Rapid analysis of benzotriazole UV absorber and phosphorus antioxidants by Direct Insertion Probe(DIP)-MS/MS

Product used：Mass spectrometer(MS)

Introduction

A lot of additives are used in plastics and other molded products, depending on the application. Thermal extraction-GC/MS and direct analysis combined with solvent extraction are used in general MS measurement of additives. Especially, direct analysis allows more rapid measurement more than GC-MS. On the other hand, the mass spectrum tend to be complex because the additives are ionized at the same time, and cannot be analyzed by NIST library search. Therefore, analysis based on accurate mass and isotope pattern is required, and it is difficult to confirm additives by direct analysis such as DIP-MS in GC-QMS, even if the target component is clear. In contrast, DIP-MS/MS can select only specific ion derived from the target component for MS/MS measurement, and thus it possible to confirm the additives from product ion scan measurement. In this report, we tried to identify the additives by DIP-MS/MS using a sample mixture of a benzotriazole UV absorber and a phosphorus antioxidant.

Method

The measurement was performed using DIP and GC triple quadrupole mass spectrometer JMS-TQ4000GC UltraQuad™ TQ. “2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol”, “Phenol, 2-(2H- Phenol, 2-(2H- benzotriazole-2-yl)-4,6-bis(1,1-dimethylpropyl)-” and “Drometrizole” were target components as benzotriazole UV absorbers. Also, “Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)” was target component as phosphorus antioxidants. These components were dissolved in THF and mixed to prepare a model sample. The measurement were performed under the measurement condition shown in Table 1.

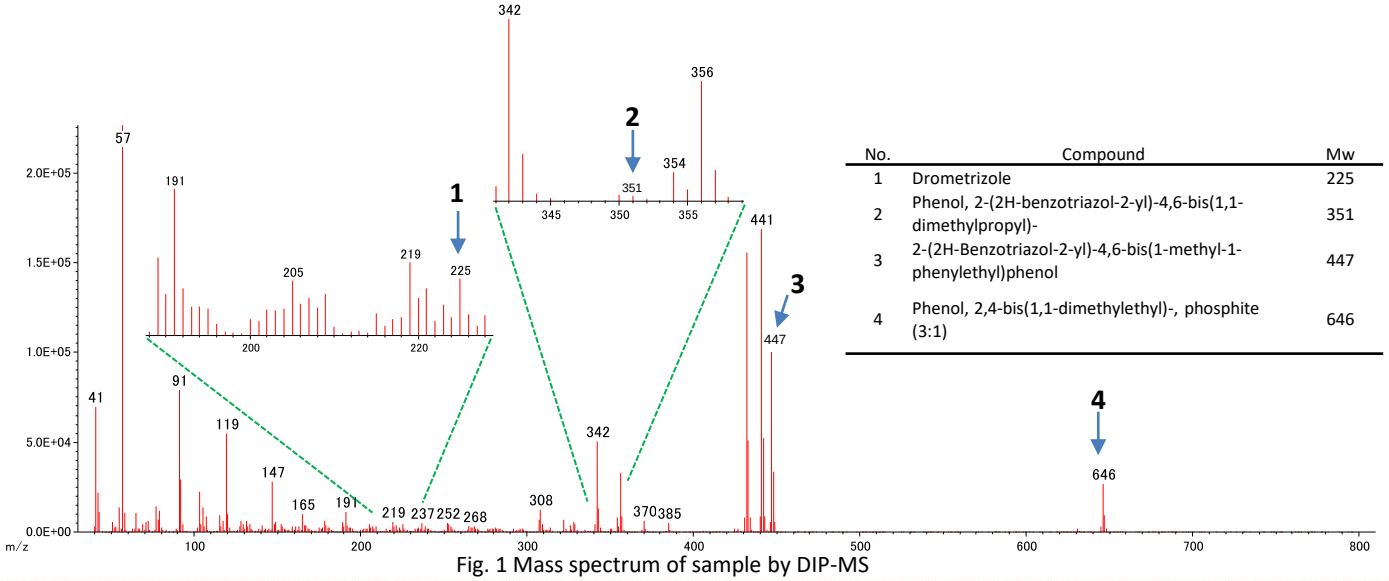
Table 1 Measurement condition

DIP condition	
Heating Program	80 ℃ (0.1 min) → 256 ℃/min → 500 ℃ (4.0 min)
MS condition	
Ion Source Temp.	250 ℃
Ionization Mode	EI+, 70 eV
Measurement Mode	SCAN, Product ion scan
Collision Gas	N_2, 10%

Result

- Measurement results by DIP-MS

The mass spectrum is shown in Fig 1. "2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol" and “Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)" were observed with high peak intensity. In addition, it is easy to confirm these peaks on the mass spectrum due to their large molecular weights. On the other hand, "Drometrizole" and "Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-" are not clear due to low peak intensity.



