

The Diels-Alder cycloaddition reaction of 1,3-butadiene to MWCNTs

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The non-polar nature of carbon nanotubes, favouring their aggregation as bundles, poses a serious limitation to a wide range of potential applications of this strong and flexible material [1]. Grafting of chemical functions on the surface of multiwall carbon nanotubes (MWCNTs) has been widely used to add new properties and improve their dispersion in solvents and/or materials. A number of chemical reactions were reported for the functionalization of the outer layer of MWCNTs, tailoring their properties and widening their applications [2]. Previous studies of Diels-Alder cycloaddition reaction of 1,3-butadiene generated *in situ* from sulfolene with carbon nanofibers showed that can be a good method to obtain high degree of functionalization without significative structural damages.[3].

In this study the functionalization of MWCNTs with 1,3-butadiene generated *in situ* from sulfolene was investigated. The reaction was studied at two different temperatures (100°C and 150°C), mass ratios (CNTs:Sulfolene of 1:1 and 1:2) and different time reaction (2, 4 and 7 days). Thermogravimetric analysis (TGA) showed high degree of functionalization in a range of 10 % to 23 % in weight loss at 800 °C. The acid properties of functionalized materials were recorded by potentiometric titration that suggests some oxidation during the functionalization process (Figure 1). In Figure 2 are summarized the results of weight loss obtained by TGA and respective acid properties of functionalized carbon nanotubes. The functionalization was also evaluated by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM).

References

- [1] Andreas Hirsch, *Angew. Chem. Int. Ed.*, **41** (2002) No. 11, 1853.
 [2] D. Tasis et al, *Chem. Rev.*, **106** (2006) 1105.
 [3] M. Fernanda et al, *J. Nanosci. Nanotechnol.*, **vol. 9** (2009), 1.

Figure 1. Possible mechanism of functionalization of MWCNTs by 1,2-butadiene.

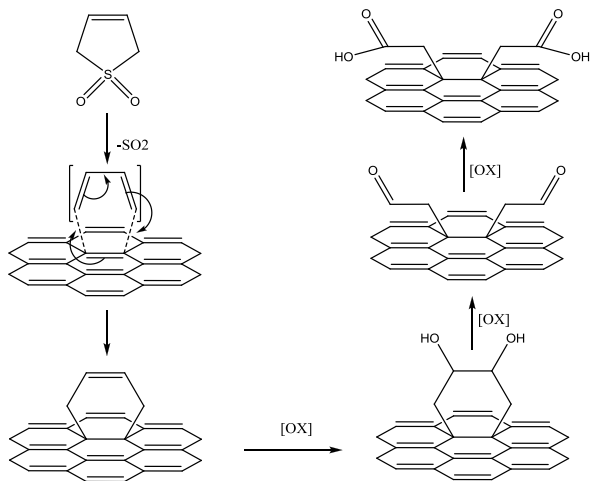


Figure 2. Degree of functionalization (%) (black line) and acidity (mmol) (blue line) of MWCNTs obtained at different conditions of functionalization.

