Structure And Fragmentation Properties Of Small Carbon Clusters And Fullerenes

Fernando Martín

Departamento de Química C-9, Universidad Autónoma de Madrid, 28049 Madrid Spain

Carbon clusters and fullerenes in excited states can be produced in collisions with ions, electrons and energetic short laser pulses [1]. The fragmentation patterns of these clusters extremely depend on the initial charge state, and on the energy transferred to the fullerene during the collision.

The knowledge of dissociation energies, ionization potentials and fission barriers is essential to analyze in detail the fragmentation patterns observed in the experiments. In this communication I present density functional theory (DFT) results on the structure and energetics of C_n^{q+} carbon clusters and fullerenes ($2 \leq n \leq 10$, $50 \leq n \leq 60$, q=0,1,2) [2] and on multicharged C_{60}^{q+} and C_{58}^{q+} (q=0-14) [3]

These calculations have allowed us to identify which are the most relevant isomers produced in the fragmentation process of neutral, singly and doubly charged of these clusters, and to compare our predicted dissociation and ionization energies with the available experimental data. Another fundamental question raised in recent experiments [4,5] is how large is the charge that the fullerene C_{60}^{q+} can sustain without spontaneously dissociating due to the repulsive Coulomb forces. Our results predict this Coulomb stability limit to be q=14. For $q \leq 8$ the lowest fission barrier corresponds to C_2^+ emission, whereas, for higher charges the emission of two charged atomic fragments is the most favorable process.

From the calculated structure, electronic energies and harmonic vibration energies of the different fragments it is possible to predict the relative importance of the different fragmentation channels. For this purpose, w have used the Microcanonical Metropolis Montecarlo method (MMMC) and the Weiskopff theory. Both methodologies have been recently applied to predict the fragmentation patterns of small neutral and singly-charged carbon clusters [6,7]

References

[1] E. E. B. Campbell, Fullerene Collision Reactions, Kluwer Academic Publishers, London, UK, 2003

[2] S. Díaz-Tendero, M. Alcamí and F. Martín. J. Chem. Phys. 119, 5545 (2003)

[3] S. Díaz-Tendero, M. Alcamí and F. Martín. Phys. Rev. Lett. 95, 013401 (2005)

[4] H. Cederquist, J. Jensen, H. T. Schmidt, H. Zettergren, S. Tomita, B. A. Huber, and B. Manil, Phys. Rev. A 67, 062719 (2003)

[5] S. Tomita, H. Lebius, A.Brenac, F. Chandezon, and B. A. Huber, Phys Rev A 67 063204 (2003).

[6] G. Martinet et al. Phys.Rev. Lett 93 063401 (2004)

[7] S. Díaz-Tendero, P.-A. Hervieux, M. Alcamí and F. Martín. Phys. Rev. A 71, 033202 (2005)