JEOL MS Data Sheet

MS Tips

Mass Spectrometry Application Group
Mass Spectrometry Business Unit
JEOL Ltd.

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JMS-T100GCV **Application Data**

Analysis of additives in plastic by thermal desorption (TD) GC-TOFMS
~ accurate mass measurement and isotope pattern matching ~

Introduction

Among various methods for characterizing plastics, qualitative and quantitative analyses using pyrolysis (Py) GC/MS and thermal desorption (TD) GC/MS are widely used. These are simple techniques, but provide detailed information.

In this application note, we report the analysis of additives in plastic by thermal desorption GC-TOFMS using a thermal desorption system and JEOL JMS-T100GCV "AccuTOF GCv" GC-TOFMS. Identification of the analytes was accomplished by library search and accurate mass measurement. Isotope cluster pattern matching was performed using the software "Mass Spec Tools™."

Methods

Sample: Plastic (0.4 mg)

Thermal desorption

Instrument:	PY-2020iD (Frontier Laboratories Ltd., Fukushima, Japan)
Temperature:	150 °C → 10 °C/min → 350 °C (20 minutes total)

GC

Instrument:	6890N (Agilent)
Column:	DB1-HT, 8 m x 0.25 mm x 0.1 μm

MS

Instrument:		JMS-T100GCV (JEOL)	
Ionization mode:	EI(+):	Electron energy:	70 eV
		Ionization current:	300 μA
Acquired mass range:		*m/z* 35 – 1,400	
Spectral recording interval:		0.4 sec	

Software: Mass Spec Tools™ (ChemSW, Inc., Fairfield, CA, U.S.A.)

Results and discussion

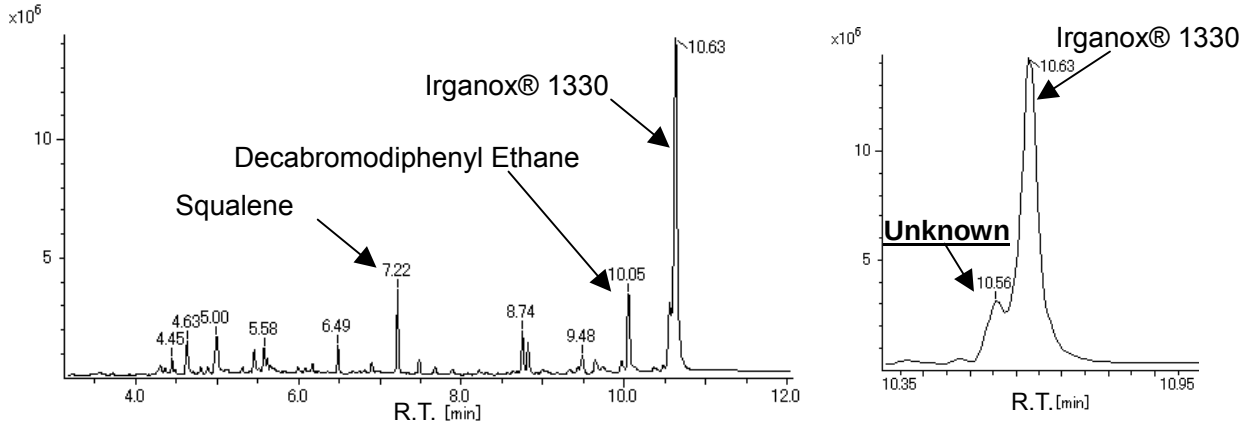

Fig.1 TIC chromatogram

The TIC chromatogram is shown in Fig. 1. Some of the peaks identified by searching NIST mass spectral library include squalene, decabromodiphenyl ethane, a brominated flame retardant, and Irganox® 1330, an antioxidant. The expansion of the TICC from 10.35 min to 10.95 min is shown in the inset of Fig. 1. There found an “unknown” component that could not be identified by the library search at the left of the Irganox® 1330 peak. The mass spectrum of this “unknown” component was analyzed by the “Elcomp™,” a part of “Mass Spec Tools™.”

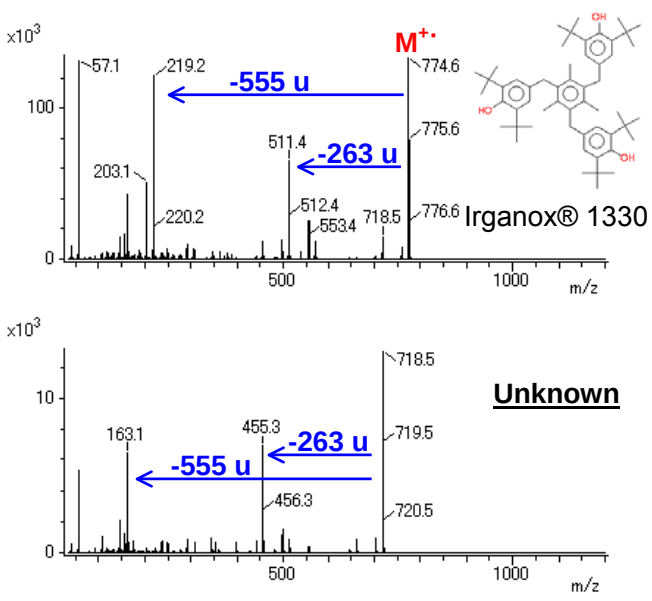

Fig.2 Mass spectra of Irganox® 1330 (upper) and unknown component (lower).

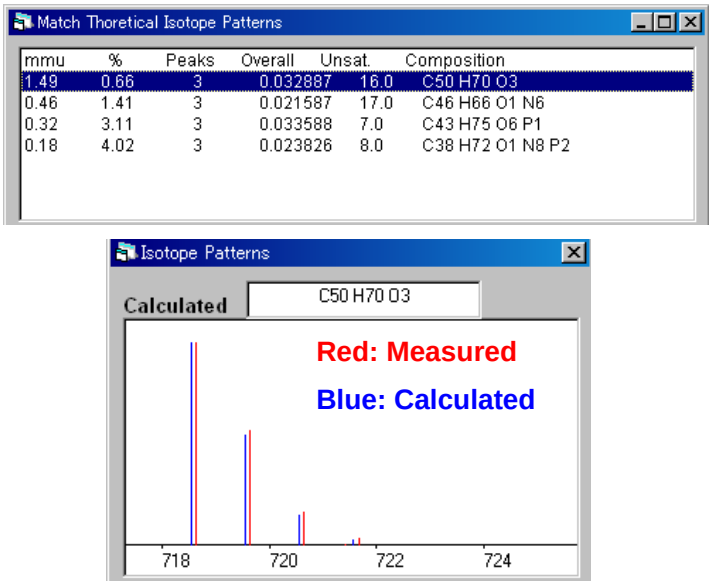

Fig.3 Analysis results table (upper) and isotope patterns (lower)

The mass spectra of Irganox® 1330 and the unknown component are shown in Fig. 2. Although *m/z* values of the major peaks in the spectra are different, the fragmentations are very similar, suggesting that they are similar in their structures. The elemental composition of the unknown was elucidated from the combinations of C, H, O, N, and P, although the spectral similarity suggests that it likely consists from C, H, and O. 21 candidates were found within the error range of ± 5 mmu. By using isotope pattern matching, they were narrowed down to 4, as shown in the top portion of Fig. 3. Among them, C50H70O3 had the smallest matching error (the smaller the “%” in Fig. 3, the better the matching) and the matching was indeed excellent, as shown in the bottom of Fig. 3. The structure of the unknown was elucidated as an analog of Irganox® 1330 with one of the t-butyl group being substituted by H.