Use of TGA for analysis of fullerenols

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Nowadays thermo-gravimetric analysis is common used for studying substances of a different nature. Thus, using this method, a determination of an amount of hydroxyl groups attached to a fullerene core can be performed.

TGA analysis was applied for three types of fullerenols having a different hydroxylation degree, $C_{60}(OH)_{12\text{-}14}$, $C_{60}(OH)_{20\text{-}24}$ and $C_{60}(OH)_{30\text{-}36}$.

To calculate an approximate amount of OH groups contained in fullerenol, it is used the following equation reported earlier in the article [1]:

$$n = \frac{molwt(C60)}{mr(C60)} X \frac{mr((OH)n)}{molwt(OH)}$$

wherein molwt(C_{60})=720 g/mol; molwt(OH) = 17 g/mol;
mr (C_{60}) is weight loss at 150ºC to 570ºC, %;
mr ((OH)n) is weight loss at 570ºC to constant weight of C_{60} (800ºC), %.

In order to ensure that for calculating correct ranges of temperatures (150ºC to 570ºC and 570ºC to 800ºC) were selected, elemental analysis of 3 samples of fullerenol $C_{60}(OH)_{30\text{-}36}$: initial, heated up to 560ºC, and heated up to 800ºC for 4 h was performed. The elemental analysis data showed that active elimination of hydroxyls takes place at heating 150ºC to 570ºC exactly, and a decomposition of fullerene core runs at above 570ºC.

Further, it can be followed from the TGA analysis data that an initial fullerene and fullerenol are decomposed in a different mechanism at heating. This event is likely to be proceeded due to opening both double bonds and single bonds at hydroxylation process to form gaps (“holes”) in fullerene framework. Therefore, at heating the fullerene framework comprising such “holes” will be piecewise decomposed, in contrast to an initial fullerene does not decayed at 800ºC, but do sublimate.

[1] Alves G., Ladeira L., Righi A., Krambrock K., Calado R., Pinheiro M. *J. Braz. Chem Soc.* **17,** 1186 (2006).