SHIMADZU

Application Data Sheet

No.33

GCMS

Gas Chromatograph Mass Spectrometer

# Analysis of Polycyclic Aromatic Hydrocarbons Using GC-MS

## Introduction

Polycyclic aromatic hydrocarbons (PAHs) are byproducts of burning fuels, such as mineral oils, and are known to be carcinogenic, mutagenic, and teratogenic. These compounds are regulated in many countries as harmful pollutants in environmental water and the atmosphere. In Japan, the "Measuring method manual for toxic air pollutants" and "Measuring method manual for polycyclic aromatic hydrocarbons (PAHs) in exhaust gas emissions" were revised in March 2011. In addition, environmental standards, including fine particle regulations ($PM_{2.5}$) and fine particles, can include PAHs. Consequently, there is an increasing need to measure PAHs. This application datasheet introduces an example of measuring 36 PAHs.

## Analysis Conditions and Results

Table 1 shows the analysis conditions and Fig. 1 shows the total ion current chromatogram. Figure 2 (Page 2) shows enlarged chromatogram sections for PAHs with 4, 5, and 6 rings.

Table 1: Analysis Conditions

| | | | |
|---|---|---|---|
| GC-MS | : GCMS-QP2010 Ultra | | |
| [GC] | | [MS] | |
| Column | : Rtx-35 (length 30 m, 0.32 mm I.D., df=0.25 µm ) | Interface temperature | : 300℃ |
| Inlet mode | : Splitless | Ion source temperature | : 230℃ |
| Vaporizing chamber temp | : 300℃ | Solvent elution time | : 3.5min |
| Column oven temperature | : 90℃ (2min) →(5℃/ min)→320℃(12min) | Data sampling time | : 4.5 – 60min |
| Carrier gas | : Helium | Measurement mode | : Scan |
| Control mode | : Constant linear velocity (43.7cm/sec) | Mass range | : *m/z* 45-450 |
| High pressure injection | : 150kPa (1.5min) | Event time | : 0.3sec |
| Purge flow rate | : 3 mL/min | | |
| Injection rate | : 1.0 µL | | |

