JEOL

Scientific / Metrology Instruments
JEOL Mass Spectrometer Material analysis solution

Solutions for Innovation

JEOL Mass Spectrometer

Material analysis solutions

JEOL Ltd.

JEOL offers solutions
for your material analysis and applications

Our complete line of mass spectrometer systems and our expertise
and years of experience help you solve the problems in analyzing functional polymer samples!

Raw mat
examinatio

- Supplier sele
- Acceptance/

High sensitivity combined with high stability for simple, easy qualitative/ quantitative analysis

JMS-Q1500GC

Gas chromatography
quadrupole mass spectrometer
GC-QMS

Various ionization techniques and exact mass analysis for unknown material identification

JMS-T200GC

Gas chromatography
time-of-flight mass spectrometer
GC-TOFMS

Simple yet robust
all-round analysis

JMS-T100LP

Liquid chromatography
time-of-flight mass spec
LC-TOFMS

Research and development

- Prototype testing
- Foreign object investigation
- Product examination

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inspection

JEOL Solutions

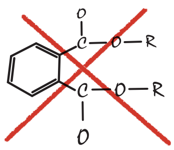
Quality control

- Product complaints
- Problems with production process steps
- Final product evaluation

Compliance

- WEEE/RoHS
- REACH
- European Directive 2005/84/EC

RoHS



design for

trometer

Direct analysis of samples in various forms without preliminary treatment

DART Ion Source

Ambient ionization
time-of-flight mass spectrometer
DART-TOFMS

High resolution observation of low to high molecular-weight ions

JMS-S3000

Matrix assisted laser desorption/ionization
time-of-flight mass spectrometer
MALDI-TOFMS

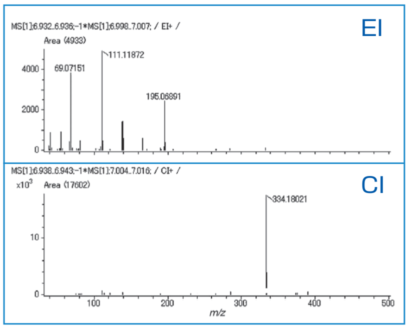
Research and development

Prototype testing

GC-TOFMS estimates the composition and structure of known and unknown materials.

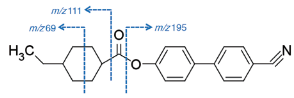
New materials used in prototypes often consist of compounds with unknown compositions and structures. Library searches by EI, which are designed for known materials, often fail to identify such compounds.
The JEOL GC-TOFMS, capable of 3 soft ionization techniques (FI, PI, and CI) and exact mass analysis, is ideal for the analysis of these prototype materials.

In this example, an unknown component in a liquid crystal mixture sample was analyzed.
A library search by EI failed to identify the component, as it was not present in the library. The GC-TOFMS, on the other hand, could identify the composition as well as the structure by utilizing molecular formula determination with CI and exact mass analysis of the EI fragment ions.
The GC-TOFMS makes it possible to determine the composition and structure of known and unknown materials.



EI and CI mass spectra of an unknown component in a liquid crystal mixture sample

Mode	Obs. *m/z*	Error (mDa)	Formula
EI+	69.0715	1.1	C_5H_9
	111.1187	1.3	C_8H_{15}
	195.0689	1.4	$C_{13}H_9NO$
	333.1743	1.4	$C_{22}H_{23}NO_2$
CI+	334.1802	-0.5	$C_{22}H_{24}NO_2$



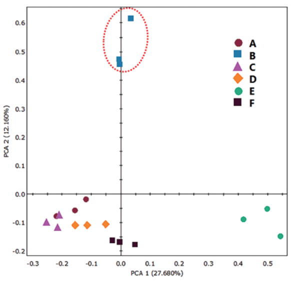
Exact mass analysis results and estimated formula for an unknown component

Product examination

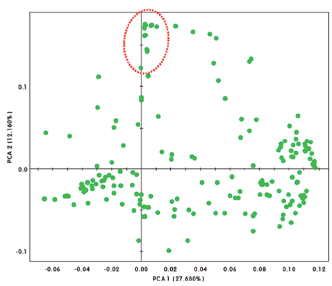
GC-MS analysis combined with multiple classification analysis enables speedy identification of characteristic components.

