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# International Journal of Mass Spectrometry

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# **Contents**

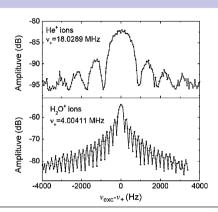
## **Regular articles**

#### 1-5

# A broad-band FT-ICR Penning trap system for KATRIN

M. Ubieto-Díaz, D. Rodríguez, S. Lukic, Sz. Nagy, S. Stahl, K. Blaum

Two three-electrode cylindrical Penning traps using the Fourier-Transform Ion-Cyclotron-Resonance detection technique in order to measure the concentration of unwanted species will be installed in the KATRIN beamline. The system is presently under commissioning at the Max-Planck-Institute for Nuclear Physics in Heidelberg.

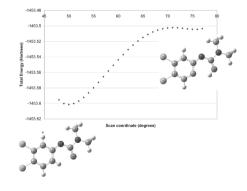


#### 6-15

# Exploring rearrangements along the fragmentation pathways of diuron anion: A combined experimental and computational investigation

Basem Kanawati, Mourad Harir, Philippe Schmitt-Kopplin

Successive two 1,3 H<sup>+</sup> shifts of the marked Proton \*H<sup>+</sup> are responsible for the elimination of dimethylamine from the Diuron anion (left). DFT studies exclude the possibility of a 1,5 proton shift in a Mclafferty like type of rearrangement. The PES shows the unfavourable energy demand for the forbidden 1,5 proton shift.

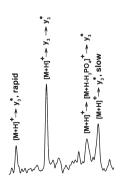


#### 16-21

Utility of reaction intermediate monitoring with photodissociation multi-stage (MS<sup>n</sup>) time-of-flight mass spectrometry for mechanistic and structural studies: Phosphopeptides

Jeong Hee Moon, Young Sik Shin, Myung Soo Kim

Photoexcitation inside a high voltage cell splits a dephosphorylated sequence peak  $(y_3^*)$  into several components.  $y_3^*$  is formed mainly via  $[M+H]^+ \rightarrow y_3 \rightarrow y_3^*$ .



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#### 22-35

# Condensation reaction of $C_4H_4^+$ with pyridine

C.Q. Jiao, J.A. Boatz, C.A. DeJoseph Jr., A. Garscadden

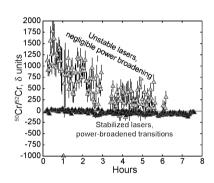
Quantum chemistry theory and FTMS experiments on the reactions of  $C_4H_4^+$  with  $C_5H_5N$  that show  $H^+$  transfer, charge transfer and condensation with H-elimination.

#### 36-43

# Resonance ionization mass spectrometry for precise measurements of isotope ratios

Jonathan Levine, Michael R. Savina<sup>,</sup> Thomas Stephan<sup>,</sup> Nicolas Dauphas, Andrew M. Davis, Kim B. Knight, Michael J. Pellin

We measure isotope ratios with sub-percent precision by resonance ionization mass spectrometry, using stabilized resonance lasers and power-broadened optical transitions.

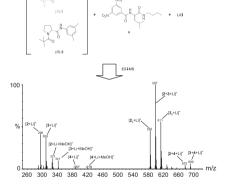


#### 44-50

# Chiral recognition and enantiomer assays of N-(3,5-dinitrobenzoyl) amino acid derivatives using electrospray ionizate i o n - m a s s spectrometry

Chengli Zu, Jonathan A. Woolfolk, Michael E. Koscho

We performed chiral recognition and enantiomer assays of *N*-(3,5-dinitrobenzoyl)amino acid derivatives in the gas phase using electrospray ionization/mass spectrometry (ESI/MS).



# 51-57

# Electrospray ionization multistage tandem mass spectrometry of penta- and hexa-substituted aryloxycyclotriphosphazenes

Zhiyu Ju<sup>,</sup>, Yong Ye<sup>,</sup>, Donghui Wei, Ruyi Zou, Yufen Zhao<sup>,</sup>

Several penta- and hexa-substituted aryloxycyclotriphosphazenes were synthesized and investigated by electro spray ionization tandem mass spectrometry (ESI-Ms $^n$ ).

$$\begin{array}{c} \text{RC3}\text{IfO} & \text{OC'}\text{H}^2\text{K} \\ \text{SC'}\text{IfO} & \text{OC'}\text{H}^2\text{K} \\ \text{OC'}\text{H}^2\text{$$

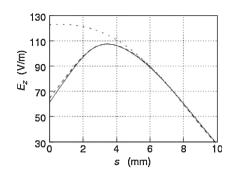
Contents

#### 58-67

# Off-axis field approximations for ion traps with apertures

#### Madhurima Chattopadhyay, Atanu K. Mohanty

This paper presents analytical approximations for the fields in ion traps with apertures.  $E_Z$  computed numerically (solid line) and by our approximation (dashed line).

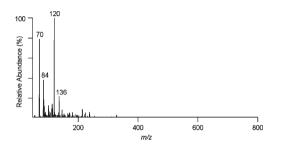


#### 68 - 74

# Fragmentation of peptides with intra-chain disulfide bonds in triple quadrupole mass spectrometry and its quantitative application to biological samples

Yun Chen, Shanlei Qiao, Ce Wang

Generation of abundant immonium ions in product ion spectrum of peptides with intra-chain disulfide bonds.



### 75-83

## Collision induced dissociation of protonated N nitrosodimethylamine by ion trap mass spectrometry: Ultimate carcinogens in gas phase

#### Natalia Kulikova, Michael Baker, Wojciech Gabryelski

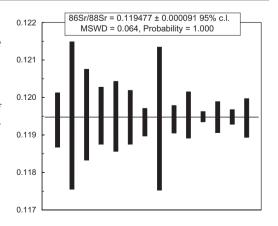
Gas phase ion chemistry of a potent carcinogen N-nitrosodimethylamine (NDMA) has been found to produce methanediazonium ion which is considered the ultimate carcinogen in metabolic pathway of NDMA in biological systems.

#### 84-91

# Rayleigh's distillation law and linear hypothesis of isotope fractionation in thermal ionization mass spectrometry

## Giancarlo Cavazzini

The relationship which exists between Rayleigh's distillation process and the linear hypothesis of instrumental isotope fractionation in thermal ionization-source mass spectrometry is investigated.



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# **Short communication**

# 92-95

Improved mass analysis of intact proteins by ion trap instrument on a chromatographic time scale via data-dependant enhanced resolution scan

## Gang Hao, Jane Gu

A novel method that improves the mass spectra resolution for multiply charged protein ions on ion trap instruments.