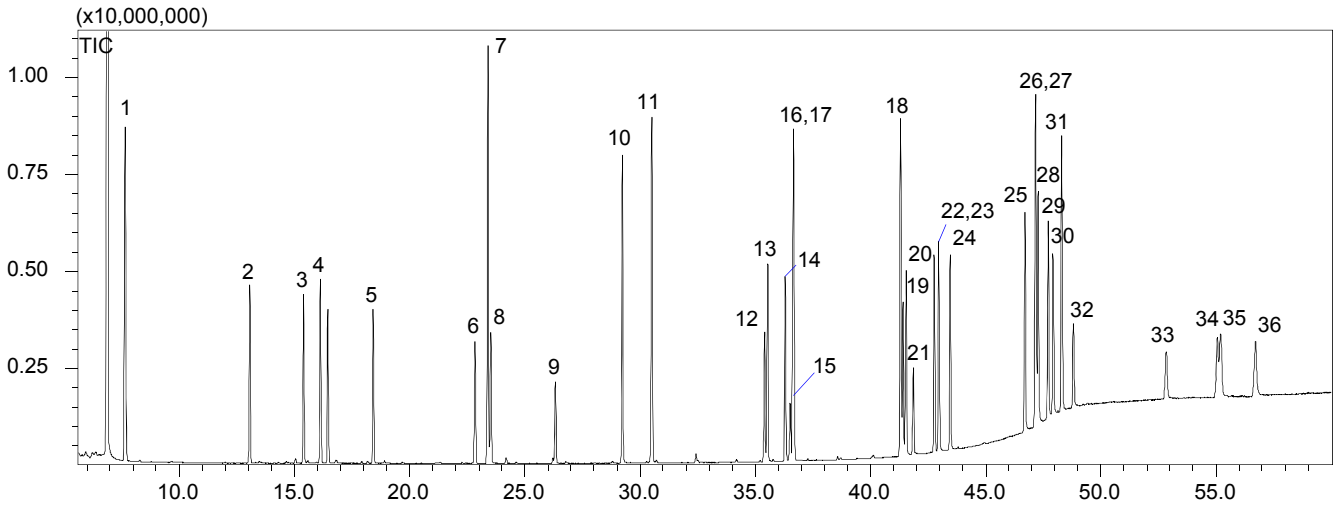
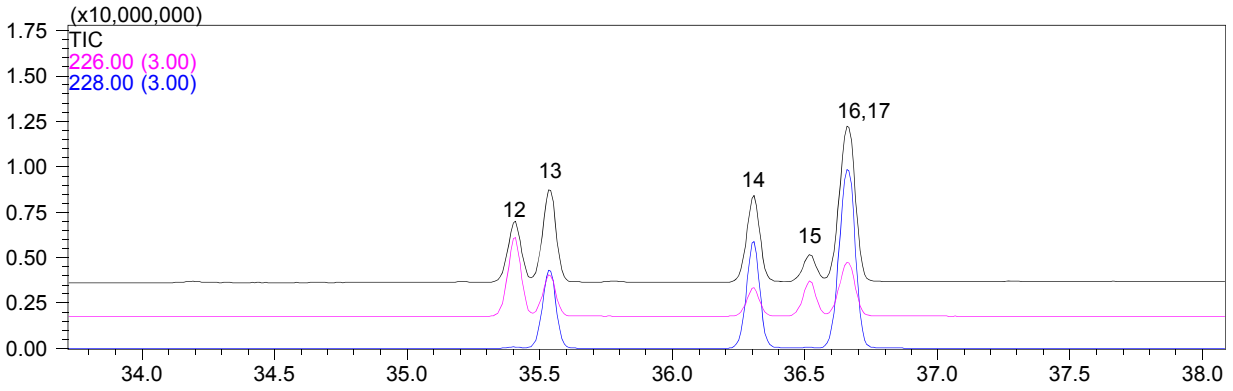
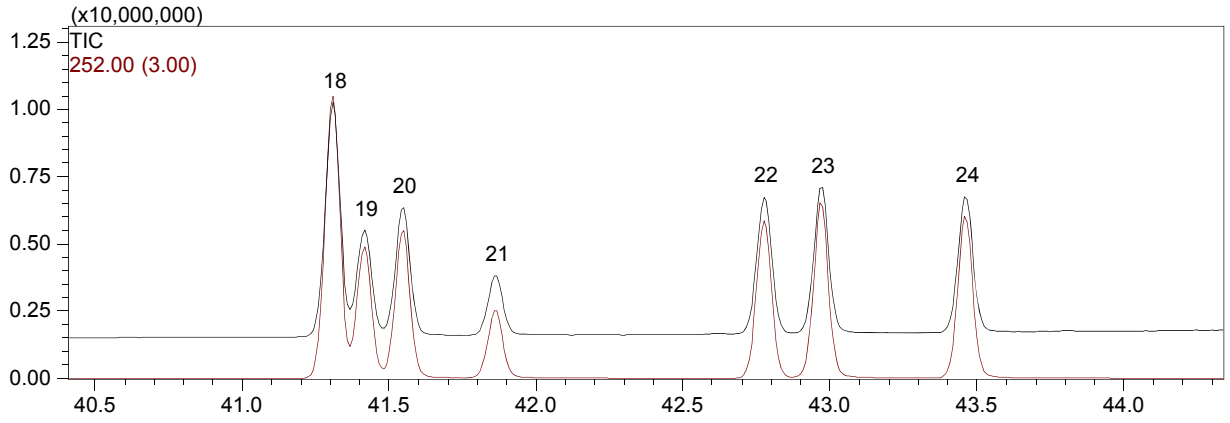



