High resolution GC/Q-TOF × MS/MS, CI measurement
Qualitative analysis of gas generated by heating fluoropolymers

The outgas from fluoropolymers, which are also used as 5G materials, may cause contamination and corrosion of surrounding materials. However, it is difficult to qualify low molecular weight fluorine compounds by GC/MS. In this paper, we would like to introduce a case study in which we attempted to qualify them by using high-resolution measurement, MS/MS, and CI (chemical ionization) measurement.

Equipment

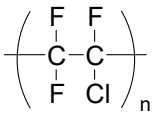
GC/Q-TOFMS with Thermal desorption system

■Features
- High-mass resolution (25000 at m/z 271)
- Equipped with re-collect system *1)
- CI measurement is possible
- Equipped with deconvolution function
- Multivariate analysis is possible
- GC × GC MS/MS analysis is available.

※1 : This is a function to re-collect components that have been thermally desorbed. Valuable gas components can be measured twice, once for EI and once for CI.

Sample and pre-treatment

■Sample
- PCTFE (Poly Chloro Tri Fluoro Ethylene)

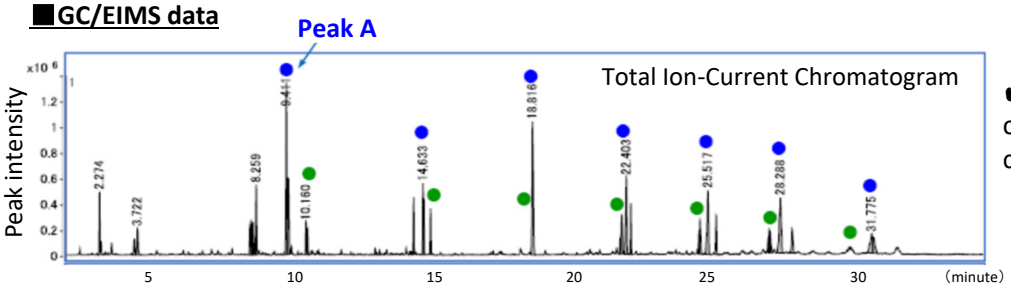


■pre-treatment
Heating conditions: 350° C, 30 minutes

Strong Point! Out gas analysis is possible!

Result

■GC/EIMS data

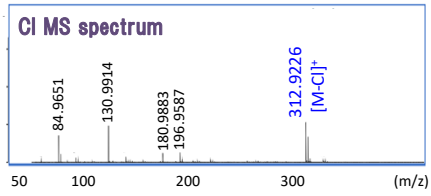


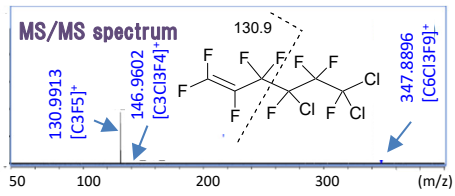
✔Confirmation of peaks consisting of two types of fluorine-containing compounds. (● and ●)

Quantitative analysis

■ Structural analysis of Peak A

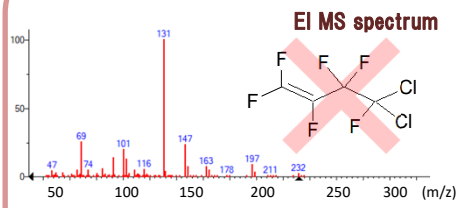
Latest MS equipment





✔CI and MS/MS measurements are also possible using re-collect system .
✔ The formula of peak A was determined to be C6Cl3F9 with CI measurement and Precise mass analysis
✔ The substructure was identified by MS/MS measurements.

Conventional MS equipment



✔C4Cl2F6 hit in library search
⇒May lead to incorrect analysis results.
✔ We only get the information that the compound contains F

■ Structural analysis of each peaks

By analyzing each peak, the following structures were deduced.

● $CF_2=CF-(CF_2-CFCl)_n-CF_2-CFCl$ ● $CF_2=CF-(CF_2-CFCl)_m-CF=CF_2$

✔Pyrolysis products of the polymer were detected as the gas components generated.

Structure identification of fluorinated gases, which are difficult to analyze, is now possible !!

Toray Research Center, Inc. can perform high-resolution GC/MS measurement of gas composition! Are there any gas compositions that you have given up on identifying the structure? Precise mass spectrometry, CI measurements, and MS/MS measurements are used to identify the structure!

Toray Research Center, Inc.