Organic Structural Analysis Using High Resolution GC/MS

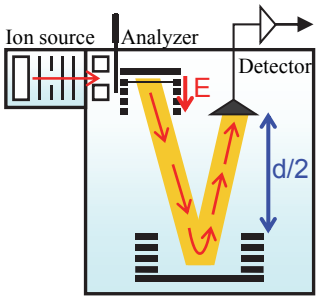
High resolution GC/TOF-MS enables us to calculate the elemental compositions of individual compounds. The field ionization (FI) method is also useful in structural analysis, as it yields molecular ions clearly.

Mass Spectrometer

Time-of-Flight Mass Spectrometer: TOF-MS

- High-resolution TOF-MS system.
- Capability for accurate mass measurement.
- Calculate possible elemental compositions for each ion.

<Diagram of TOF-MS>



$m/z = (2E/d^2)\,t^2$

E: Acceleration energy,
d: Distance, t: Time of flight

Benefits

- High sensitivity
  1pg OFN* S/N ≧ 100
  *OFN: Octafluoronaphthalene
- High mass accuracy
  Accuracy: ≦4 ppm
- High speed data acquisition
  Max: 50 spectra/sec.

Soft Ionization Methods

Chemical Ionization: CI

☺Provides molecular ion information (Ions $[M+H]^+$ are mainly observed).

☹The molecular ion may be absent for some compounds because of their fragmentation.

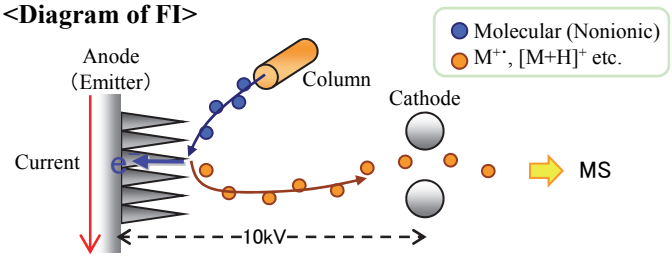
Field Ionization: FI

☺Generally yields intact molecular ions $[M]^{+\cdot}$.

☺Produce very few fragment ions.

Useful technique for determination of molecular weight.

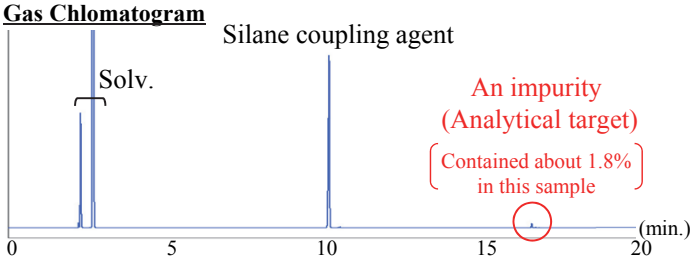
<Diagram of FI>



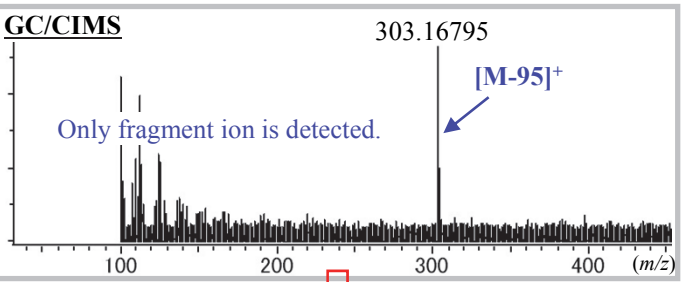
The analyte molecules are ionized by electron tunneling at the tip of the emitter.

Examples of Observation: An Impurity in Silane Coupling Agent

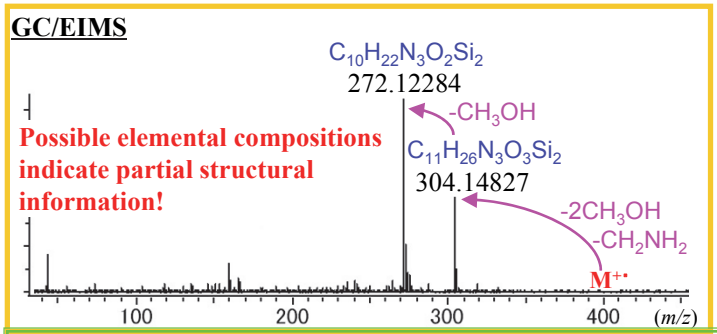
Gas Chlomatogram



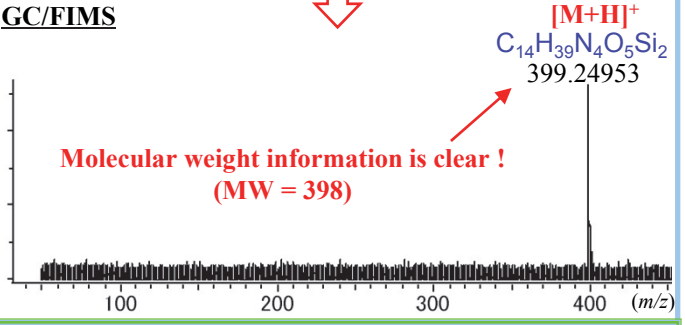
GC/CIMS

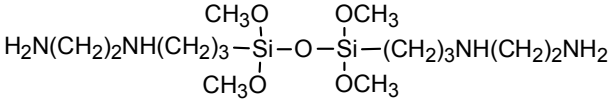


GC/EIMS



GC/FIMS





Using high resolution GC/MS measurement of each ionization mode, the structure of this target is estimated as left figure.

RAPID and RELIABLE qualitative analysis of additives, impurities, degradant and so on!