

## Detection of molecular ions of fluorine compounds by GC/FI-TOFMS

Chlorofluorocarbon (CFC) and hydrochlorofluorocarbon (HCFC) have been used extensively as solvent, cleaning agent and foaming agent. Unfortunately CFC and HCFC have negative effects on the environment like ozone depletion and global warming. For this reason, CFC's substitutes, such a hydrofluorocarbon (HFC) and hydrofluorocarbon ether (HFE), have been developed.

In general, fluorine compounds are analyzed by gas chromatography (GC) / mass spectrometry (MS). However, molecular ions of these compounds are often not observed with electron ionization (EI) and chemical ionization (CI). Therefore, molecular weight determination is often difficult for unknown compounds when they are present as by-product or impurity.

On the other hand, field ionization (FI) is a very soft ionization technique capable to observe the molecular ion of volatile compounds. This application note shows that FI is a suitable technique to determine the molecular weight of compounds which are not producing molecular ions in EI or CI.

### 【Measurement Conditions】

Mass Spectrometer: JEOL JMS-T100GC

Gas Chromatograph: Agilent 6890N

Sample:

Fluorinated ether (MW174) and AK225 (Mixture)

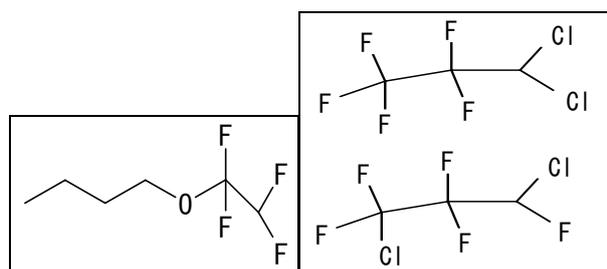


Fig.1 Structure of fluorinated ether (Left) and AK225 (Right)

|                             |  |
|-----------------------------|--|
| GC                          |  |
| Carrier Gas                 | He   |
| Flow rate                   | 0.8 ml/min (const. flow)                       |
| Temperature (Injection)     | 200 degree C                                   |
| Injection mode              | Split (10:1)                                   |
| Oven temperature            | 40C (2min) - <5C/min> - 60C - <15C/min> - 200C |
| MS                          |  |
| Ionization mode             | FI+  |
| Acquired m/z range          | 35 -450  |
| Spectrum recording interval | 0.4 sec  |

### 【Result】

Each TIC and FI mass spectrum of 2 samples are shown in Fig.2 and Fig.3. Although the molecular ion of these compounds are not observed by EI or CI, FI works well and produces the molecular ion of each compound clearly.

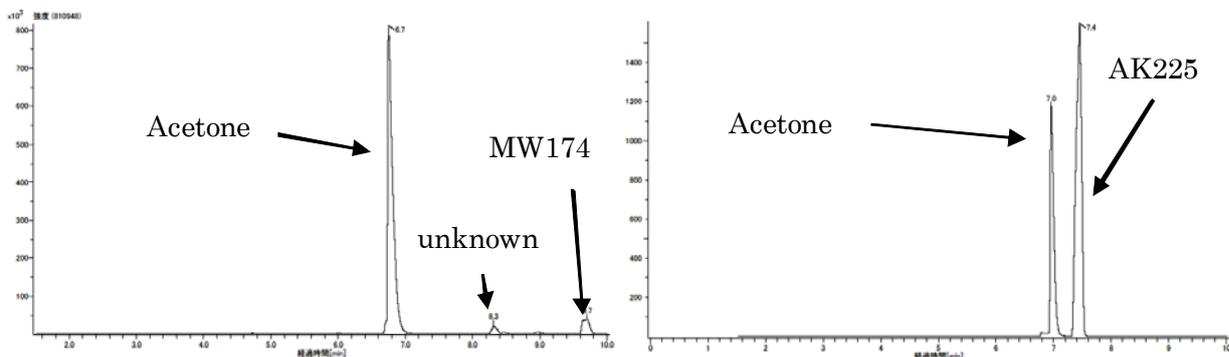


Fig.2 TIC of fluorinated ether (left) and AK225 (right)

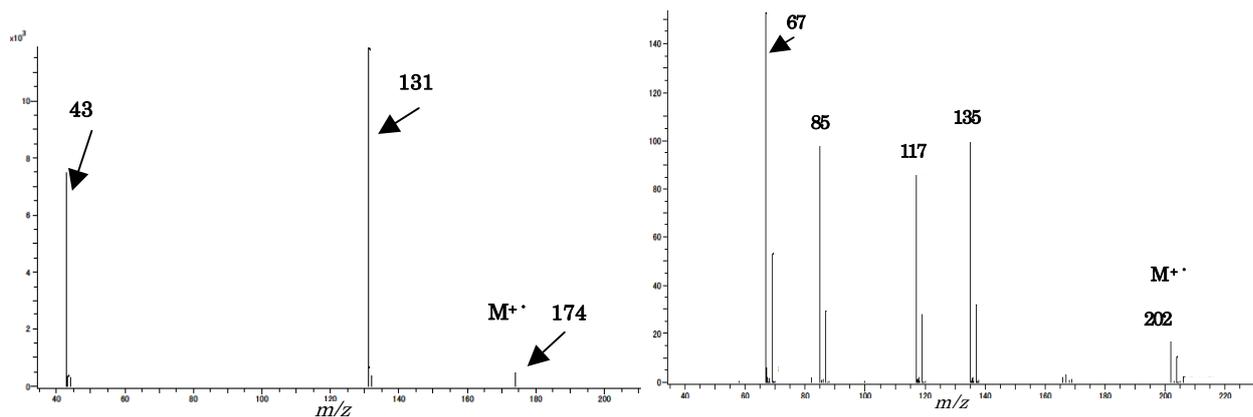


Fig.3 FI spectra of fluorinated ether (left) and AK225 (right)

Both compounds produce not only fragment ions but also the molecular ion with FI. It is very clear to confirm the molecular weight of compounds in comparison with EI and CI. In addition, the elemental composition of the molecular ion and fragment ions were determined with accurate mass. This result is very useful to identify the unknown compound.

Table 2 Result of elemental composition determination for fluorinated ether (left) and AK225 (right)

| Observed  | Calculated | Diff.(mDa) | Formula   |
|-----------|------------|------------|---|
| 43.05632  | 43.05478   | 1.55       | C <sub>3</sub> F <sub>7</sub>                   |
| 131.01407 | 131.01200  | 2.07       | C <sub>3</sub> H <sub>3</sub> F <sub>4</sub> O  |
|           | 131.01086  | 3.21       | C <sub>6</sub> H <sub>2</sub> F <sub>3</sub>    |
| 174.06348 | 174.06678  | -3.29      | C <sub>6</sub> H <sub>10</sub> F <sub>4</sub> O |

| Observed  | Calculated | Diff.(mDa) | Formula  |
|-----------|------------|------------|--|
| 66.97379  | 66.97508   | -1.29      | CHClF  |
| 84.96424  | 84.96566   | -1.42      | CClF <sub>2</sub>                              |
| 116.97270 | 116.97189  | 0.81       | C <sub>2</sub> HClF <sub>3</sub>               |
| 134.96324 | 134.96347  | 0.78       | C <sub>2</sub> ClF <sub>4</sub>                |
| 201.93481 | 201.93755  | -2.74      | C <sub>3</sub> HCl <sub>2</sub> F <sub>5</sub> |

**【Acknowledgement】**

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**【Reference】**

T. Isemura, R. Kakita, A. Tamaoki, S. Yonemori, J. Fluor. Chem., 80(1996)81-85