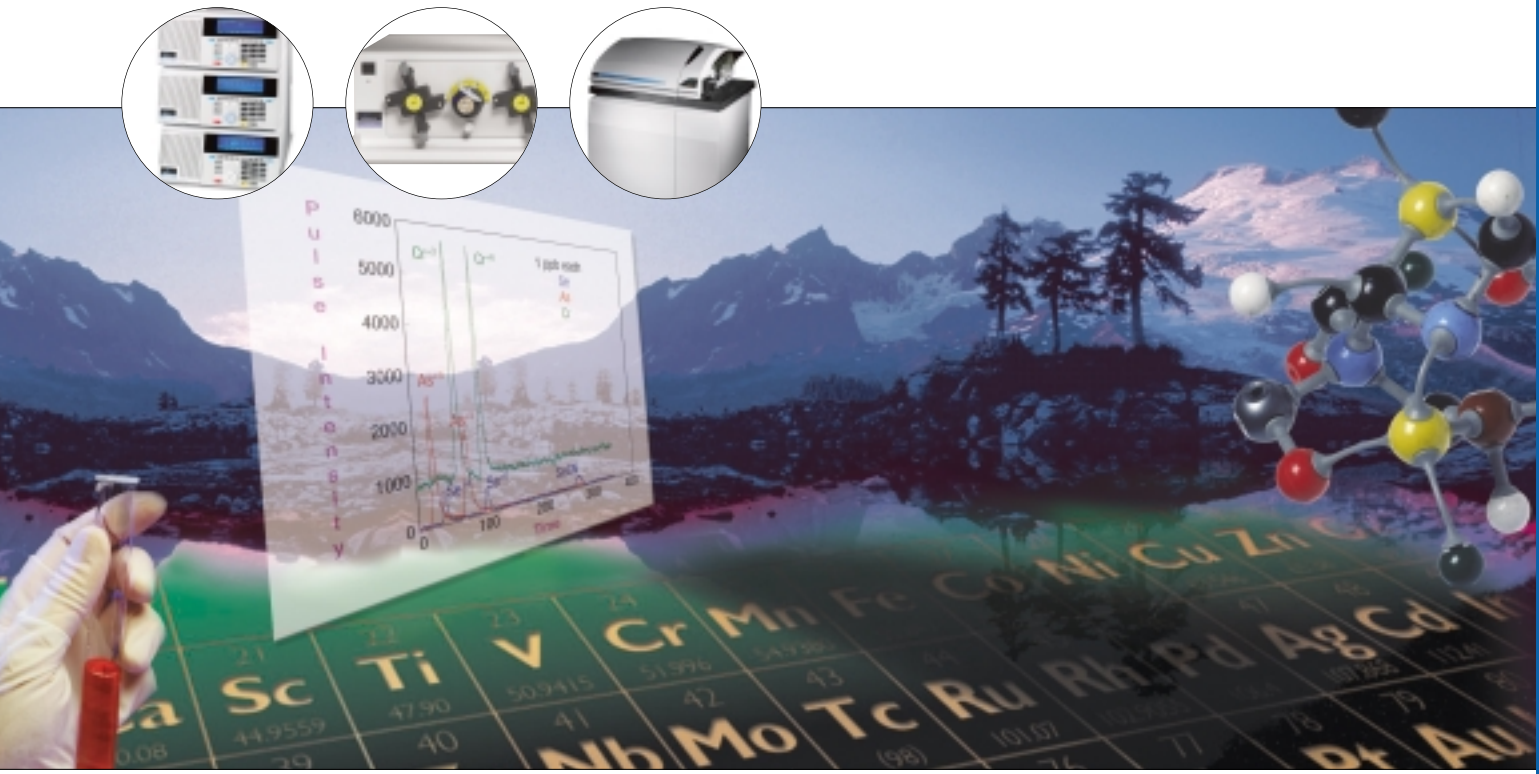
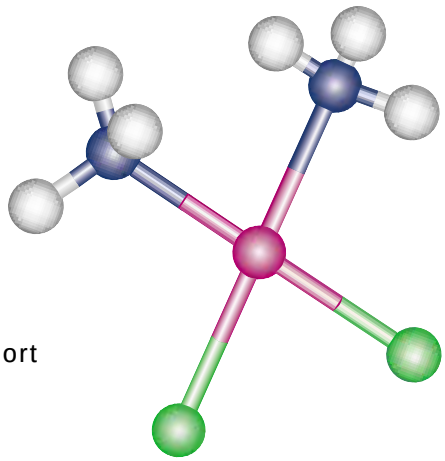
inorganic speciation solutions



working **together** for **results**

PerkinElmer®
precisely.