While industrial polymer materials contain numerous compounds, those which "differentiate" the materials are limited. Multiple classification analysis, designed to survey multiple sets of data at a time, is effective in searching for such compounds.

In this example, 6 different vinyl acetate resins were analyzed by pyrolysis GC-EI-TOFMS.
PCA analysis of the data acquired separated the materials and extracted the characteristic compounds.
GC-MS analysis combined with multiple classification analysis enables speedy identification of characteristic components.



PCA score plot of 6 vinyl acetate resins



PCA loading plot of 6 vinyl acetate resins

Applications

MSTips 040: The power of exact mass measurement: an example of unknown compound identification
MSTips 108: Analysis of photo polymerization initiator in UV light curing adhesives by GC/TOFMS
MSTips 220: Analysis of cyanoacrylate adhesive using the JMS-S3000 "SpiralTOF™"
— Application of Kendrick Mass Defect plot analysis —

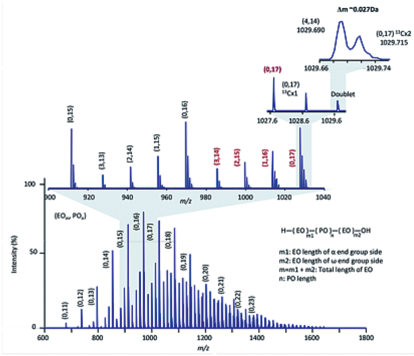
Raw material examination

Base material identification

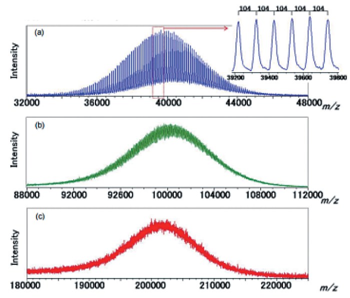
MALDI-TOFMS enables precise structural analysis of synthetic polymers in polymer materials.

Physical properties of any polymer material change according to the structure of the oligomers, as well as the terminal groups, degree of polymerization, and molecular weight distribution. Analysis of the terminal group composition and degree of polymerization requires the direct observation of molecules.
MALDI-TOFMS, capable of observing low to high molecular weight samples with high resolution measurements, is ideal for this type of analysis.

In this example, a surfactant was analyzed.
The data shows 2 repeat structures, EO and PO, as well as their end structures and molecular weight distributions.
MALDI-TOFMS enables precise structural analysis of synthetic polymers in polymer materials.



MALDI mass spectrum of a surfactant



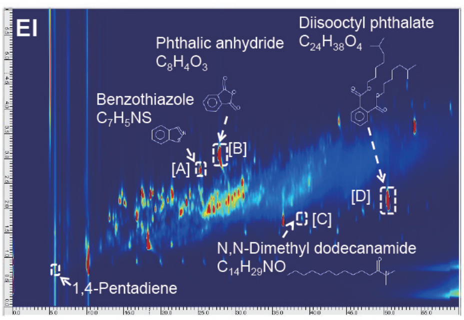
MALDI mass spectrum of a high molecular weight polymer

Additives

Py-GC-MS analysis rapidly identifies additives in materials.

Today, a wide variety of additives are developed, produced, and distributed to provide polymers with new functions. Since these functions vary depending on the type and amount of additives in the polymer materials, it is critical to identify additives during material examination and quality control.
While pyrolysis (Py)-GC-MS is designed for direct analysis of materials which makes it effective in studying additives in polymers, this technique analyzes additives simultaneously with pyrolysates of matrix macromolecules. As a result, it can be difficult to identify all of these compounds by conventional one-dimensional chromatography. Comprehensive 2D GC (GCxGC) is effective for analyzing complex mixtures of components.

In this example, a commercial “X-ring” made of nitrile rubber (NBR) was analyzed.
The high resolution GCxGC measurement separated 4 additives from the numerous pyrolysate background components.
Py-GC-MS analysis combined with GCxGC makes it easier to identify additives.



