

## Contents

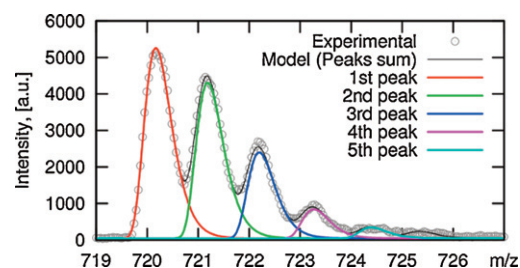
### Regular articles

#### 1–6

#### The peak shape model for magnetic sector and time-of-flight mass spectrometers

Oleg N. Peregudov, Oleksandr M. Buhay

Phenomenological peak shape model for mass spectra processing and studying of physical and chemical processes of ion formation in TOF-MS is proposed.

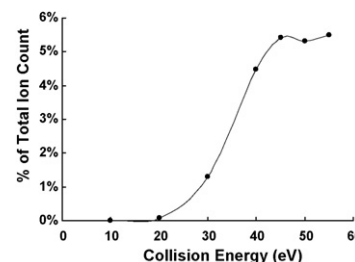


#### 7–12

#### An investigation into fragmentation of hEGF in triple quadrupole mass spectrometry and its quantitative application to human plasma

Yun Chen, Shanlei Qiao, Xianlong Wang, Yuan Liu

Fragmentation efficiency as a function of collision energy for the transition of  $m/z$  1037  $\rightarrow$  86.

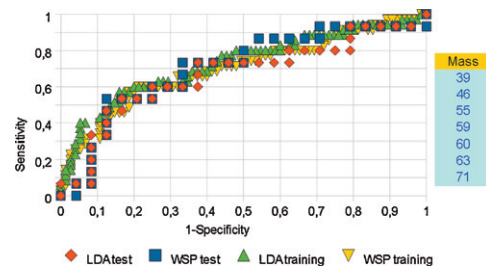


#### 13–20

#### Multidimensional statistical analysis of PTR-MS breath samples: A test study on irradiation detection

Mattia Fedrigo, Christoph Hoeschen, Uwe Oeh

A multidimensional statistical analysis for PTR-MS data associated to breath gas samples is proposed, based on a chemical-diffusion equilibrium approach. It is demonstrated on the problem of detecting exposure of human beings to ionizing radiation.

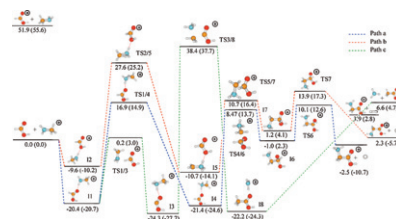


## 21–25

### Could the reactions of formic acid with $\text{CH}_3\text{NH}_2^+/\text{CH}_3\text{NH}_3^+$ produce protonated glycine?

Laura Largo, Carmen Barrientos, Víctor M. Rayón, Antonio Largo, Pilar Redondo

Energy profile, in kcal/mol, for the reaction of  $\text{CH}_3\text{NH}_2^+$  with  $\text{HCOOH}$  at the CCSD(T)/aug-ccpVTZ and MP2/cc-pVTZ (in parentheses) levels. Zero-point vibrational energy differences are included.

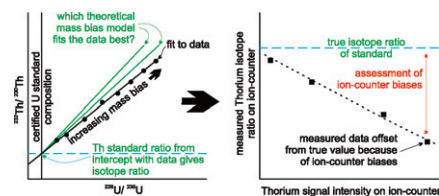


## 26–35

### Correction of multi-collector-ICP-MS instrumental biases in high-precision uranium–thorium chronology

Andrew J. Mason, Gideon M. Henderson

New in-house thorium standards have been calibrated and used to assess instrumental biases in thorium isotope measurement on a Nu Plasma ICP-MS.

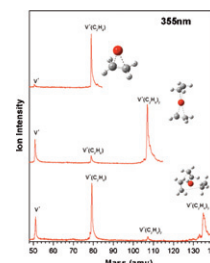


## 36–42

### Photodissociation and DFT investigation of $\text{V}^+(\text{C}_2\text{H}_4)_n$ ( $n = 1-3$ ) complexes

Jinyun Yuan, Zeng-Guang Zhang, Yuchao Zhao, Gao-Lei Hou, Hong-Guang Xu, Weijun Zheng

$\text{V}^+(\text{C}_2\text{H}_4)_n$  ( $n = 1-3$ ) were photodissociated with 1064, 532 and 355nm photons. The dissociation occurred by elimination of neutral ethene molecules.

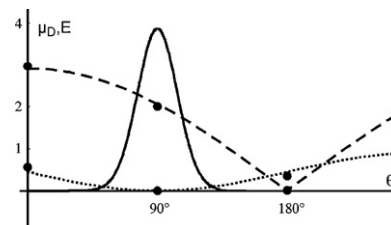


## 43–48

### Proton transfer reaction rate coefficients between $\text{H}_3\text{O}^+$ and some sulphur compounds

Luca Cappellin, Michael Probst, Jumras Limtrakul, Franco Biasoli, Erna Schuhfried, Christos Soukoulis, Tilmann D. Märk, Flavia Gasperi

We provide estimations of the reaction rate coefficients between  $\text{H}_3\text{O}^+$  and sulphur compounds at more realistic conditions than the ones usually found in the available literature.

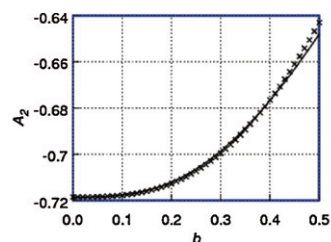


49–59

### Approximate multipole coefficients of RF ion traps as functions of aperture size

Madhurima Chattopadhyay, Atanu K. Mohanty

This paper presents analytical approximations for the variation in multipole expansion coefficients in ion traps as a function of the size of the apertures.