solving your speciation needs



➤ Options ➤ Technology ➤ Data handling ➤ Support

Options to meet regulatory needs now and in the future, a variety of instrument hardware choices for separation and detection, software to view and process the results – PerkinElmer® can provide this and the support you need to get started rapidly and stay productive. Join many of the world's leading speciation researchers in using our knowledge, products and comprehensive support. Together, we can solve your speciation needs.

Speciation:

1. *Chemical species*. Chemical elements: specific form of an element defined as to isotopic composition, electronic or oxidation state, and/or complex or molecular structure
2. *Speciation analysis*. Analytical chemistry: analytical activities of identifying and/or measuring the quantities of one or more individual chemical species in a sample
3. *Speciation of an element; speciation*. Distribution of an element amongst defined chemical species in a system

Pure Appl. Chem., Vol. 72, No. 8, pp. 1453–1470, 2000.

Why perform speciated analyses?

Regulations generally drive environmental measurements, but speciation is also becoming more important in medical research, clinical analysis and drug discovery. One basic reason to consider performing speciated analyses is to obtain additional information that will aid in determining a compound's toxicity, bioavailability or mobility in a system of interest. Table 1 shows selected current regulations, indicating that government agencies are now beginning to consider these analyses feasible on a routine basis. As life science begins to study proteins, speciation techniques will provide integral clues to understanding metalloproteins and their actions in a given biological system.

What methods are available for speciation?

Methods have been in development for more than 20 years, but have only recently been included in publications by environmental agencies. The U.S. Environmental Protection Agency (EPA) has published Method 321.8 describing the speciation of bromine compounds in drinking water and wastewater, using ion chromatographic separation and ICP-MS detection. The U.S. EPA solid waste Method 6800 has been published for the measurement of a variety of metals in water and waste using a speciated isotope dilution procedure. Method 1632 uses hydride-generation quartz-furnace atomic absorption to measure arsenic species in water and tissue. Several draft methods are also under consideration to measure tin, chromium and mercury species. The development of methods by regulatory agencies in the U.S. and other countries indicates the technology is beginning to mature and more routine laboratories may begin to adopt it.

Table 1. Selected Regulations.

Country	Elements
International	Methyl mercury Tributyl tin compounds
Japan	Cr (VI) in water Hg, Methyl mercury
Germany	Cr (VI) in water Methyl mercury Organo tin compounds Tetraethyl and tetramethyl lead
United States	Cr (VI) Se (IV) and Se (VI) Tributyltin (TBT) Hg, Methyl mercury As (III), As (V), MMAs, DMAs

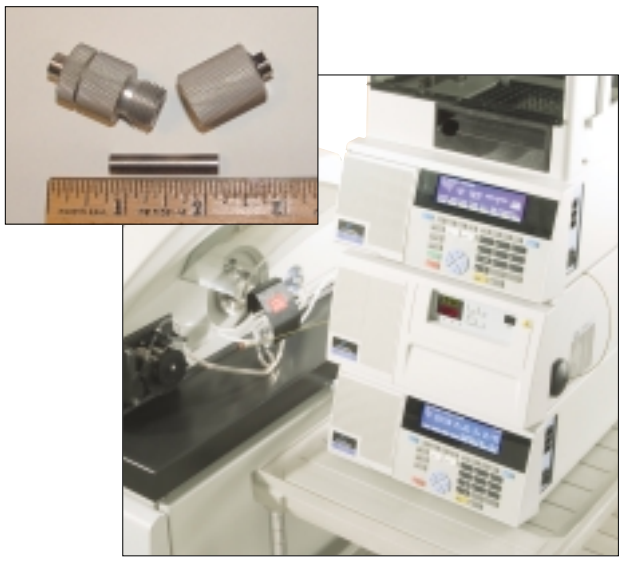
choosing the best instrumentation for your lab

Many types of instrumentation have been coupled together to achieve the separation and detection steps required for speciated analysis. Speciated analyses generally require lower detection limits than total analyses because the measurement is divided amongst the various species. Species that can be made volatile can be measured with hydride analysis, either with or without some type of pre-concentration. The types of instrumentation that can help with sample preparation, separation and detection of speciated compounds will be discussed.

