Application Note TA6004

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TA6004 - Analysis of mixture gases for production of volatile organic compounds

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 programed 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.

Simultaneous measurement of thermogravimetry and differential thermal analysis equipped with skimmer-type interface system and photoionization method, ThermoMassPhoto, can be measured the unchanged molecular ion state which never broken the detected gas molecule. Thus, it is possible to discriminate in real time the evolved mixture organic gas's components without gas separation module. We evaluated the mixture of solvents and polymethylmethacrylate using electron ionization-MS (EIMS) and photoionization-MS (PIMS), in terms of its ability to produce fragment-free species during the ionization process.

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

Evolved gases mass spectra of a mixture of solvents (benzene, toluene and xylene) obtained in photoionization (PI) and electron-impac (EI) ionization modes are shown in Figure 1. In EI mode, the molecular ion component and the fragment ion are laid on top of each other and consisted complicated spectrum. On the other hand in PI mode, each molecular ion is

selectively ionized; for example, m/z=78 (benzene), m/z=92 (toluene) and m/z=106 (xylene). Thus, using PI mode, it is possible to measure and discriminate in real time only for the molecular ion in the multiple-evolved organic gases.

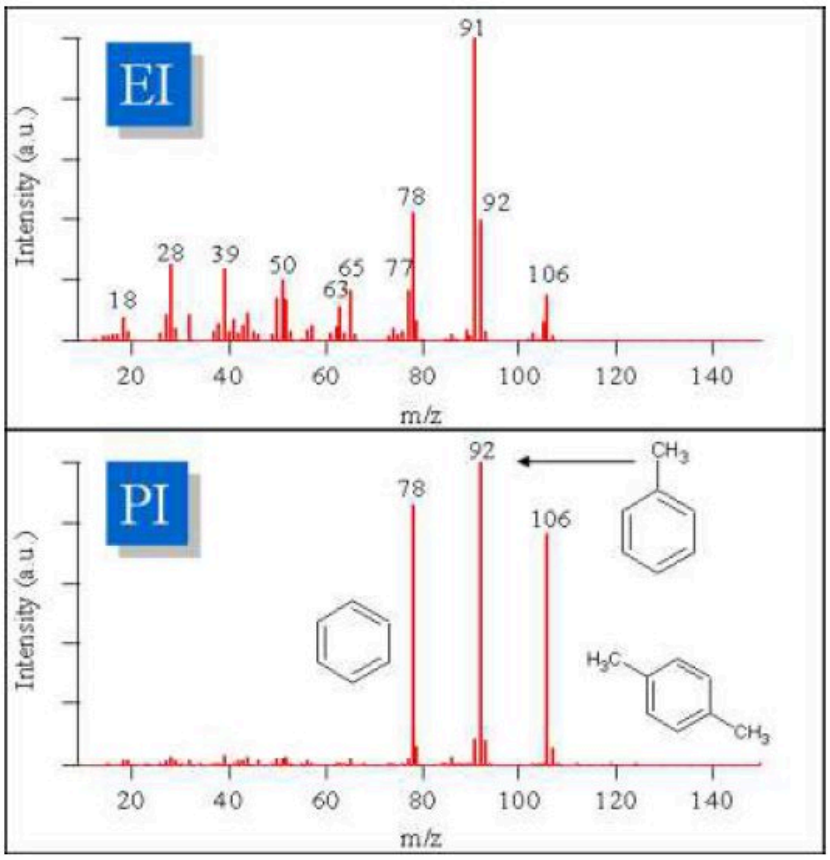

Figure 1: Analysis of a mixture of gases

In an example of the thermal decomposition of polymer, multiple organic gases evolve simultaneously by heating. Mass spectra of polymethylmethacrylate (PMMA) due to thermal decomposition, obtained by PI and EI at heating rate 20℃/min are shown in Figure 2.

Both ionization modes are observed total ion current curve shows same behavior, however, the mass spectra are remarkably different.

