An investigation of the effects of oxidation and reduction on the energy gaps of C_{60} and C_{70} fulerenes

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The C_{60} and C_{70} fulerenes exhibit non conventional optical and electrical properties with important potential technological applications. The transfer or withdrawal of electrons (oxidation, reduction) from the neutral C_{70} results in a redistribution of the electronic level, |HOMO-LUMO|, such that the electronic properties related to the band gaps can be modified. The cause for the possible variety of oxidation and reduction numbers has been attributed to the large number of π electrons. We have used and compared both semi-empirical and ab initio methods in order to investigate the total energies, conformations, HOMO-LUMO gaps as a function of charge, multiplicity and number of occupied levels of the systems. Our results suggests that the HOMO-LUMO can be modified by reduction and oxidation of the C_{60} and C_{70} fulerenes.

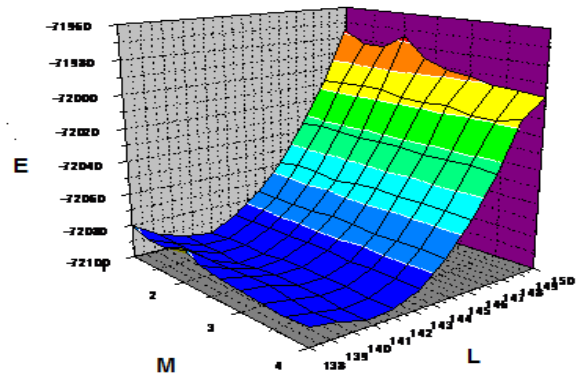

Fig. 1 Total energy as a function of multiplicity and levels

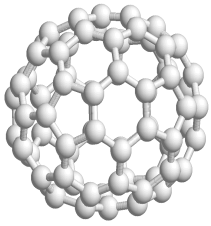

Fig. 2 C_{70} fulerene

References

[1] J. D. Santos, E. Longo, C. A. Taft, Journal of Molecular Structure 538 (2001) 211.