No.	Compound	Mw
1	Drometrizole	225
2	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-	351
3	2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol	447
4	Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)	646

Fig. 1 Mass spectrum of sample by DIP-MS

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- Measurement results by DIP-MS/MS

The obtained product ion spectra by product ion scan and private library search results are shown in Fig. 2. Molecular ions of each component were used as precursor ions. Private library was created by product ion spectra from each standard sample in advance. Product ion spectra were derived from "Drometrizole" and "Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-" which were difficult to analyze by DIP-MS, can be obtained by DIP-MS/MS, and they were confirmed to be the target components by private library search results. Similarly, product ion spectra were obtained from "2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol" and "Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)", and they were confirmed to be the target components by private library search results.

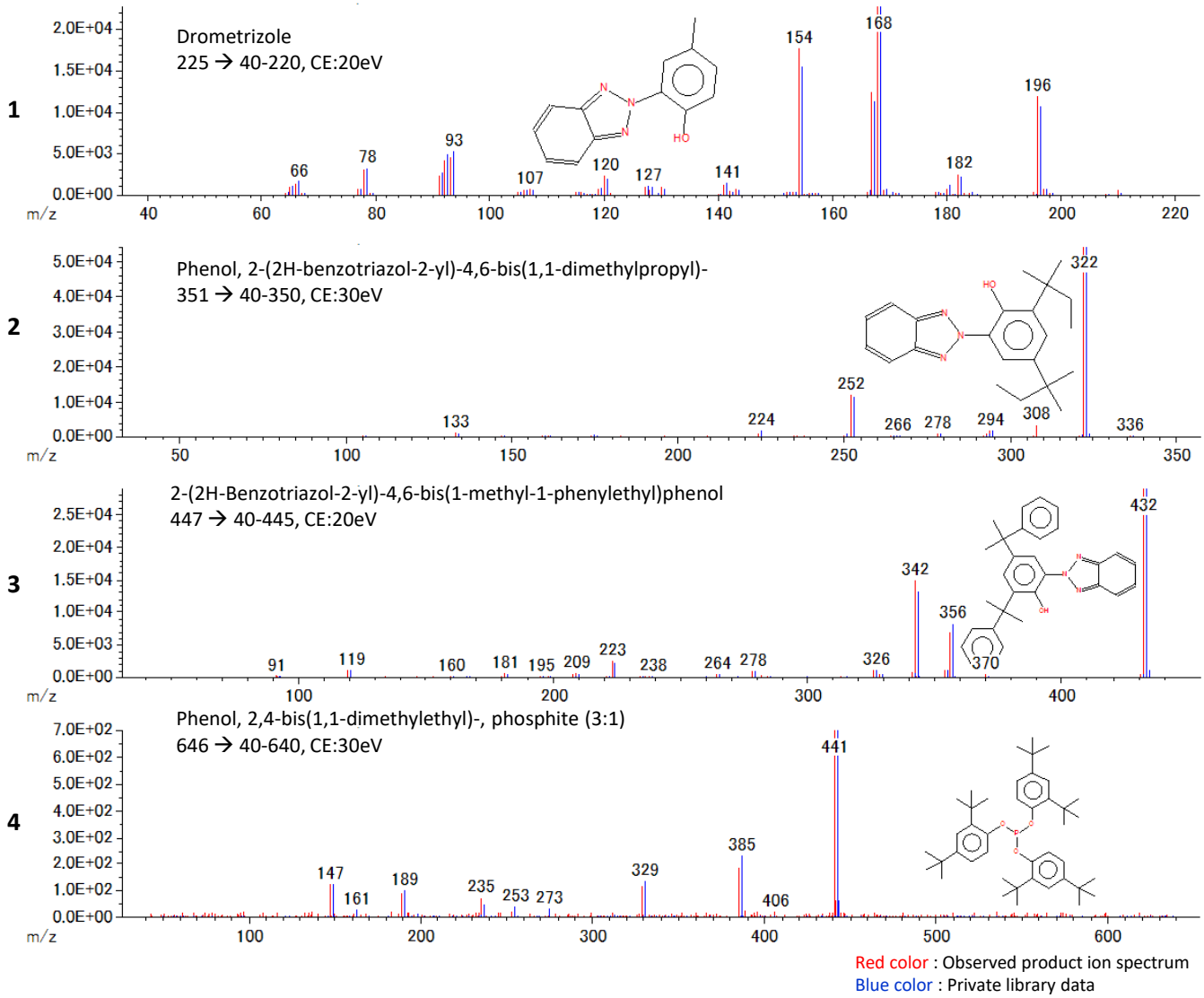

Fig. 2 Product ion spectra of each additive and private library results

Conclusion

For DIP-MS measurement of sample including multiple components, it is difficult to confirm the target component because complex mass spectrum is obtained. However, in DIP-MS/MS, product ion spectrum can be obtained from a selected specific ion. Therefore, it is possible to confirm whether the target component is contained by comparing product ion spectra. Furthermore, it is possible to confirm target component by using private library which components are registered in advance. Thus, the JMS-TQ4000 GC UltraQuad™ TQ was shown to be an effective analysis instrument for direct analysis.

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