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### **Contents**

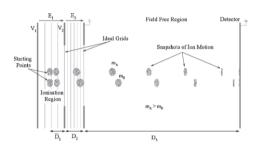
#### **Regular articles**

#### 1-12

## Designing multi-field linear time-of-flight mass spectrometers with higher-order space focusing

Murat Yildirim, Omer Sise, Mevlut Dogan, Hamdi S. Kilic

Simulation of a two-field linear TOFMS with second-order space focusing. Identical ions formed at slightly different distances (s) from the center of the source region shall have the same flight time.

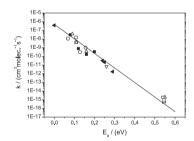


#### 13-16

## The influence of the temperature on electron attachment to some halocontaining molecules

Janina Kopyra, Jolanta Wnorowska, Mieczysław Foryś, Iwona Szamrei

The obtained rate coefficients for thermal electron capture by  $CH_2CICH_2CI$ ,  $CH_2CICH_2Br$ ,  $CH_2CICH_2Br$  and  $CF_2CICFCI_2$  show an Arrhenius-type rise with increasing the temperature. At constant temperature the  $\log(k)$  on  $E_a$  gives, to good approximation, a linear dependence.



#### 17-23

Coordinated dissociative proton transfers of external proton and thiocarbamide hydrogen: MS experimental and theoretical studies on the fragmentation of protonated S-methyl benzenylmethylenehydrazine dithiocarboxylate in gas phase

Kezhi Jiang, Gaofeng Bian, Nan Hu, Yuanjiang Pan, Guoqiao Lai

The added proton and the thiocarbamide hydrogen have different transferring directions in the fragmentations: fragment ion, neutral product, or both.

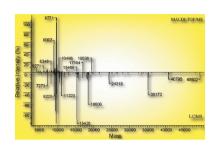
iv Contents

#### 24-32

### Comparison of MALDI-TOF/MS and LC-QTOF/MS methods for the identification of enteric bacteria

Tiffany M. Mott, Robert A. Everley, Shane A. Wyatt, Denise M. Toney, Timothy R. Croley

A comparison of MALDI-TOF/MS and LC-QTOF/MS for the analysis of intact proteins.

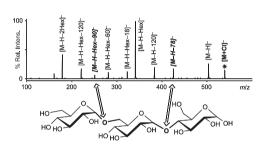


#### 33-40

#### Structural analysis and differentiation of reducing and nonreducing neutral model starch oligosaccharides by negative-ion electrospray ionization ion-trap mass spectrometry

Richard Čmelík, Josef Chmelík

The identification of nonreducing saccharides, as well as the differentiation between  $\alpha$ - $(1 \rightarrow 4)$  and  $\alpha$ - $(1 \rightarrow 6)$  linkage were obtained on the basis of presence of diagnostic ions.

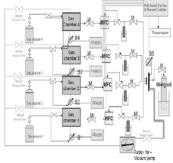


#### 41-47

### Preparation of argon Primary Measurement Standards for the calibration of ion current ratios measured in argon

S. Valkiers, D. Vendelbo, M. Berglund, M. de Podesta

In this work a procedure is described to prepare SI-traceable argon isotope amount ratios in high purity argon.



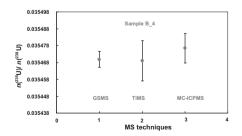
Schematic presentation of the gas mixing line.

#### 48-54

# Demonstrating the metrological compatibility of uranium isotope amount ratio measurement results obtained by GSMS, TIMS and MC-ICPMS techniques

O. Pereira de Oliveira Junior, W. De Bolle, A. Alonso, S. Richter, R. Wellum, E. Ponzevera, J.E.S. Sarkis, R. Kessel

The metrological compatibility of isotope ratios obtained by GSMS, TIMS and MC-ICPMS in uranium samples is demonstrated in this study. Correlation between certified isotope ratio materials has a great impact in this kind of comparison.