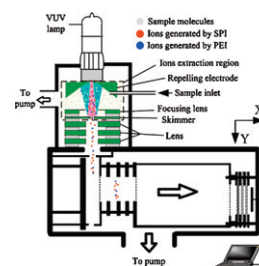
$A_2$  computed numerically (crosses) and by our approximation (continuous line)

60–64

### A combined single photon ionization and photoelectron ionization source for orthogonal acceleration time-of-flight mass spectrometer

Qinghao Wu, Lei Hua, Keyong Hou, Huapeng Cui, Ping Chen, Weiguo Wang, Jinghua Li, Haiyang Li

A novel ion source has been introduced in the present study, which combines the characteristics of single photon ionization (SPI) and photoelectron ionization (PEI).

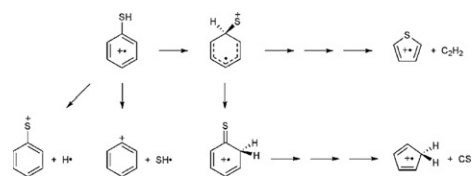


65–71

### Dissociation of the thiophenol molecular ion: A theoretical study

Sun Young Kim, Joong Chul Choe

The competitive losses of H, SH, C<sub>2</sub>H<sub>2</sub> and CS from the thiophenol molecular ion were investigated to understand their kinetics and mechanisms from G3//B3LYP and RRKM calculations.

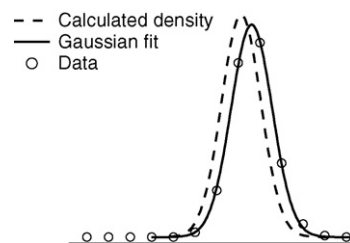


72–77

### Improved peak analysis of signals based on counting systems: Illustrated for proton-transfer-reaction time-of-flight mass spectrometry

Thorsten Titzmann, Martin Graus, Markus Müller, Armin Hansel, Alexander Ostermann

We present a correct method to analyze peaks of histograms by fitting distributions instead of densities and show the influences on peak areas and peak positions.

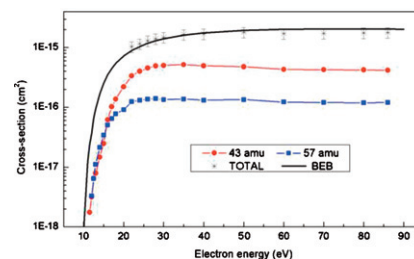


## 78–84

Electron impact ionization cross-sections of *n*-heptane

J.R. Vacher, F. Jorand, N. Blin-Simiand, S. Pasquiers

Electron impact ionization cross-sections of the two major cations issued from *n*-heptane from 10 eV to 90 eV. Total ionization cross-section measured and calculated with the BEB theory.

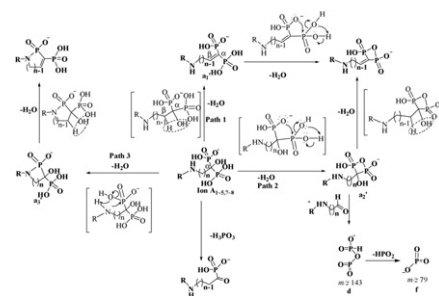


## 85–93

Fragmentation pathways of eight nitrogen-containing bisphosphonates (BPs) investigated by ESI-MS<sup>n</sup> in negative ion mode

Zhibo Qu, Xiaolan Chen, Chen Qu, Lingbo Qu, Jinwei Yuan, Donghui Wei, Huina Li, Xiaoying Huang, Yuqin Jiang, Yufen Zhao

Fragmentation pathways of eight nitrogen-containing bisphosphonates (BPs) were investigated by ESI-MS<sup>n</sup>. The hydrogen/deuterium exchange experiment, theoretical calculations, and HRMS were appropriately employed to rationalize the proposed fragmentation pathways.



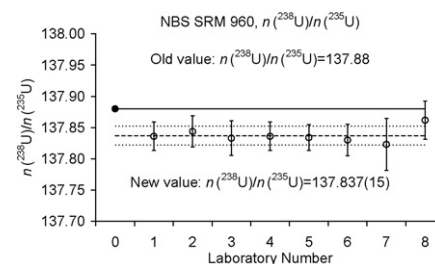
## Short communications

## 94–97

New average values for the  $n(^{238}\text{U})/n(^{235}\text{U})$  isotope ratios of natural uranium standards

S. Richter, R. Eykens, H. Kühn, Y. Aregbe, A. Verbruggen, S. Weyer

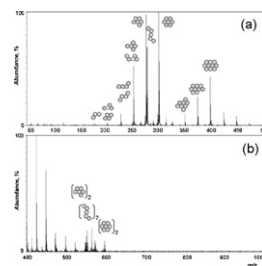
New 'multi-lab and multi-standard average values' for the  $n(^{238}\text{U})/n(^{235}\text{U})$  isotope ratios for NBS SRM 960 (NBL CRM 112a) and NBS SRM 950a are presented.



**98–102****Advantages and limitations of laser desorption/ionization mass spectrometric techniques in the chemical characterization of complex carbonaceous materials**

B. Apicella, M. Alfè, A. Amoresano, E. Galano, A. Ciajolo

The effect of experimental parameters on mass ranges detectable by laser desorption/ionization techniques has been investigated for polycyclic aromatic hydrocarbons, fullerenes, polyacenaphthylene and complex carbonaceous materials.



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