

Application News

Gas Chromatography Mass Spectrometry

No.M247

Search of Polymer Additives Using Mass Spectral Libraries

Commercial MS libraries can be used to identify compounds detected using GC/MS. Such MS libraries include the NIST spectral library (spectra for 160,000 compounds) and the Wiley spectral library (310,000 spectra). In addition, a specific MS library (ADD-MS06 Library: Frontier Laboratories Ltd.) has recently been developed for polymer additives. This library consists of the mass spectra

and retention indices (RI) of the main peaks and pyrograms observed following Pyrolysis (Py)-GC/MS (pyrolysis at 600°C) of the 329 main commercial organic additives. This Application News introduces an investigation using the abovementioned three libraries to identify the additives contained in various polymers.

The polymer beads used in this analysis are shown in Fig. 1.

The temperature settings that were used for pyrolysis (Py)-GC/MS and thermal desorption (TD)-GC/MS are 550°C and 300°C (5 min), respectively, using the EGA (evolved gas analysis)-MS method. The polymer additive constituents were predicted from the measured chromatogram (TIC).



Fig.1 Polymer Beads Used in Analysis

■ GC/MS Analysis Using Pyrolysis: 550°C

The chromatogram (TIC) obtained from pyrolytic analysis ((Py)-GC/MS) of the polymer beads is shown in Fig. 2.

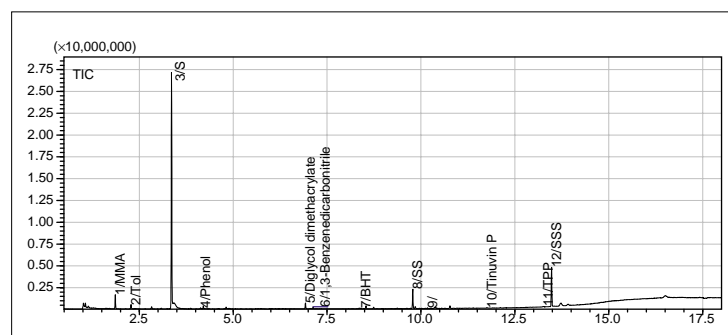


Fig.2 Py-GC/MS (TIC) 550°C

Table 1 Polymer Beads Used in Analysis

Model	: GCMS-QP210 Plus
	: PY-2020iD
-GC-	
Column	: Ultra ALLOY+5 (30 m × 0.25 mm I.D. df = 0.25 μm)
Column Temp.	: 50°C (1 min) - 20°C/min - 330°C (5 min)
Carrier Gas	: He 100 kPa at 50°C (1.75 mL/min)
Injector Temp.	: 300°C
Injection Method	: Split 1:50
-MS-	
Interface Temp.	: 300°C
Ionization Method	: EI
Scan Range	: m/z 35 - 800
Scan Interval	: 0.2 sec

Reference Records:

Polymer/Additive	EntryID	Qual[%]
1 Polystyrene ; PS (C1-C40)	PYGCT-016	98
2 Styrene-maleic anhydride copolymer ; P(S-Mah) (C1-C40)	PYGCT-027	98
3 Styrene-ethylene-butadiene-styrene-block copolymer (C1-C40)	PYGCT-080	98
4 Acrylonitrile acrylate styrene copolymer ; AAS (C1-C40)	PYGCT-025	97
5 Acrylonitrile-butadiene-styrene copolymer ; ABS (C1-C40)	PYGCT-024	97
6 Acrylonitrile acrylate styrene copolymer ; AAS (C1-C20)	PYGCT-025	96

Fig.3 Library Search Results

GC/MS Analysis Using Thermal Desorption (TD): 300°C/5 min

Next, the chromatogram (TIC) obtained from thermal desorption (TD)-GC/MS analysis for additive investigation is shown in Fig. 4.