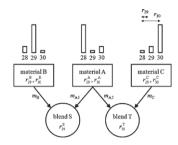
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#### 55-60

#### The calibration of Si isotope ratio measurements

#### G. Mana, O. Rienitz

The determination of absolute isotope amount ratios requires the calibration of mass spectrometric measurements. For the very first time, the relevant calibration factors are explicitly given for a three-isotope system. The conditions ensuring the existence and uniqueness of the calibration-equation solutions are related as well.

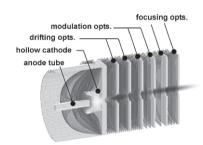


#### 61-66

### Ionizing nonvolatile samples using laser desorption–proton-transfer reaction with cluster reagent ions

#### Chi-Wei Liang, Yuan Tseh Lee, Chung-Hsuan Chen, Yi-Sheng Wang

A soft ionization reaction is demonstrated to produce protonated intact biomolecules by combining laser desorption and proton-transfer reaction with protonated reagent clusters.

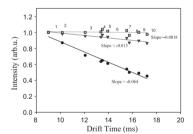


#### 67-72

#### Relative transmission of different ions through shutter grid

#### M. Tabrizchi, H.R. Shamlouei

In this work, we study the transmission of different ions through a shutter grid which is a key part in ion mobility instruments. It will be shown that the relative transmission of ions through the shutter grid depends not only on the opening time but also on the nature of ion and the voltage applied to the grid electrodes. The effect of shutter grid can be corrected by multiplying the intensities by a factor of  $(1 + \alpha t_d)$  where  $\alpha$  is a small correction factor which depends on the geometry of both the shutter grid and the drift tube and on the opening time. In figure the corrected intensities can be seen.

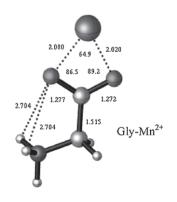


#### 73-83

## Complexation of glycine by manganese (II) in the gas phase: A theoretical study

#### M. Hassan Khodabandeh, Mehdi D. Davari, Mansour Zahedi, Gilles Ohanessian

Detailed description of gas-phase interaction between Mn(II) ion in three possible spin states and various conformers of glycine has been performed using quantum chemical calculations.



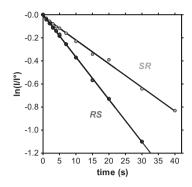
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#### 84-89

### Diastereoselective gas-phase ion/molecule reactions of ethanolamine neurotransmitter/amido[4]resorcinarene adducts

Maurizio Speranza, Ilaria D'Acquarica, Caterina Fraschetti, Bruno Botta, Andrea Tafi, Luca Bellucci, Giovanni Zappia

The factors influencing the stability and selectivity of diastereomeric ethanolamine neurotrasmitter/amido[4]resorcinarene adducts have been determined in the gas phase by FT-ICR and computational methods.



#### 90-95

# Quantification of interferences in PTR-MS measurements of monoterpene emissions from *Fagus sylvatica* L. using simultaneous TD-GC-MS measurements

É. Joó, J. Dewulf, M. Demarcke, C. Amelynck, N. Schoon, J.-F. Müller, M. Šimpraga, K. Steppe, H. Van Langenhove

Simultaneous GC-MS and PTR-MS measurements showed that one should remain cautious when quantifying MT emissions from vegetation by PTR-MS based on the ion signal at m/z 137.



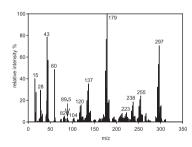
#### **Short communication**

#### 96-99

### Generation of "unstable" complexes of carbon dioxide with $Pb^{2+}$ and $Sn^{2+}$ under electron ionization conditions

Rafał Frański, Błażej Gierczyk, Ewa Szymańska, Piotr Kirszensztejn

The acetates of Sn(II) and Pb(II/IV) yield, on EI mass spectra, peaks of the asymptotically unstable complexes of Sn<sup>2+</sup> and Pb<sup>2+</sup> with CO<sub>2</sub> molecule(s). [Sn + (CO<sub>2</sub>)<sub>2</sub>]<sup>2+</sup> m/z 104, [Sn + CO<sub>2</sub>]<sup>2+</sup> m/z 82.



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