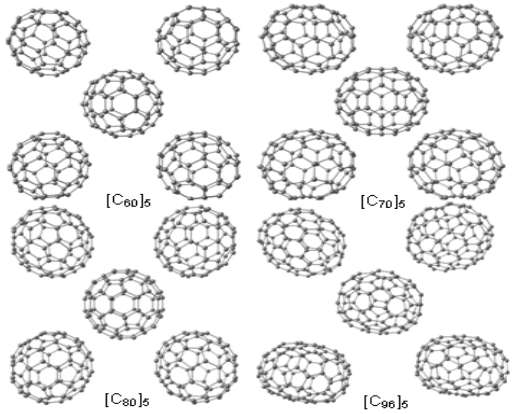


**Figure 1. Models of $[C_{60}]_5$, $[C_{70}]_5$, $[C_{80}]_5$ and $[C_{96}]_5$, used in the calculations.**

**Table 1. Gap values with MNDO method**

| Model | HOMO-LUMO – MNDO method |
|---|---|
| $C_{60}$ | 6.56513 |
| $C_{70}$ | 5.83214 |
| $C_{80}$ | 3.92447 |
| $C_{96}$ | 4.37741 |
| $[C_{60}]_5$ | 6.51499 |
| $[C_{70}]_5$ | 5.72331 |
| $[C_{80}]_5$ | 3.74716 |
| $[C_{96}]_5$ | 4.32311 |

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[2] R. W. Lof, M. A. Van Veenendaal, H. T. Jonkman and G. A. Sawatzky, J. Electron Spectrosc. Relat. Phenom. 94 (1995) 023085.