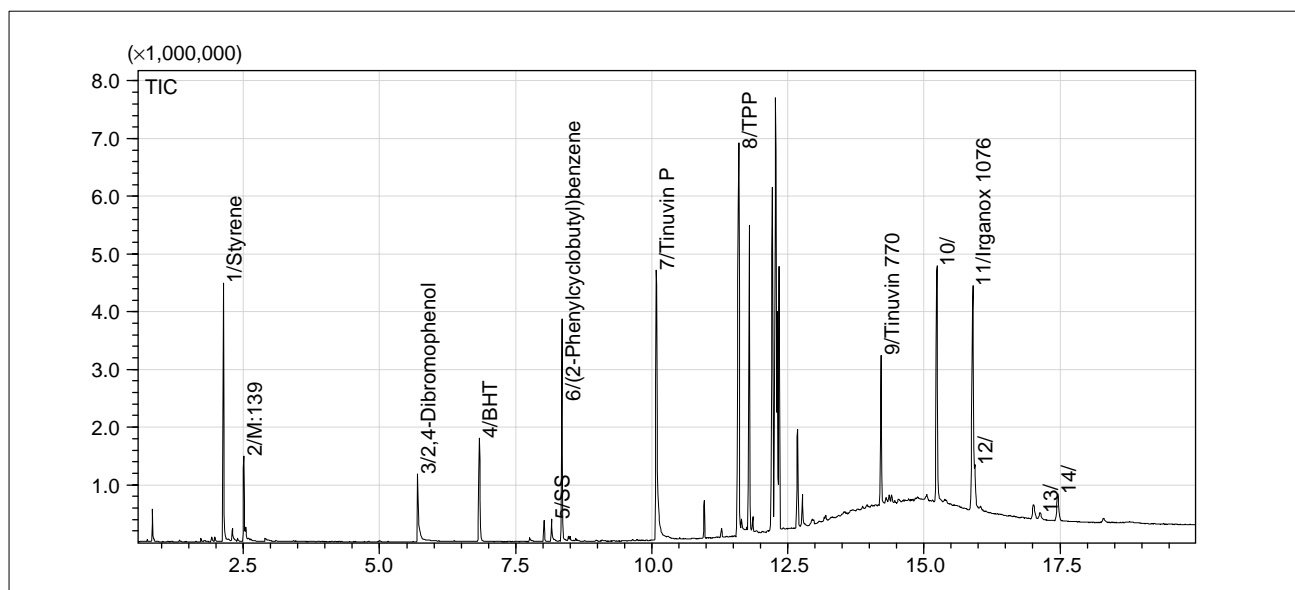


Fig.4 TD-GC/MS (TIC) 300°C/5 min

Table 2 shows the search result for chromatographic peaks obtained in TD-GC/MS analysis.

Table 2 Peak Search Results

Peak No	NIST		Wiley		Qaul	ADD-MS06 Entry ID	
	SI	1st	SI	1st			
1	98	100-42-5	98	100-42-5			Styrene
2	89	3088-41-3	89	3088-41-3		B(9)300	Tetrakis(2,2,6,6-
3	95	615-58-7	96	615-58-7	76	K(2)206	Br ₂ phenol
4	91	128-37-0	91	128-37-0	92	A(2)093	BHT
5	79	1667-00-1	78	4368-68-7			
6	97	20071-09-4	97	20071-09-4			SS
7	96	2440-22-4	95	2440-22-4	86	H(1)040	Tinuvin P
8	95	115-86-6	96	115-86-6	98	K(4)020	TPP
9	91	52829-07-9	84	0-00-0	99	B(9)160	Tinuvin770
10	59	134868-71-6	68	0-00-0	99	A(2)080	Tetrakis(2,4-di-t
11	93	2082-79-3	79	2082-79-3	86	A(1)-040	Irganox 1076
12	53	56771-86-9	45	60705-62-6			
13	59	121955-26-8	47	0-00-0			
14	64	0-00-0	43	37163-54-5	95	A(2)093	Cyclcneptane-

Six compounds were identified by searching the NIST library and 5 compounds were identified using the Wiley library (excluded Tinuvin770 of Peak 9). However, in 3 of the Wiley search result compounds, the CAS No. was not registered. Since there are many entries in the NIST and Wiley libraries and numerous positive search results are possible, some interpretation is frequently required. Sometimes, some knowledge as to which candidate compounds may be present in a sample can be

used to select the most probable of the candidate library spectra.

On the other hand, using the ADD-MS06 library, 9 compounds were identified, including 3 that were not identified by searching the NIST library. While prior knowledge of a sample may still be required to assist in the interpretation of library search results, it is apparent that the polymer additive library is a powerful tool for this application.

NOTES:

*This Application News has been produced and edited using information that was available when the data was acquired for each article. This Application News is subject to revision without prior notice.



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