

Development of an additive mass spectral library for the qualitative analysis in polymeric materials by pyrolysis-GC/MS

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Pyrolysis-GC/MS (Py-GC/MS) is applied to both the characterization of polymeric materials and the determination of additives in polymeric materials. While the degradation products for a large number of polymers have been cataloged, there are not so much data on the degradation products of versatile additives used in polymer formulations. Conventional mass spectrum (MS) libraries such as Wiley and NIST are not always applicable to the pyrolysis data; consequently, there exists a strong demand upon a pyrolysis-based library containing spectral data for the associated pyrolyzates of additives used for polymeric materials.

In this work, a new mass spectral library (ADD-MS06) containing the spectra of the main pyrolyzates obtained from the pyrolysis (at 600°C) of about 400 different additives together with their pyrograms. In the pyrograms, the pyrolyzates usually contains a variety of fragmented compounds relating to its original additives which are very useful for the identification of unknown additives in the polymeric materials.

For a given unknown polymeric material, conventional evolved gas analysis (EGA) is first tried by temperature programming at 20°C /min from 100 to 700°C in order to find the volatile additive zone on the resulting thermogram and then the thermal desorption (TD)-capillary GC/MS run is carried out for the method for the selected zone to obtain its detailed compositional information.

The search algorithm and the trial search results for several additives present in a variety of polymeric materials will also be discussed using the new ADD-MS06, conventional Wiley and NIST libraries for comparison.

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