Application Note TA6006

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TA6006 - Thermal behavior analysis of over-the-counter (OTC) drugs

Introduction

The detection or analysis of the gases evolved during a chemical reaction, as a function of temperature, constitute the techniques of thermal analysis called evolved gas detection (EGD) and evolved gas analysis (EGA), respectively.

Thermal analysis using mass spectrometry covers a large number of related and analytical powerful techniques such as evolved gas analysis using mass spectrometry (EGA-MA) including thermogravimetry-mass spectrometry (TG-MS), temperature programmed pyrolysis-mass spectrometry and temperature programmed desorption mass spectrometry.

In conventional EGA-MS, the evolved gaseous products, which are introduced rapidly to MS, are generally ionized by electron ionization (EI) at 70 eV. In this case, a part of the evolved gaseous molecular ion undergoes further decomposition, and observed simultaneously ions. Especially in the thermal processes, since the evolved gases consists of multiple gaseous species in almost all cases, the resulting fragment ions are overlapped, while the fragment ions provide significant information concerning the structure of the molecule, the apparent mass spectra can be quite complicated. In order to differentiate in real-time the multiple organic species that are evolved in the thermal process, one feasible approach is the use of MS with a selective and soft (fragment-free) ionization technique which avoids fragmentation during ionization.

We evaluate the thermal behavior of over-the-counter products employed the combination of thermogravimetry (TG), differential thermal analysis (DTA) and photo ionization mass spectrometery (PI-MS). The photo ionization mass spectrometer is available to detect and discriminate in real time the molecular state of decomposition gas which corresponded to mass change by heating, it is useful to analyze the thermal cracking process of drug and, it improves the analytical precision and measurement efficiency.

Instrument: ThermoMass Photo

ThermoMass Photo is an evolved gas analytical system designed for real-time simultaneous measurements of thermogravimetry – differential thermal analysis (TG-DTA) coupled with electron impact ionization (EI) and the fragment-free photoionization (PI) mass spectrometry (MS) that performs measurements as a function of temperature or time.

Measurement and analysis

A comparison between the results from EIMS and PIMS for remedy (major component is metoprolol tartrate for high-blood pressure, angina and irregular heartbeat) obtained evolved gas peak at around 200℃ employed TG-DTA-EI/PIMS are shown in Figure 1. The EI mass spectrum consisted of molecular ions along with numerous fragment ions formed by the high ionization energy of the EI. Since the detected fragmentation and molecular ions were mutually mixed, the

identification of the evolved gas species was complicated and difficult. The PI mass spectrum shows that those evolved gas species were easily real-time characterized by the m/z 96, 110, 126, 144 and 152 ions assigned to 5 molecular ions due to soft-photoionization effect.

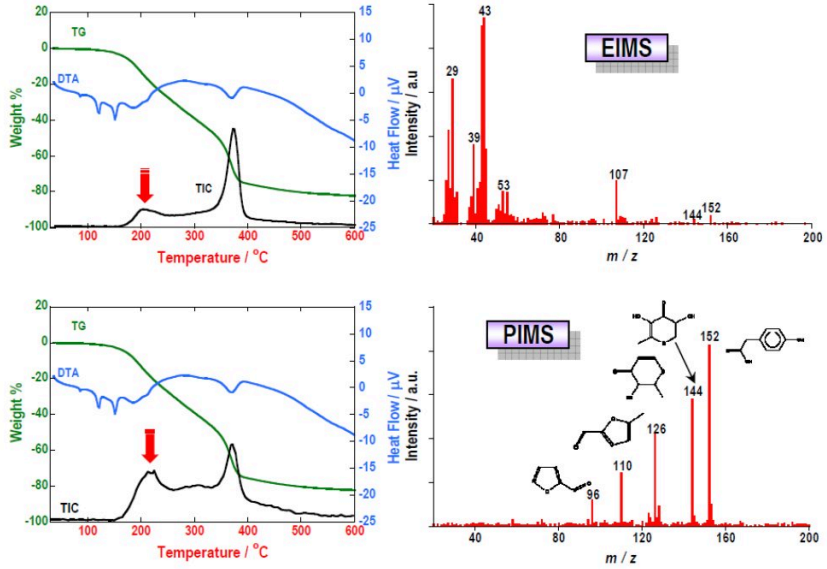
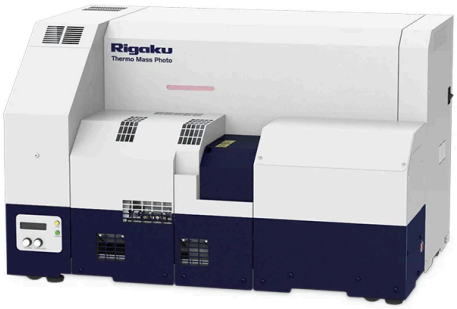


Figure 1: Comparison of TG-DTA-EI/PIMS curves and mass spectra for OTC drug
Top: TG-DTA-EIMA and EI mass spectrum; Bottom: TG-DTA-PIMS and PI mass spectrum

Related products



ThermoMass Photo

An integrated thermal analysis instrument capable of high-precision mass analysis of evolved gases without breaking the molecules, allowing direct measurement.