## 1.9 Analysis of kerosene (1) - GCMS

## Explanation

The primary products of petroleum - gasoline, kerosene, light oils etc - are hydrocarbon mixtures refined through distillation. A Gas Chromatography Mass Spectrometer (GCMS) is used for qualitative determination, since measurement by Gas Chromatography (GC) using a capillary column produces a large number of peaks.

Fig. 1.9.1 is the TIC of kerosene by a non-polar column (methyl silicon). Chemical compounds up to toluene can be seen because of the small amount of gasoline contained in this kerosene.

Fig. 1.9.2 is a TIC chromatogram by a polar column. This kerosene is standard and compounds up to  $C_8$ -paraffin are not contained. As shown in Fig. 1.9.3 (polar column), paraffin hydrocarbons from  $C_9$  to  $C_{16}$  are contained, with  $C_{10}$  and  $C_{11}$  as the main components. A lot of aromatic hydrocarbons are contained as well.

## Analytical Conditions

Model : Shimadzu GCMS-QP1000EX

Column ① : CBJ1 0.25mm  $\times 30$ m i.d. df=0.25 $\mu$ m

Column Temp. : 40°C (2min)-220°C (5°C/min)

Column (2) : CBP20 0.25mm  $\times 30$ m i.d. df=0.25 $\mu$ m

Column Temp. : 80°C (2min)-5°C/min-150°C

-15°C/min-200°C

Carrier Gas : He 50kPa Injector Temp. : 300°C Interface Temp. : 200°C Split : 1:50

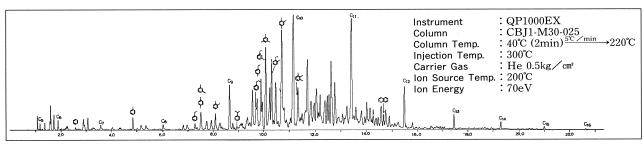


Fig. 1.9.1 TIC chromatogram by a non-polar column

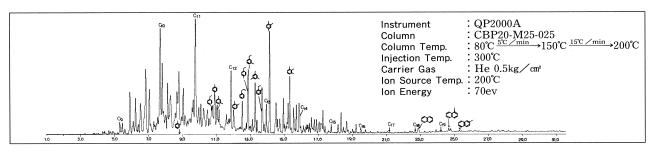


Fig. 1.9.2 TIC chromatogram by a polar column

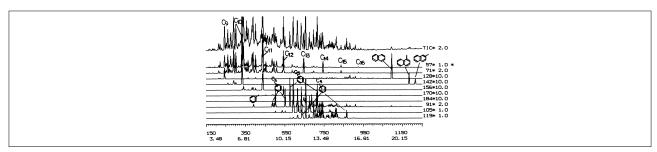


Fig. 1.9.3 Mass chromatogram by a polar column



## 1.9 Analysis of kerosene (2) - GCMS

Fig.1.9.4 is the mass chromatogram obtained by analysis with a nonpolar column. C<sub>3</sub>-alkylbenzene is eluted from in between the main components of paraffin, n-nonane (C<sub>9</sub>H<sub>20</sub>) and n-decane (C<sub>10</sub>H<sub>22</sub>). Fig. 1.9.5 is the mass chromatogram obtained by a polar column (PEG). The component ratio of kerosene A and kerosene B differ somewhat, and the C<sub>3</sub>-alkylbenzene has moved to between n-undecane (C<sub>12</sub>H<sub>26</sub>) and n-tetradecane (C<sub>14</sub>H<sub>30</sub>), and there is less interference by paraffin hydrocarbons.

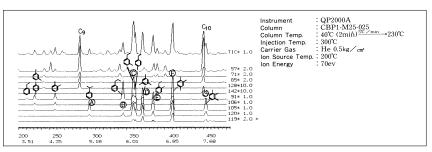


Fig. 1.9.4 Mass chromatogram by a non-polar column

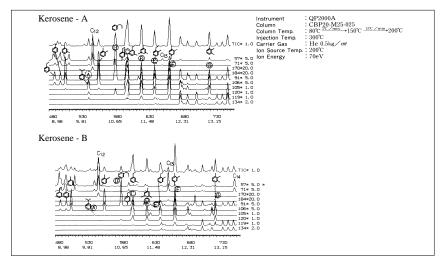


Fig. 1.9.5 Mass chromatogram by a polar column

As indicated in Fig. 1.9.6, there are 8 types of C<sub>3</sub>-alkylbenzene isomers. Identification from the mass spectra becomes extremely difficult. In this case, if a capillary column with good separation is used, C<sub>3</sub>-alkylbenzene can be completely separated, with the exception of m,p-ethylmethylbenzene, making identification from a mass chromatogram easy.

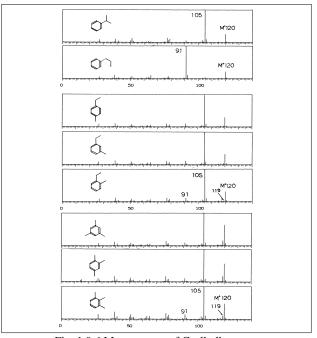


Fig. 1.9.6 Mass spectra of C3-alkylbenzene