Sample preparation

Sample preservation and preparation remain the most difficult steps of a speciated analysis. Sample preparation can range from keeping a sample cold and performing the analysis within 24 hours for water samples to a mild extraction for soil samples. The challenge is to separate the species of interest from the matrix, while preserving them in the organic form or oxidation state in which they were originally found. If the separation of the various species is done through the sample-preparation step, rather than by using an instrumental separation, the extraction can become quite complex.

The Multiwave™ microwave digestion system can help in both digestion and extraction by providing a very controlled sample preparation procedure. The procedure can be reproduced very precisely from sample to sample to provide more comparable results.



PerkinElmer HPLC/ICP-MS system. A small column developed for fast HPLC separations is shown.

Speciation helps define the form of tin that may contaminate marine waters.

species separation techniques

The separation and determination of each individual species can be accomplished by wet chemical methods or with instrumentation, such as high performance liquid chromatography (HPLC), gas chromatography (GC) or flow injection (FI).

Wet chemical methods

Wet chemical methods are usually labor-intensive and can be less reproducible than an instrumental method. As speciation becomes more routinely required, automated methods bring productivity and greater control to the separation process.

HPLC

High performance liquid chromatography, including ion chromatography (IC), is an excellent choice for separating most species of interest. As reflected in the literature, HPLC is one of the most popular instrumental methods for this task because of its wide range of separation capabilities. HPLC has the ability to separate non-volatile species, which comprise the majority of species of interest, as well as volatile. Once the compounds are separated, the output of the HPLC is easily coupled to a variety of detection techniques. The combination of HPLC with ICP-MS provides a rugged and sensitive system and has become one of the most capable and widely used systems today for speciation analysis.

The PerkinElmer Series 200 HPLC pump, autosampler, column oven and vacuum degasser provide a powerful system for separation. Reversed-phase or ion-exchange columns are typically used. The system can easily be connected and disconnected from the detection system, such as ICP-MS, to provide the most laboratory flexibility. For ICP-MS, we also provide quick connection kits that will give you all the parts you need to connect your ELAN® ICP-MS system to the Series 200 HPLC system.

GC

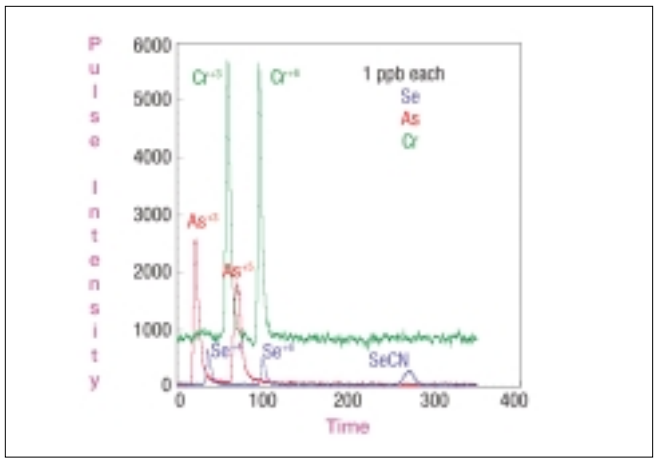
Gas chromatography can also be used to achieve separation, provided the compounds of interest are either volatile or semivolatile compounds. However, in general, it does not apply to the majority of compounds of interest, since they are non-volatile. In some limited cases, derivatization can be used to convert a non-volatile compound to a volatile one, enabling gas chromatography to be used. Unfortunately, this adds additional sample-preparation steps and may result in species interconversion if extreme care is not taken. For researchers that require gas chromatographic separation, the Clarus® GC offers robustness with sophisticated features such as Pneumatic Pressure Control (PPC) and large volume injection.

Flow injection

Flow injection can be used for simple separation procedures. PerkinElmer is the leading supplier of inorganic flow-injection systems and has provided systems for this purpose for many years. The flow-injection atomic spectroscopy (FIAS) models provide a variety of features to automate flow procedures. Flow injection is best suited for binary separations or when other components can be calculated by difference measurements.

Data handling

The selected separation system can be coupled with either dedicated speciation software or TotalChrom® chromatography data handling for complete data handling and reporting of the acquired chromatograms and results.



