

## Analysis of organic pigments using a direct exposure probe on JMS-T100GC "AccuTOF GC"

### Introduction

With the direct exposure probe (DEP), the analyte solution (or suspension) is placed on a coiled platinum filament at the end of the probe (Fig. 3). The probe is introduced into the ion source and the analyte is rapidly heated and vaporized by passing an electric current through the filament. Since the analyte is vaporized by rapid heating with DEP, it is efficient and suitable for the analysis of high boiling point and thermally labile compounds. When used with electron ionization (EI), the method may be called desorption electron ionization (DEI). When used with chemical ionization (CI), the method may be called desorption chemical ionization (DCI).

Commercially available organic pigments, which are widely used in paints, inks, or plastic coloring, are analyzed by DEI.

### Methods

Sample commercial organic pigments (Pigment Yellow 83 and Pigment Red 144)

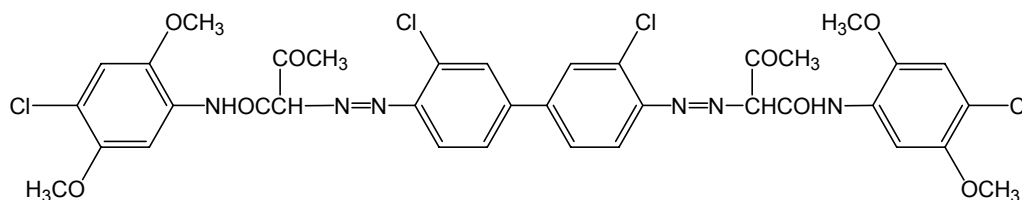


Fig. 1 Pigment Yellow 83 ( $C_{36}H_{32}Cl_4N_6O_8$ )

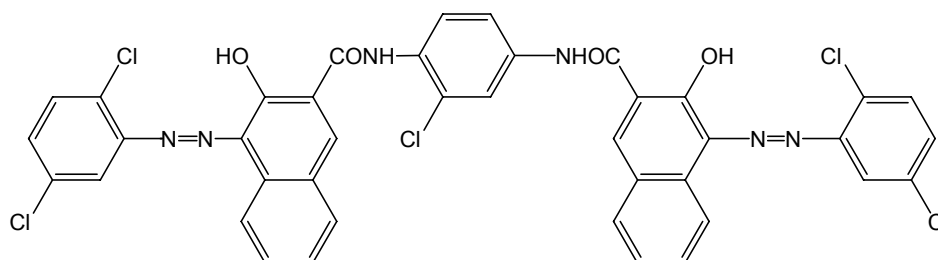


Fig. 2 Pigment Red 144 ( $C_{40}H_{23}Cl_5N_6O_4$ )

DEI conditions	EI conditions:	70 eV, 300 $\mu$ A
	DEP conditions:	0 A $\rightarrow$ 5.12 A/min $\rightarrow$ 1.0A
Ion source temperature:		250 $^{\circ}$ C
Acquired mass range:		m/z 35 – 900
Spectral recording interval:		0.3 sec



Fig. 3 DEP tip

## Results and discussion

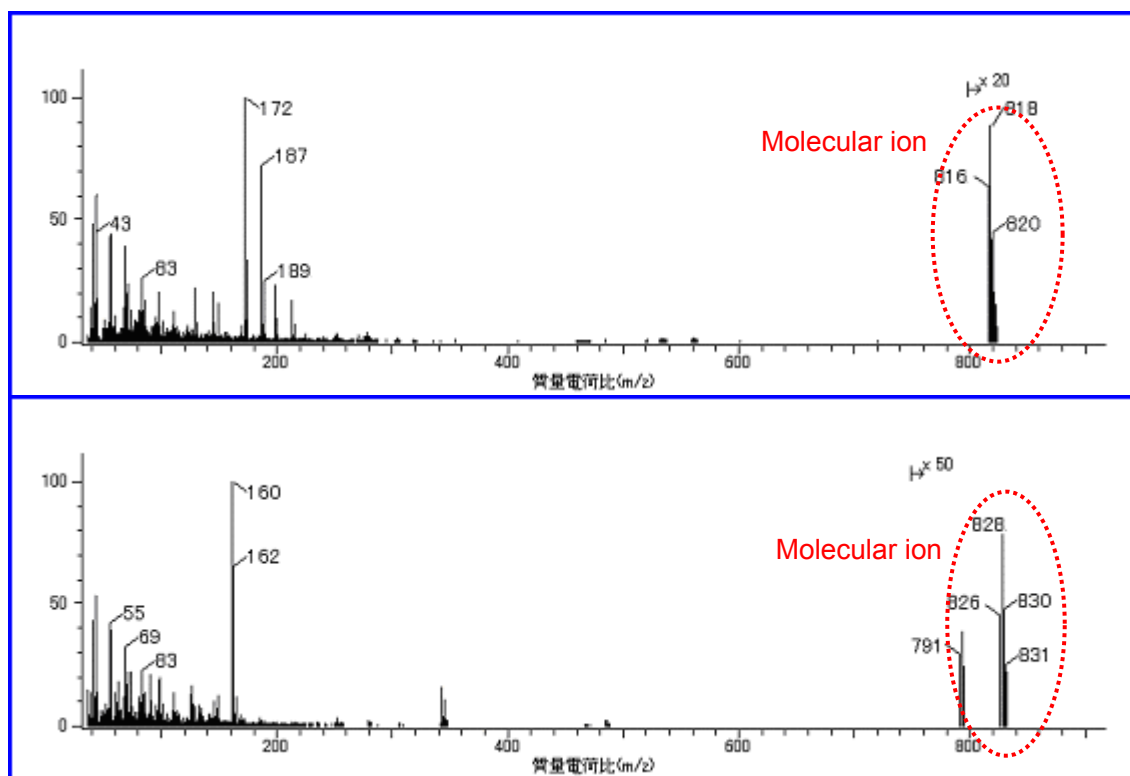


Fig. 4 Mass spectra (top: Pigment Yellow 83, bottom: Pigment Red 144)

As shown in Fig. 4, the mass spectra for the organic pigments were obtained and the molecular ions of both analytes were detected. By applying one of the analytes and 2, 4, 6-tris(pentadecafluoroheptyl) - 1, 3, 5-triazine (the triazine hereafter) to the filament and perform the analysis, the accurate mass of the molecular ions were obtained. A fragment ion from the triazine,  $C_{18}F_{32}N_3$  ( $m/z$  865.95812) was used as an internal mass reference for single point drift correction. The results of the accurate mass measurements are shown below.

Table 1 Accurate mass measurement results

Sample	Measured accurate mass	Calculated exact mass	Error (ppm)	Elucidated composition	Unsaturation
Pigment Yellow 83	816.10205	816.10357	-1.86	$C_{36}H_{32}Cl_4N_6O_8$	22
Pigment Red 144	826.02515	826.02234	3.40	$C_{40}H_{23}Cl_5N_6O_4$	30

The JMS-T100GC “AccuTOF GC” has high mass accuracy as it has very low inherent systematic mass error. Only a single mass reference ion peak is required to perform an accurate mass measurement. Even for DEI, accurate mass can be readily measured by applying the analyte and a mass reference sample to the probe simultaneously and highly reliable structural elucidation is possible.

### Acknowledgement

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