Py-GCxGC-EI TIC chromatogram of nitrile rubber

Applications

MALDI for Polymer Analysis: Synthetic Polymers and Additives
MSTips 138: Analysis of additives in plastic by thermal desorption (TD) GC-TOFMS: accurate mass measurement and isotope pattern matching
MSTips 111: Analysis of block copolymer by field desorption (FD) using JMS-T100GC “AccuTOF GC”

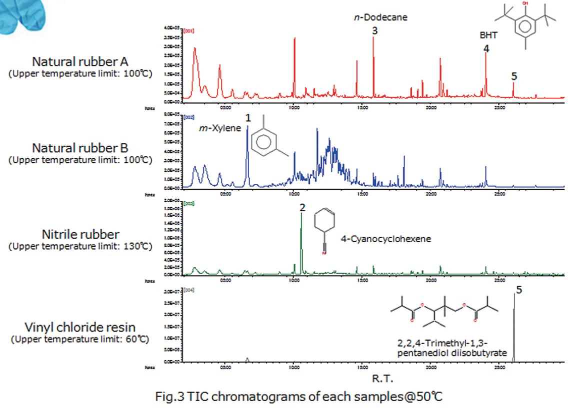
Quality control

Failure analysis

A variety of sampling techniques for GC-MS are effective in investigating product failures.

Quality control to investigate odor, foreign objects, and defects in products requires a number of analytical techniques since samples come in different types and forms.
GC-MS, a general purpose analytical system, supports multiple and diverse types of analysis and applications by combining different preliminary treatment devices.

In this example, gases produced from industrial rubber gloves were analyzed by HS-GC-MS using a head space (HS) technique for preliminary treatment. Four different gloves (two natural rubbers, a nitrile rubber, and a vinyl chloride resin) were heated at 50 °C, and the components of the resulting gases were compared. Each had a different profile with characteristic compounds detected from each glove sample.
A variety of preliminary sampling devices like HS are available for GC-MS, thus allowing the effective investigation of product failures.



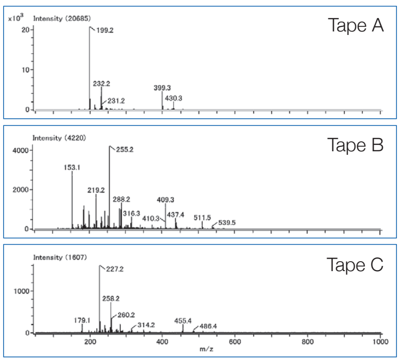
HS-GC-EI TIC chromatograms of 4 rubber gloves

Surface deposit analysis

DART directly analyzes samples without preliminary treatment, and is effective in analyzing surface deposits and surface contamination.

DART (Direct Analysis in Real Time) is an ambient ionization technique capable of direct analysis of samples in different states such as gas, liquid, and solid.

In this example, cassette tapes were analyzed by DART to examine the surface deposits.
Base peaks were detected at *m/z* 199 for Tape A, *m/z* 255 for Tape B, and *m/z* 227 for Tape C. When these ions were subjected to exact mass analysis, the results suggested that these components were fatty acid used as a lubricant.



DART mass spectra of cassette tapes

Cassette tape being analyzed in DART

Applications

Direct analysis of stains on cloth caused by cosmetic
MSTips 043: Analysis of Impurities in Ethylene glycols with JMS-T100GC AccuTOF GC

