infiTOF Application

High-resolution time-of-flight mass spectrometer infiTOF

Heating gas analysis using TG/DTA-MS

KANOMAX FMT
A Kanomax Company

A simultaneous differential thermogravimetry analyzer (TG/DTA) changes the temperature of the sample and measures the resulting weight change and the temperature difference with a reference sample to investigate the behavior of physical and chemical changes due to heat in the sample. This method is used in a wide range of fields, including inorganic materials, polymer materials, and pharmaceuticals. TG-MS is a device that connects a mass spectrometer (MS) to this TG/DTA. TG/DTA-MS enables qualitative analysis of gases generated from samples and analysis of decomposition reactions. Generally, a quadrupole mass spectrometer (QMS) is used in TG/DTA-MS, but with QMS it is sometimes difficult to characterize the generated gas and analyze its behavior due to mass resolution and mass accurac w,. By using the multi-turn time-of-flight mass spectrometer infiTOF, it is possible to characterize the generated gas and analyze its generation behavior using accurate mass spectrometry, which is difficult to do with QMS. The multi-turn time-of-flight mass spectrometer infiTOF achieves high mass resolution despite its small size by orbiting the same flight space. By changing the number of laps, it is possible to set the resolution as desired.

Multi-turn time-of-flight mass spectrometer (infiTOF)

TG/DTA Simultaneous differential thermogravimetry measurement device STA7300

Calcium oxalate TG-MS analysis

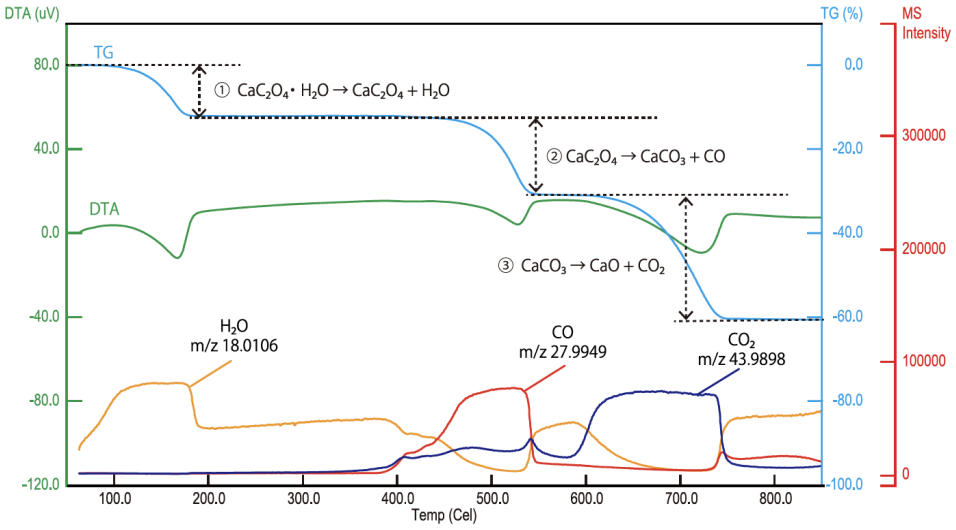
We will introduce an example of high mass resolution measurement using TG-MS using calcium oxalate hydrate. As the temperature is raised by TG in a helium atmosphere, a three-stage weight loss reaction and MS analysis of the resulting components show that (1) water (H_2O) from the reaction at 100 to 200 °C changes to carbon monoxide (CO) at around 450 to 550 °C., carbon dioxide (CO_2) was confirmed at around 600-700 °C. By measuring with high mass resolution, it is possible to separate carbon monoxide (CO) and nitrogen (N_2), which have the same integer mass number (m/z 28), with accurate mass, which is generally impossible to separate using QMS. It is possible to accurately analyze CO (m/z 27.994) by mass. In this way, by using the high-resolution time-of-flight mass spectrometer infiTOF, it is possible to perform mass separation analysis using accurate mass for compounds that are difficult to separate using integer mass.

TG/DTA Conditions

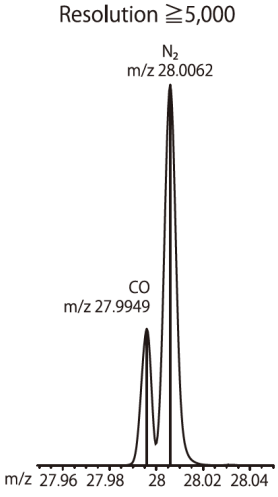
Sample: 5 mg calcium oxalate hydrate
Temperature Conditions: 45 - 1000 °C @ 40 °C/min
Transfer Line Temperature: 300 °C
Measurement Atmosphere: He 100 mL/min

TOF-MS Conditions

Ionization method: EI
Ionization voltage: 20eV.
Ion source temperature: 300 °C
MultiMode cycles= 8, resolution>=5000



Example of TG/DTA-MS analysis of calcium oxalate hydrate



With the same integer mass number (m/z 28) accurate mass separation of CO and N_2

High-resolution time-of-flight mass spectrometer infiTOF Heating gas analysis using TG/DTA-MS

