Isotope ratio measurements: new developments and applications

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After 2004 and 2008 (Vols. 378/2 and 390/2) this is the third issue of *Analytical and Bioanalytical Chemistry* to contain papers on new developments and applications in isotope ratio measurements. Whereas Klaus Heumann was guest editor for the two previous special issues, in this issue Torsten Schmidt joins him as guest editor for the first time. His involvement with this collection of papers strongly reflects the increasing importance of compound-specific stable isotope analysis, one of his core research areas, on which, with Maik Jochmann, he has recently published a monograph “Compound-specific Stable Isotope Analysis” (see corresponding book review in this issue). A total of 24 manuscripts describing new instrumentation, methodological questions, for example normalization and the use of certified isotope reference materials, isotope-labeling experiments, determination of natural isotope signatures, applications in archeology and in clinical and nuclear chemistry, and isotope dilution analysis demonstrate the broad range of modern precise and accurate isotope ratio measurements. This great variety of applications also clearly shows that increasing attention is being focused on isotope ratio determinations in modern analytical chemistry. A recently published textbook “Isotopic Analysis” by Frank Vanhaecke and Patrick Degryse, which is also reviewed in this issue, confirms this trend. Another interesting trend compared with the earlier collections of papers on this topic is that thermal

ionization mass spectrometry (TIMS) is no longer predominant in current applications. Although TIMS still has some important niches of application in nuclear and geochemistry, it has frequently been substituted by ICP–MS, because of its advantages of simpler sample preparation and multi-element capability and also because some elements, for example refractory and precious metals, are not easily accessible to TIMS. On the other hand, gas chromatography coupled with an isotope ratio mass spectrometer (GC–IRMS) and a combustion interface for converting organic molecules into CO₂ and N₂ for ¹³C/¹²C and ¹⁵N/¹⁴N ratio measurements, respectively, by electron impact ionization is increasingly used for new applications in compound-specific isotope analysis. Furthermore, the more recently introduced hyphenation with liquid chromatography for carbon-isotope analysis of compounds not or hardly amenable to GC separation has been demonstrated. One “Technical Note” reports the first isotope ratio measurements with a commercially available Mattauch–Herzog ICP–MS, which was constructed for simultaneous mass detection. However, future improvements of this instrument will show whether this type of mass spectrometer can become an alternative to high-resolution multi-collector systems for precise isotope ratio determinations.

A Feature Article by Willi Brand on “Atomic weights: not so constant after all” may be of general interest to all natural scientists. This article explains why IUPAC’s Commission on Isotopic Abundances and Atomic Weights recently decided to substitute fixed atomic weights for ten elements by atomic weight intervals. More precise isotope ratio measurements of the isotope variation of the corresponding natural and commercial substances during the last two decades led to this decision. Whereas for the light elements, for example hydrogen, carbon, and oxygen, isotope variations have been known for a long time, those for heavy metals, for example thallium, which is one of the ten elements for which the change has been made, were discovered by highly precise isotope ratio measurements especially by use of multi-collector (MC)-ICP–MS systems. This substantial improvement in isotope ratio determinations is

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also the reason why natural isotope variations of so called “non-traditional” heavy elements are increasingly investigated. The review by T. Hirata emphasizes the importance of this topic. The early isotope-abundance determinations of Alfred O.C. Nier lasted for a long time, but the introduction of MC-ICP-MS systems to isotope ratio measurements has substantially improved knowledge of natural isotope variations in the past, especially for heavy metals. Thus, it must be expected that, in the future, the fixed atomic weight will be substituted by an interval for other elements also.

Klaus Gustav Heumann is Emeritus Professor of Analytical Chemistry at Johannes Gutenberg University Mainz. His research interests are in the development and application of analytical methods for determination of trace elements and trace amounts of elemental species, by use of inductively coupled plasma mass spectrometry, thermal ionization mass spectrometry, different types of optical atomic spectrometry,

and electroanalysis as detection methods, and high-performance liquid chromatography, capillary electrophoresis, and capillary gas chromatography as separation methods. He has received several awards, including the Clemens Winkler Medal of the German Society for Analytical Chemistry in 2004 for his scientific lifework and for his continuous support of analytical chemistry in Germany. In 2007 he received the European Award for Plasma Spectrochemistry. He is a member of several national and international scientific societies, and was a member of the IUPAC Commission on Atomic Weights and Isotopic Abundances for 12 years, including chairman from 1991 to 1995.

As a tribute to the pioneering work of A.O.C. Nier the cover of this issue, prepared by Maik Jochmann, shows an adaptation of a popular photograph of Nier as a young scientist in front of a nuclide chart sketch, holding the glass mass spectrometer with which he conducted measurements relating to uranium fission.

The guest editors are very pleased by the great number of manuscripts received, their high quality, and the many different aspects covered. We therefore hope that readers of ABC will also enjoy this collection of papers on new developments and applications in isotope ratio measurements.

Torsten C. Schmidt obtained his PhD degree in Analytical Chemistry in 1997 from Philipps University Marburg. After a postdoctoral stay at EAWAG/ETH Zurich he became senior scientist at the Center for Applied Geoscience at Eberhard Karls University of Tuebingen where he finished his habilitation 2006. In the same year he was appointed Chair of Instrumental Analytical Chemistry at the University of Duisburg-Essen (W3) and scientific director at the IWW Water Centre in Muelheim an der

Ruhr. He has been interested in stable isotope analysis since his postdoctoral work and, in the meantime, been involved in the set-up of four stable isotope laboratories. Research focus in isotope analysis is on compound-specific stable isotope analysis of biogeochemically relevant elements using chromatographic separations with online coupled isotope ratio mass spectrometry. On that topic, with his coworker Maik A. Jochmann, he recently published the first comprehensive textbook. Apart from stable isotope analysis, his current research interests comprise sample preparation in environmental analysis, separation techniques, sorption in natural and engineered systems, and advanced oxidation processes. This year he became chairman of the executive board of the German Water Chemistry Society within GDCh.