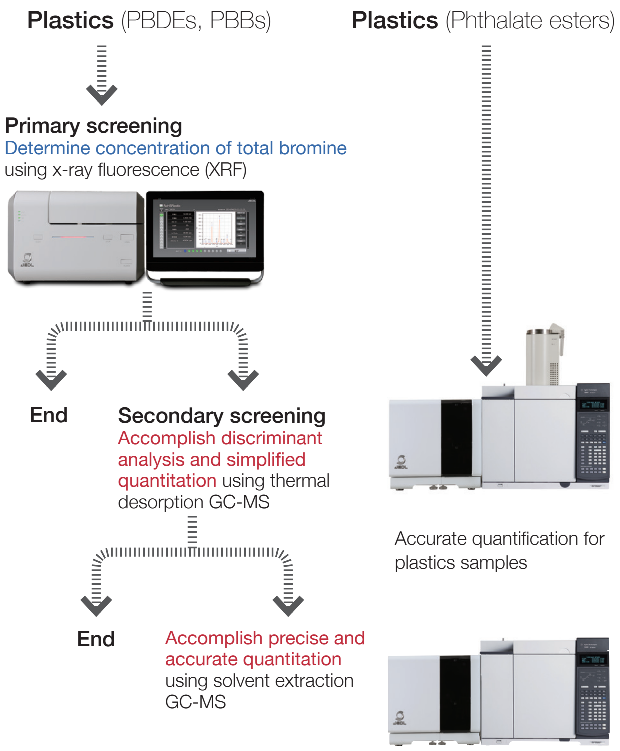
RoHS

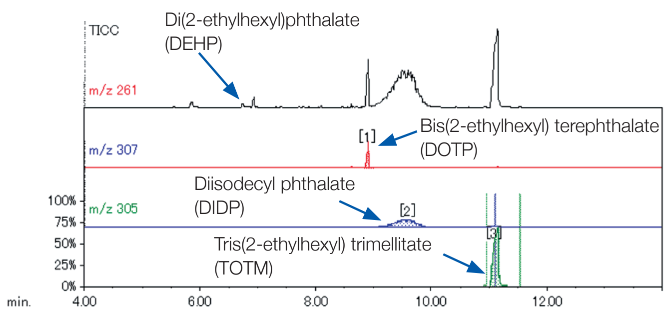
GC-MS is capable of speedy qualitative/quantitative analysis of substances on the RoHS list.

The polybrominated diphenyl ethers (PBDEs) and polybrominated biphenyls (PBBs) currently used as polymer flame retardants are suspected of being endocrine disrupters. The European Union specifically regulates the use of PBDEs and PBBs.

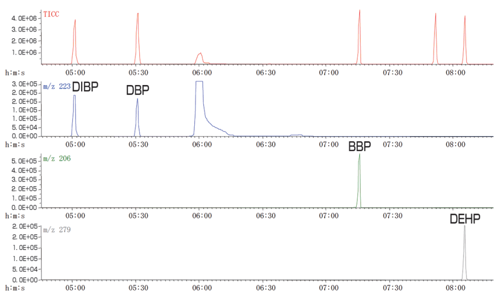
PBDEs and PBBs are bromine containing organic compounds that can be subjected to X-ray fluorescence (XRF) for primary screening to determine the concentration of total bromine. For resins and other materials found to have high concentrations during the primary screening, secondary screening with thermal extraction GC-MS and precision quantitative analysis with solvent extraction GC-MS are effective. Shown on the left is a flow chart for the analysis of PBDEs and PBBs. A single GC-MS can be used for both secondary screening and precision quantitative analysis.
In 2014, the RoHS directive was amended to include an additional 4 phthalate esters. Unlike PBDEs and PBBs, phthalate esters are organic compounds made up of C, H, and O so they cannot be subjected to primary screening with XRF. However, GC-MS is capable of analyzing phthalate esters, using the same techniques of simplified quantitative analysis and precise quantitative analysis that were used for PBDEs and PBBs.

The data shown here were acquired by thermal extraction GC-MS of a sample that contained the alternative materials DOTP, DIDP, and TOTM as plasticizers. Additionally, this sample was suspected to contain 4 additional phthalate ester impurities (DIBP, DBP, BBP, DEHP), which are on the amended RoHS list.
This technique facilitates sampling with speedy qualitative/quantitative analysis at a rate of 30 minutes per sample.

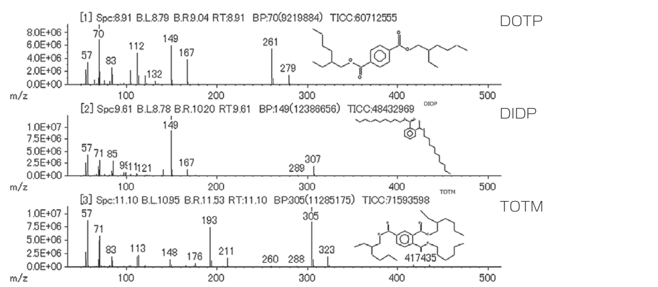




Extracted ion chromatograms of a resin additive
(*m/z* 261: DOTP, *m/z* 307: DIDP, *m/z* 305: TOTM)



Chromatograms of 4 phthalate esters added to amended RoHS



Mass spectra and library search results of alternate materials (DODP, DIDP, TOTM)

*Appearance or specifications subject to change without notice.

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