Application Note TA6002

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TA6002 - Evolved gas analysis for 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 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 evaluated the volatile organic compounds employed electron ionization-MS (EIMS) and photoionization-MS (PIMS) in terms of is ability to produce fragment-free species during the ionization process. The findings herein suggest that unique PI mass spectra obtained in real time by EGA-PIMS can be satisfactorily used to characterize the decomposition products, based on only the parent ions with no contribution as a result of fragmentation during the ionization.

Instrument: ThemoMass 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

This measurement can measure and discriminate the simultaneous evolved gases of volatile organic compounds in real time.

Using photo ionization mass analysis method (PIMS), it is possible to perform the mass analysis detecting as molecular ion state directly without gas molecule break (see Figure 1).

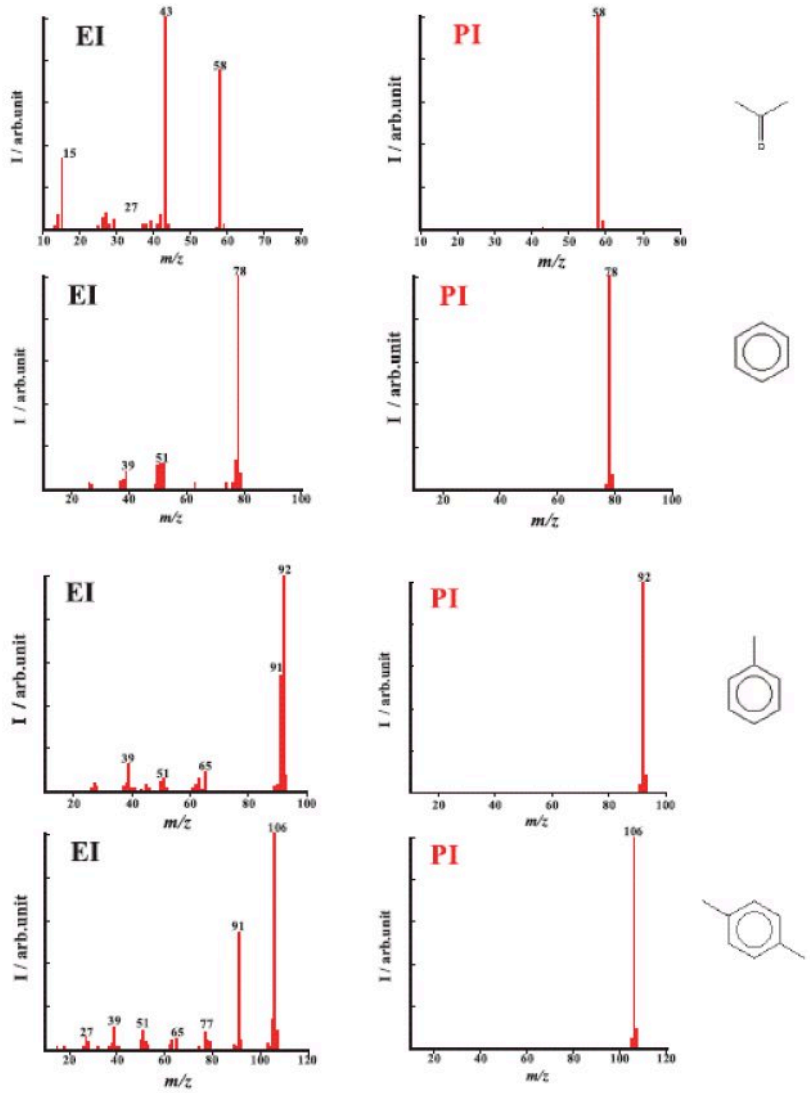

Figure 1: EI and PI mass spectra of several volatile organic compounds.

On the other hand, electron impact ionization method (EI), it causes the complex mass spectra overlapping between molecular ions and fragment ions. Thus, PI method which only generated molecular peak ion can be obtained as the simple mass spectra, it is available to discriminate the gases in real time even when multi-component gases are generated simultaneously (see Figure 2).

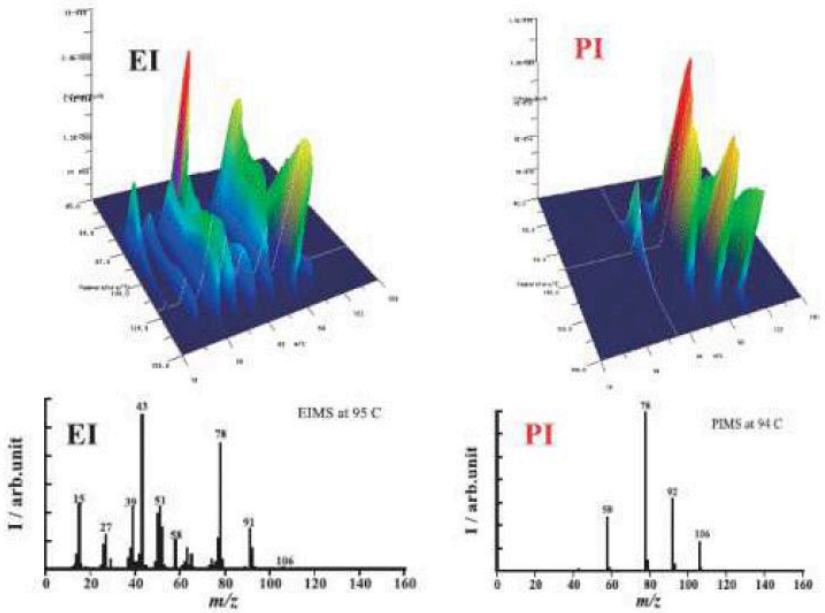

Figure 2: EI and PI mass spectra of volatile organic compounds, total figure of 3D images for above and at around 95℃ for below

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.