



TG-PIMS

THERMOGRAVIMETRY - PHOTOIONIZATION MASS SPECTROMETRY

Decomposition of polymers Characterization of crude oil Characterization of tobacco and coffee

TG-PINS THERMOGRAVIMETRY - PHOTOIONIZATION MASS SPECTROMETRY

Investigation of chemicals released during thermal analysis

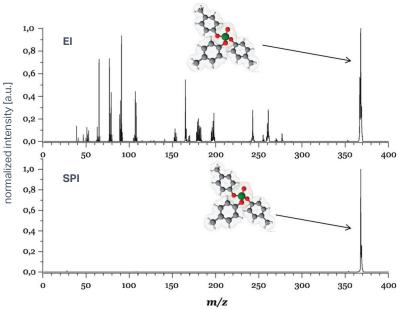
One of the most powerful methods to analyze the gaseous products evolving from thermal analysis is mass spectrometry using electron ionization (EI). As the kinetic energies of the electrons ($E_{kin} = 70 \text{ eV}$) thereby are typically far above the ionization energies of the released molecules, particularly organic compounds are heavily fragmented.

The correlation of the ion signals to the gaseous compounds, especially for complex mixtures, is very difficult or even impossible.

Soft ionization methods, specially the ionization with VUV light can reduce or even circumvent the fragmentation. Photonion uses single-photon ionization (SPI), based on an innovative vacuum ultraviolet light source. The advantage of this ionization method is that substances can be measured directly in complex mixtures.

Time-consuming separation techniques combined with MS (e.g. GC) are not needed. That is why MS containing soft ionization is ideally suited for process monitoring and quality control.

VUV [vacuum ultra violet]



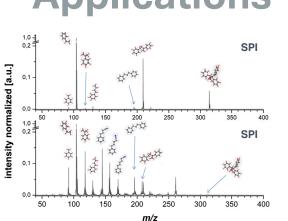
Ionization of tricresyl phosphate (TCP) with standard ionization EI (top) and soft ionization SPI (bottom)

Specifications

mass range	10-600 Th
mass resolving power	900 Th/Th FWHM *
mass accuracy	100 mTh
extraction rate	up to 80 kHz
spectra rate	10 Hz
ionization	EI, SPI, EI/SPI
Quad Filter	low cut-off
dynamic range	10 ⁶
gas flow into ion source	1 std ml/min = 1 sccm
matrix gas	He, N2, Ar also air or O2
ion rate	1000 ions/extraction
different VUV sources	for different energies

* mass resolving power of 900 Th/Th at 500 Th with dynamic range 100





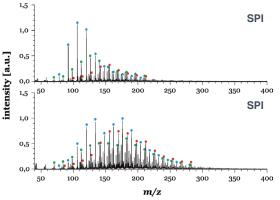
Applications



DECOMPOSITION OF POLYMERES

Polystyrene (PS): The SPI mass spectrum shows that in addition to the dominating styrene monomer peak at 104 m/z, also the styrene dimer (208 m/z) and styrene trimer (312 m/z) are formed. Due to the resonance stabilization of the styrene monomer the alkane backbone of the PS polymer readily is breaking after every second chain carbon, forming predominately styrene (C2-phenyl unit). However, the occurrence of toluene (C1-phenyl unit), phenyl propene (C3-phenyl unit) and phenyl butadiene (C4-phenyl unit) shows that other chain braking positions are possible, although less probable.

Acronitrile-Butadiene-Styrene (ABS): The most dominant species in the evolved gas phase SPI mass spectrum is styrene (104 m/z) surrounded by the C1 and C3-benzene products from the polymer chain degradation (toluene and propenyl benzene). At 157 m/z the condensation product of acrylonitrile and styrene is visible and at 208 m/z the styrene dimer can be seen in the SPI mass spectrum.



The result of the thermogravimetrical analysis of light Californian oil (top) and a heavy crude oil sample from Turkey (bottom) are presented here.

CHARACTERIZATION OF CRUDE OIL

Crude oils are often characterized according to their physical properties such as density, viscosity, color, and odor. Furthermore, they may be distinguished by determining their chemical composition on a molecular level, which is challenging due to the enormous number of components present in the oils. In the displayed mass spectra alkanes (linear and branched), cycloalkanes and substituted benzenes occur in long homologous series and are assigned by the different colored dots red, green and blue, respectively. The SPI mass spectra from thermal analysis of different crude oils clearly show the advantageofsoftphotoionizationforthecharacterization of the evolving gases. Since fragmentation does not occur, each hydrocarbon may be identified according to its molecular peak. Different crude oils can be easily identified and characterized based on their distinct molecular patterns of the released compounds.

Features + Design

The thermogravimetry SPI-MS setup consists of a thermobalance which is coupled to an oaTOF mass spectrometer. The coupling is carried out via a heated capillary, which transfers the gas molecules evolving in the thermobalance into the ion source. There, the molecules are ionized either by VUV photons or by 70eV-electrons in case of conventional El.



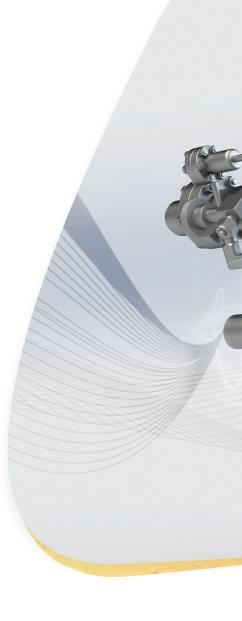




Applications

Thermal analysis and characterization of evolving gases by soft ionization mass spectrometry







PHOTONION GmbH Hagenower Str. 73 19061 Schwerin Deutschland / Germany

 T
 (+49 385) 3993 288

 F
 (+49 385) 3993 281

 E
 info@photonion.de

 W
 www.photonion.de