Simultaneous separation and detection of three elements and their species in water using HPLC/ICP-MS.

species detection technologies

Atomic absorption

Atomic absorption (AA) is an easy-to-use, inexpensive technology. Either flame atomic absorption spectroscopy (FAAS) or graphite furnace atomic absorption (GFAA) can be used to measure an element after chemical separation of the species has been completed. It can sensitively detect volatile elements at very low concentrations when set up with a quartz cell for hydride generation. Flow-injection hydride generation can also be coupled with graphite furnace to directly adsorb the metallic element on the inside of the graphite tube before atomization. Although graphite furnace AA is a very sensitive technology, it is not continuous and therefore is not well matched to the continuous mode of most separation techniques. However, it is often used after wet chemical separation.

The AAnalyst™ series of atomic absorption instruments is well suited for this type of measurement. They can be coupled with the flow-injection system for automated hydride or hydride/furnace measurement. Flow injection can also be used for simple separations using adsorbent cartridges.

ICP-MS

Inductively coupled plasma mass spectrometry (ICP-MS) provides the ultimate in sensitive, interference-free measurements for speciation. The ELAN series of ICP-MS instruments provides excellent detection limits, especially with patented Dynamic Reaction Cell™ (DRC™) technology to preserve detection limits in complex samples. In addition, since ICP-MS is a multielement technology, the species of several elements can be examined simultaneously in a speciated sample using this detection method.

ICP-MS has been coupled with a variety of separation techniques, including high performance liquid chromatography, capillary zone electrophoresis (CZE) and gas chromatography to perform speciated analyses. ICP-MS is especially compatible with HPLC, providing rapid connection and disconnection to the instrument for flexibility. In fact, since HPLC/ICP-MS is such a popular speciation technique, we made it even easier by developing quick-connect kits that contain everything you need to connect your HPLC (or ion chromatography) system to the ELAN ICP-MS, including the relevant sample introduction system compatible with your separation system's flow rates.

ICP-OES

Inductively coupled plasma optical emission spectroscopy (ICP-OES) is a fast, multielement technology also suitable for speciation detection. The Optima™ series of spectrometers can be used off- or on-line for sensitive and rapid detection of one or several elements. Our latest version of WinLab32™ software for ICP-OES also includes the ability to perform time-resolved data acquisition, enabling speciation analysis by this popular multielement technology. Integrated FIAS control also provides the ability to combine separation by flow injection with ICP-OES detection.

AAnalyst 400 atomic absorption spectrometer

complementary technologies

MALDI-TOF

As speciation analysis becomes more popular in the life sciences, complementary techniques such as Electrospray (ES) and matrix assisted laser desorption ionization (MALDI) mass spectrometry (MS) will increasingly supplement inorganic information with structural information. Metallobiomolecules, specifically metalloproteins, are a growing area of speciation research. The PerkinElmer prOTOF™ MALDI O-TOF is a mass spectrometer with unique capabilities. Ion focusing and fragmentation are better controlled utilizing collisional cooling. The prOTOF also provides the advantages of orthogonal extraction, which decouples the time of flight (TOF) analysis from the ionization process, minimizing or eliminating the typical error sources related to axial MALDI MS analysis. The prOTOF offers enhanced mass accuracy and stability which is critical to developing fields of research in biomarker discovery, as well as peptide mass fingerprinting for protein identification.

LIMS

Many labs are moving to laboratory information management systems (LIMS) to manage the data from several techniques and to handle some of the business systems. Connecting PerkinElmer instruments to an existing or new LIMS system is straightforward and can be easily accomplished. For a full system, PerkinElmer offers the scalable LABWORKS™ LIMS system that evolves when your needs change. The unique ability to build the database and learn the system in a virtual environment before installation makes the transition seamless.

prOTOF MALDI O-TOF

Worldwide support

With over 60 years of experience and as a world leader in analytical instrumentation, PerkinElmer is the right partner for your industry. In concert with global distribution of instruments, turnkey systems, and consumables, we provide global factory-trained service and support.

PerkinElmer's OneSource℠ Laboratory Services provides you with a comprehensive worldwide service offering that lets you take care of business and set your sights on what matters most – results. With over 1000 factory-trained professionals serving more than 125 countries worldwide, PerkinElmer is your single source for instrument care and repair, validation services, software and hardware upgrades, education and more.

Join many of the world's leading speciation researchers in using our knowledge, products and comprehensive support. Together, we can solve your speciation needs.

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