Identification of Unknown Polymeric Materials using a Polymer MS Library

[Background] The qualitative analysis of unknown polymeric materials has historically been based on the identification of the major peaks in the pyrogram using a general-purpose MS library such as NIST. However, relatively high molecular-weight pyrolyzates which often reflect the polymeric structure are often not found in general-purpose libraries. In response to this deficiency, Frontier Laboratories has developed a pyrolyzate MS library for 165 typical polymers.

[Library structure] The new MS library includes approximately 4,000 mass spectra of compounds found in the pyrograms of 165 polymers when pyrolyzed at 600ºC. Compound names, retention indices (RI), polymer names and the individual pyrograms, are included in the pyrozate library.

[Results] Figure 1, shows the major peaks (A)-(G) found in the pyrogram of an unknown polymer sample. Each peak is identified using the newly constructed MS library. (C)-(G) are relatively high molecular-weight pyrolyzates and can be used to tentatively identify the backbone structure of the polymer. The new library contains data on the parent polymer as well as the pyrolyzates identified in the pyrograms. Four candidate polymers, see Figure 2, are reported. Comparing the peaks on the four pyrograms, especially the hybrid trimers eluting around 12 min, suggests that the unknown polymer is Acrylonitrile-styrene copolymer. Further confirmation can be obtained using Frontier Laboratories' EGA-MS library. This simple example illustrates how the new pyrolyzates library can assist in polymer identification.
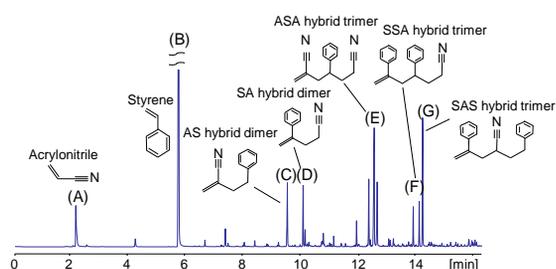

Fig. 1 Pyrogram of unknown polymer sample and peak identifications
Furnace temp.: 600ºC, GC oven temp.: 40(2 min)-320ºC(20ºC/min, 10 min)
Column: Ultra ALLOY-5 (MS/HT) (length 30 m, id 0.25 mm, film thickness 0.25 μm)

Table 1 Searching compounds for peak (A)

| Rank	Compound	Polymer	Quality[%]
1	Acrylonitrile	Acrylonitrile-EPDM-styrene copolymer	99
2	Acrylonitrile	Acrylonitrile styrene copolymer	99
3	Acrylonitrile	Acrylonitrile-styrene alternating copolymer	99
4	Acrylonitrile	Acrylonitrile-acrylate-styrene copolymer	99
5	Acrylonitrile	Acrylonitrile-methyl acrylate copolymer	97
6	Acrylonitrile	Acrylonitrile-vinyl chloride copolymer	96
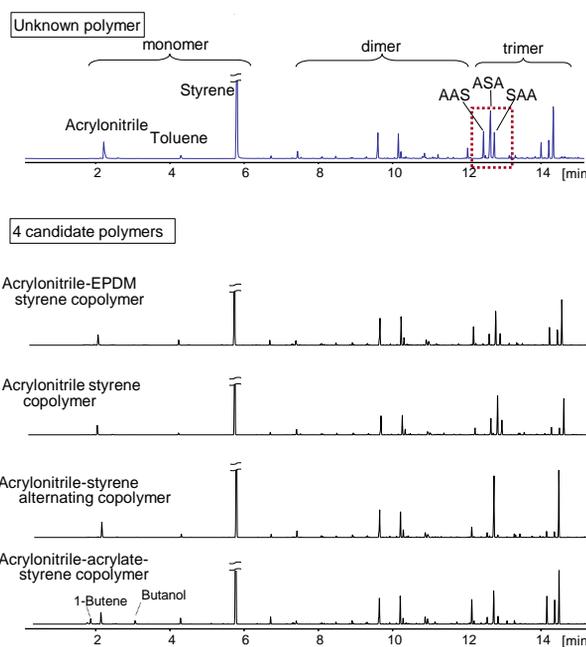
Fig. 2 Comparison of pyrograms of unknown and candidate polymers

Ref : K. Matsui et al., 12th Polymer Analysis & Characterization Japan 2007 II-15

Keywords : Polymer, MS Library

Products used : Multi-functional pyrolyzer, Auto-Shot Sampler, Vent-free GC/MS adapter, F-Search, UA-5 (MS/HT)

Applications : General polymer analysis

Related technical notes :