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An XPS characterization of novel fulleropyrrolidine derivatives

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The study of positively charged fullerene derivatives is relevant because fulleropyrrolidinium ions have interesting applications in photovoltaics [1]. In addition, amphiphilic compounds, such as those studied here, have interesting aggregation properties [2]. The pyrrolidine nitrogen atom is located close to the fullerene sphere and as a consequence its chemical properties are affected to some extent. There are only a few studies on how the fullerene substituent modifies the chemical properties of groups linked to it. On the other hand additional groups fused to the pyrrolidine nitrogen atom also affect the chemical properties of the pyrrolidine nitrogen atom. In this work we studied the influence of the C₆₀-sphere and that of positively charged ions onto the binding energy of nitrogen atoms in fulleropyrrolidine and fulleropyrrolidinium ion derivatives by means of X-ray photoelectron spectroscopy. XPS is an ideal tool for this purpose because it can be used to obtain information about the chemical bonding by comparing the binding energies of the same atom in different environments.

The results show that the pyrrolidine nitrogen (N 1s) has a binding energy value of 399.2 eV which is by 0.7 eV lower than the value observed when the fullerene sphere is present (399.9 eV). The influence of the fullerene sphere on the pyrrolidinium ion has the same effect on the binding energy. When the C₆₀-cage is present the binding energy increases from 402.1 eV to 403.1 eV. This increase is due to delocalization of the nitrogen lone pair into the fullerene core [3]. Further, the influence of the counter ion is found to be an important factor for the final stability of the derivatives. It is observed that in the case of iodide, the nitrogen of pyrrolidinium is partly unstable. The stability of the pyrrolidinium nitrogen is improved by changing the counter ion from iodide to tetrafluoroborate without affecting the binding energy of the nitrogen atom. Finally, for fulleropyrrolidine derivatives having an ammonium end group in the alkyl side chain the N 1s photoelectron line is observed at 401.9 eV while for a secondary amine protected by a tert-butoxycarbonyl group it is observed at 400.1 eV.

[1] D.M. Guldi, C. Luo, D. Koktysh, N.A. Kotov, T. Da Ros, S. Bosi, M. Prato, *Nano, Letters*, 2002, 2, 775.

[2] V. Georgakilas, F. Pellarini, M. Prato, D.M. Guldi, M. Melle-Franco, F. Zerbetto, *Proc. Natl. Acad. Sci. USA*, 2002, 99, 5075.

[3] A. Bagno, S. Claeson, M. Maggini, M.L. Martini, M. Prato, G. Corrono, *Chem. Eur. J.*, 2002, 8/5, 1016.