TG-MS analysis of polycarbonate resin

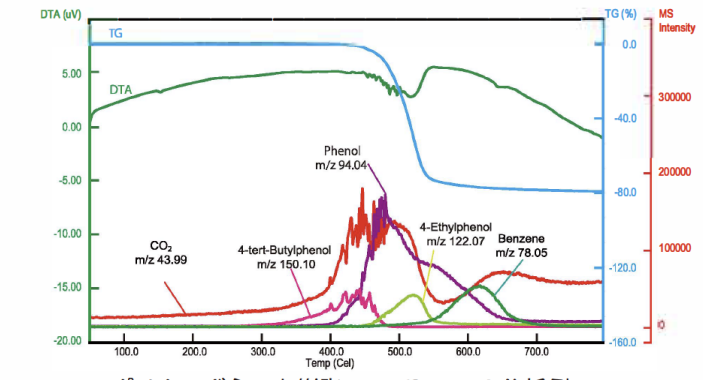
The TG-MS method is a method in which the gas generated from a sample by heating with a TG is qualitatively determined using an MS. In particular, when decomposing polymers, multiple gases are emitted simultaneously. With TG-MS using a quadrupole mass spectrometer (QMS), it is possible to analyze even samples in which it is difficult to identify the evolved gas components due to mass resolution.
Identification can be easily performed using accurate mass analysis using infiTOF's high mass resolution.
We will introduce an example of qualitative analysis of gas generated by the TG-MS method of polycarbonate resin using infiTOF in a helium atmosphere.
The results of accurate mass analysis of the gases generated by polycarbonate resin show that CO_2 and CO are generated and that they are derived from bisphenol A, which is the raw material for polycarbonate resin. Phenols and hydrocarbons were confirmed.

TG/DTA Conditions

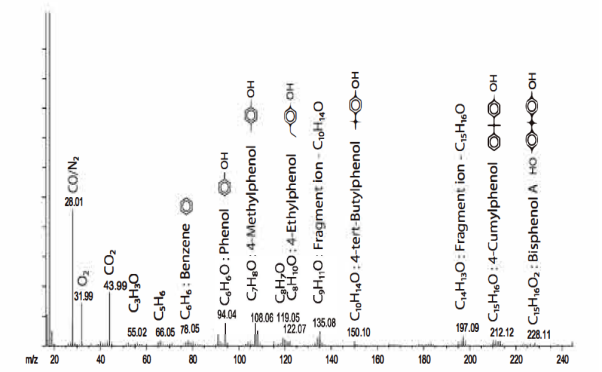
Sample: 5 mg polycarbonate resin
Temperature Conditions: 45 - 800 °C @ 20 °C/min
Transfer Line Temperature: 300 °C
Measurement Atmosphere: He 100 mL/min

TOF-MS Conditions

Ionization method: EI
Ionization voltage: 20eV.
Ion source temperature: 300 °C
MultiMode cycles= 8, resolution>=3000



Example of TG/DTA-MS analysis of polycarbonate resin



TG/DTA-MS analysis average mass spectrum of polycarbonate resin

TG-MS analysis of pharmaceuticals (commercial cold medicines)

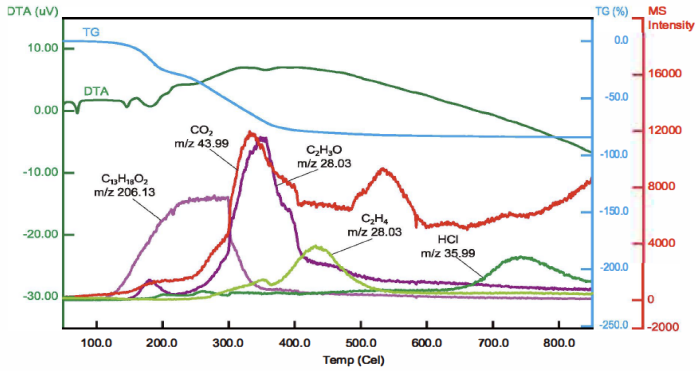
TG/DTA analysis is used to confirm the thermal stability of pharmaceuticals for safety reasons. Also, as a qualitative analysis of the gas components generated at that time.TG/DTA-MS is beginning to be used. Introducing an example of TG/DTA-MS analysis of commercially available cold medicine using a high-resolution time-of-flight mass spectrometer infiTOF. The high mass resolution of inifiTOF enables the emission of ethylene C_2H_2 with the same integer mass (m/z 28), which is difficult to separate by mass using a quadrupole mass spectrometer (QMS). It is possible to confirm the raw product and identify generated components derived from ibuprofen and caffeine by accurate mass analysis.

TG/DTA Conditions

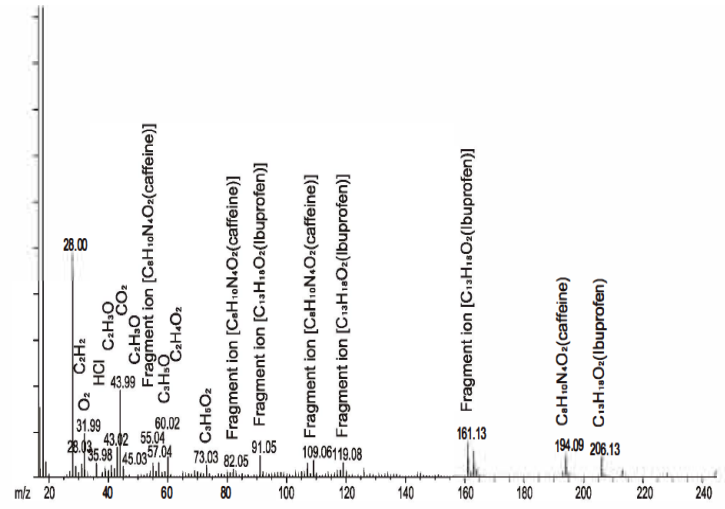
Sample: 5 mg over-the-counter cold medicine
Temperature Conditions: 45 - 850 °C @ 25 °C/min
Transfer Line Temperature: 300 °C
Measurement Atmosphere: He 200 mL/min

TOF-MS Conditions

Ionization method: EI
Ionization voltage: 20eV.
Ion source temperature: 300 °C
MultiMode cycles= 8, resolution>=3000



Example of TG/DTA-MS analysis of commercially available cold medicines



Average mass spectrum of commercial cold medicine TG/DTA-MS analysis

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