Fig. 1: Total Ion Current Chromatogram of 36 PAHs

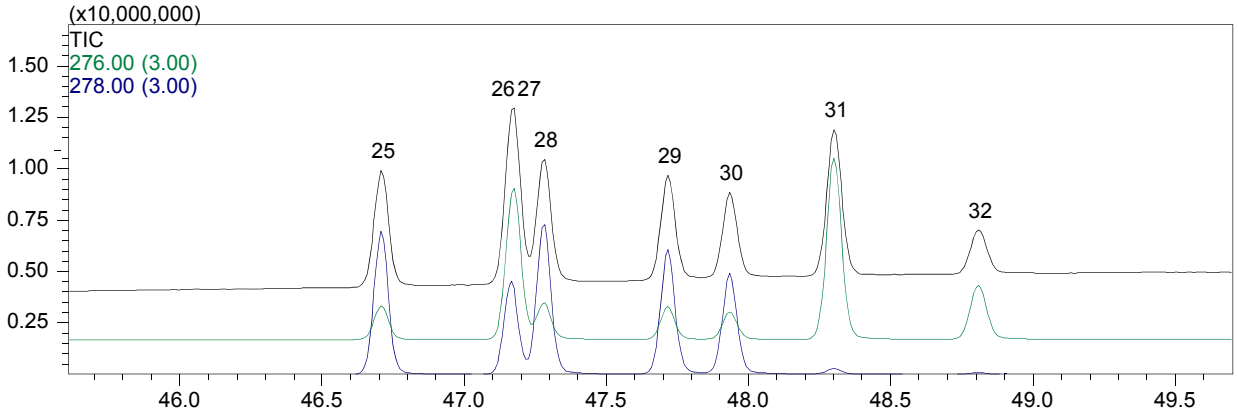
1.Naphthalene, 2.Biphenyl 3.Acenaphthylene 4.Acenaphthene 5.Fluorene 6.Dibenzothiophene 7.Phenanthrene 8.Anthracene 9.4H-Cyclopenta[*def*]phenanthrene 10.Fluoranthene 11.Pyrene 12.Benzo[*ghi*]fluoranthene 13.Benzo[*c*]phenanthrene 14.Benzo[*a*]anthracene 15.Cyclopenta[*cd*]pyrene 16,17.Chrysene & Triphenylene 18.Benzo[*b*]fluoranthene 19.Benzo[*k*]fluoranthene 20.Benzo[*j*]fluoranthene 21.Benzo[*a*]fluoranthene 22.Benzo[*e*]pyrene 23.Benzo[*a*]pyrene 24.Perylene 25.Dibenz[*a,j*]anthracene 26.Dibenz[*a,c*]anthracene 27.Indeno[1,2,3-*cd*]pyrene 28.Dibenz[a,h]anthracene 29.Benzo[b]chrysene 30.Picene 31.Benzo[*ghi*]perylene 32.Anthanthrene 33.Dibenzo[*b,k*]fluoranthene 34.Dibenzo[*a,h*]pyrene 35.Coronene 36.Dibenzo[*a,e*]pyrene




12.Benzo[*ghi*]fluoranthene 13.Benzo[*c*]phenanthrene 14.Benzo[*a*]anthracene 15.Cyclopenta[*cd*]pyrene
16,17.Chrysene&Triphenylene




18.Benzo[*b*]fluoranthene 19.Benzo[*k*]fluoranthene 20.Benzo[*j*]fluoranthene 21.Benzo[*a*]fluoranthene
22.Benzo[*e*]pyrene 23.Benzo[*a*]pyrene 24.Perylene




25.Dibenz[*a,j*]anthracene 26.Dibenz[*a,c*]anthracene 27.Indeno[1,2,3-*cd*]pyrene 28.Dibenz[*a,h*]anthracene
29.Benzo[*b*]chrysene 30.Picene 31.Benzo[*ghi*]perylene 32.Anthanthrene
26 and 27 can be resolved between *m/z* 276 and 278.

Fig. 2: Enlarged Chromatograms
Upper: 4-Ring Section (retention time 33.5 to 38.0 minutes);
Middle: 5-Ring Section (retention time 40.5 to 44.5 minutes);
Lower: 6-Ring Section (retention time 45.5 to 49.5 minutes)

## Summary

Because there are so many PAH isomers, separation by column is more important than separation by mass. Of the 36 polycyclic aromatic hydrocarbons, the Rtx-35 column can separate all except chrysene and triphenylene. Therefore, it enables separating PAHs with a wide range of boiling points.

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First Edition: November 2011