In EI mode, although the MMA molecular ion can be observed at m/z 100 and fragment ions are observed at m/z 69, 41, 39 and 15 respectively and the mass spectra become complex (see Figure 2(a)). On the other hand, in PI mode, only the molecular ion can be observed at m/z 100 due to soft ionization,. From these results, it is easy to understand that the thermal decomposition of PMMA progresses due to depolymerization so the decomposition product only consists of MMA (see Figure 2(b))

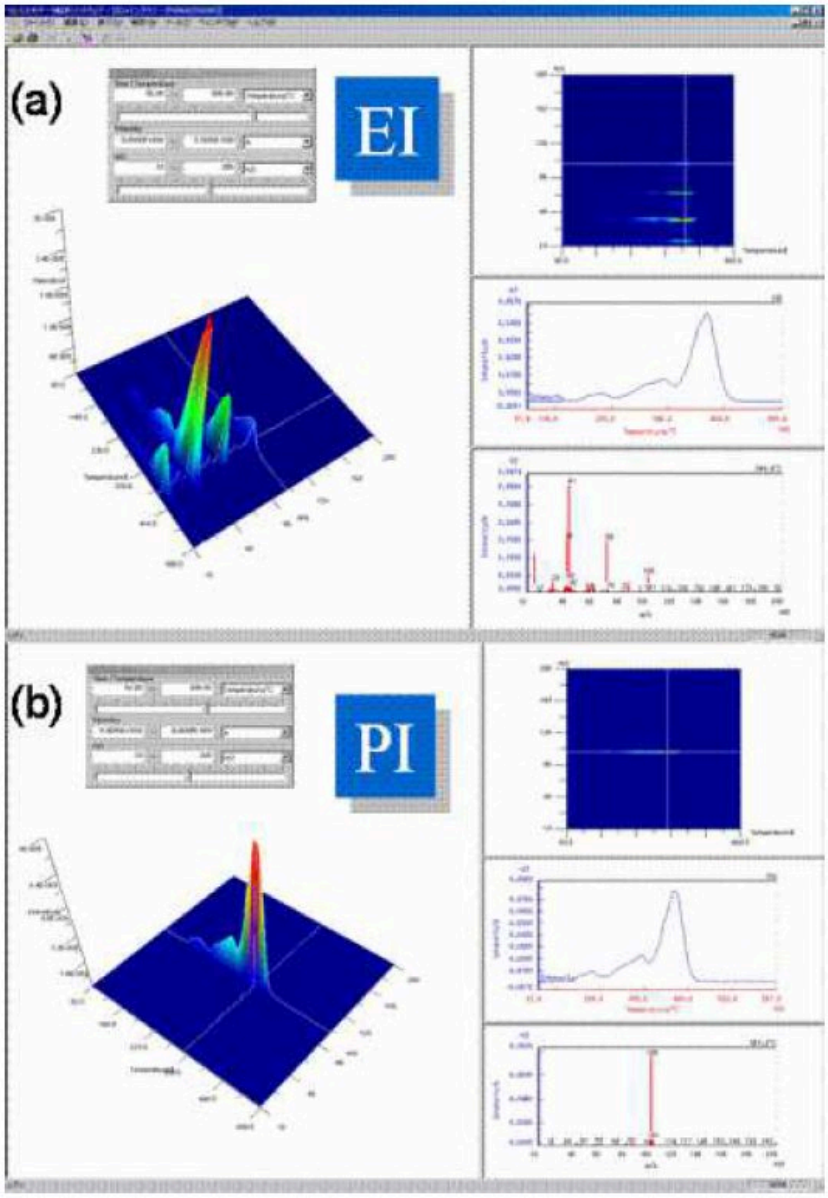

Figure 2: Thermal decomposition of PMMA

Related products

ThermoMass Photo

An integrated thermal analysis instrument capable of high-p
recision mass analysis of evolved gases without breaking t
he molecules, allowing direct measurement.