Identification of the additives in polystyrene using the F-Search additive library

[Background] Polymeric materials generally contain a variety of additives such as antioxidants, UV absorbers, etc. The method of choice for characterizing the various additives in a given polymeric matrix is thermal desorption (TD)-GC/MS. The sample is analyzed directly which means that cumbersome and time-consuming sample pretreatments (e.g., solvent extraction, filtration, etc.) are unnecessary. Generally, compounds are identified using commercial mass spectral (MS) libraries such as Wiley or NIST; however, these general purpose MS libraries contain very few entries for pyrolyzates and additives which severely limits their utility for polymer characterization. This note illustrates how the F-Search additive library (ADD-MS08B) can be used to identify unknown additives in polystyrene (PS). The library includes both chromatographic and mass spectral data for 358 additives.

[Experimental] A double-shot pyrolyzer (model 2020iD) was installed on a GC/MS. Both the deactivated metal capillary tube (EGA) and the metal capillary separation column (TD) were interfaced to the MS using a vent-free GC/MS adaptor. 50µL of a 20 mg/mL dichloromethane solution was added to a sample cup and the solvent was allowed to evaporate prior to analysis. The analytical conditions are provided in the figure captions.

[Results] (EGA)-MS was utilized to determine the thermal desorption zone of the volatile additives - see Fig. 1. This thermal zone ((100-300ºC) was analyzed using TD-GC/MS. Each peaks was tentatively identified using the F-Search additive library. Ten "additive" were identified based on mass spectral match quality and retention indices.

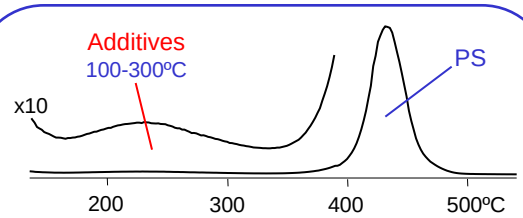

Fig.1 EGA Thermogram of PS

Py furnace temp.: 100 - 700ºC (20ºC/min),
GC oven temp.: 300ºC,
EGA tube: UADTM-2.5N(L=2.5 m, i.d. 0.15 mm),
column flow rate: 1 mL/min He, split ratio: 1/50,
sample: 0.1 mg

TD-GC/MS: total ion chromatogram

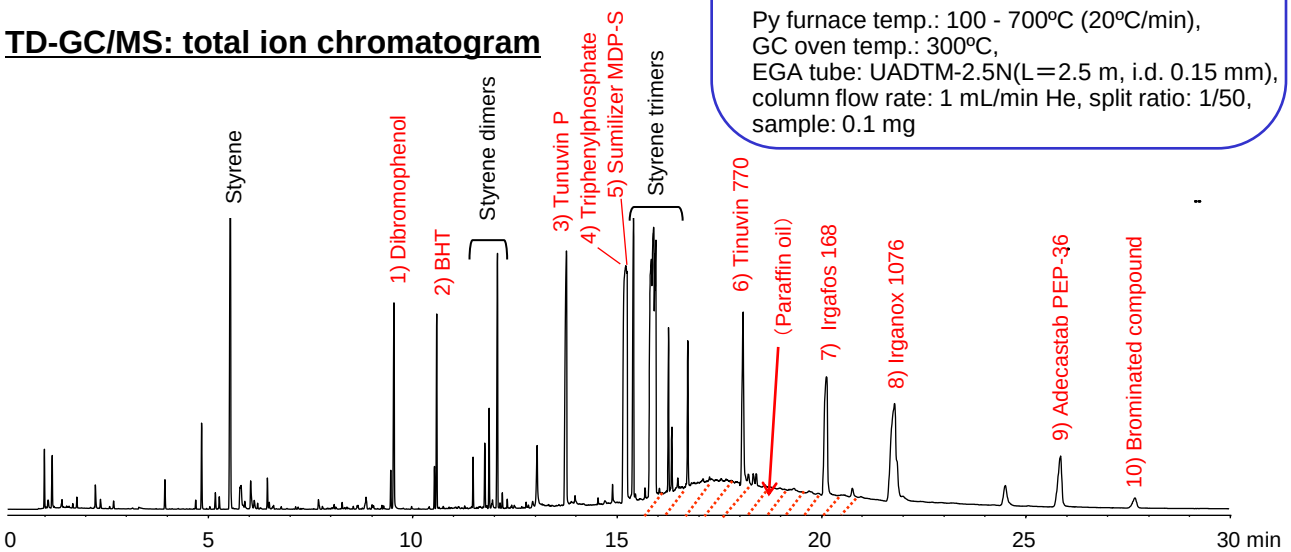

Fig. 2 Library search results

Pyrolyzer temp.: 100 - 300ºC (20ºC/min, 5 min), GC oven temp.: 40ºC (2 min) - 320ºC (20ºC/min), separation column: Ultra ALLOY⁺-5 (5% diphenyl 95% dimethylpolysiloxane) (L=30 m, i.d.=0.25 mm, df=0.05 µm), column flow rate: 1 mL/min He, split ratio: 1/20, scan rate: 2 scans/sec, scan range: 29 - 810 (m/z), sample: 1 mg

Reference: K. Odagiri et al., 13th Polymer Analysis and Characterization (2008), II-11

Keyword : F-Search, Additives MS library, Polystyrene, Additive, Thermal desorption analysis, Evolved gas analysis

Applications : Additives analysis

Related technical notes : PYA1-054E, PYA1-057E

Please forward your inquiries via our web page or send us a fax message.

R&D and manufactured by :
Frontier Laboratories Ltd.
1-8-14 Saikon, Koriyama,
Fukushima 963-8862 JAPAN
Phone: (81)24-935-5100 Fax: (81)24-935-5102
http://www.frontier-lab.com/

SIM
Scientific Instruments Manufacturer GmbH
Im Erlengrund 21-23
D-46149 Oberhausen
Phone: +49-208-941078-0 Fax: +49-208-941078-88
http://www.sim-gmbh.de info@sim-gmbh.de