

## Contents

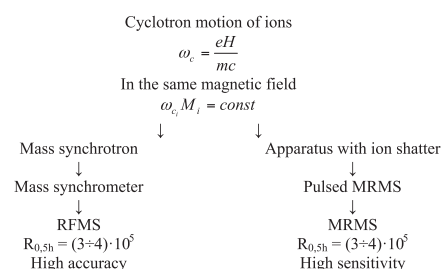
### Review

1–19

#### Magnetic resonance and radio frequency mass spectrometers and their application

N.N. Aruev

► Two schemes of dynamic mass spectrometers based on cyclotron motion of ions in the magnetic field are considered. ► High analytical parameters of these instruments make it possible to use them in different fields of science and technics



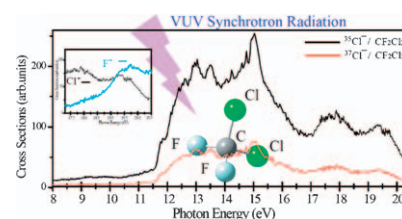
### Regular articles

20–25

#### Vacuum ultraviolet negative photoion spectroscopy of dichlorodifluoromethane

Liu-Li Chen, Shan Xi Tian, Yun-Feng Xu, Gen-Bai Chu, Fu-Yi Liu, Xiao-Bin Shan, Liu-Si Sheng

► Photolysis of freon molecules is closely related to the destructions of atmosphere. Negative ions  $^{35}\text{Cl}^-$ ,  $^{37}\text{Cl}^-$ , and  $\text{F}^-$  are observed in the vacuum ultraviolet photodissociations of  $\text{CF}_2\text{Cl}_2$  using synchrotron radiation and their ion production efficiency curves are recorded in the photon energy range of 8.00–20.50 eV. The appearance energy of  $\text{Cl}^-$  is experimentally determined to be  $8.20 \pm 0.04$  eV, in excellent agreement with the theoretical thermochemical value 8.19 eV. A novel competition between the ion-pair photodissociations to  $\text{Cl}^-$  and  $\text{F}^-$  anions is found in the photon energy range of 17.30–20.50 eV.

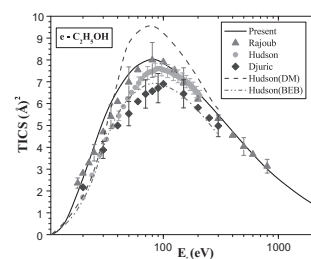


26–29

#### Computation of the electron impact total ionization cross sections of $\text{C}_n\text{H}_{(2n+1)}\text{OH}$ molecules from the threshold to 2 keV energy range

Minaxi Vinodkumar, Kirti Korot, P.C. Vinodkumar

► Electron impact ionization for simple alcohols ( $\text{CH}_3\text{OH}$ ,  $\text{C}_2\text{H}_5\text{OH}$ ,  $1\text{-C}_3\text{H}_7\text{OH}$ ). ► We have used improved complex scattering potential- ionization contribution (ICSP-ic) method for the calculation of  $Q_{\text{ion}}$ . ► The total inelastic cross sections ( $Q_{\text{inel}}$ ) are calculated using SCOP formalism.

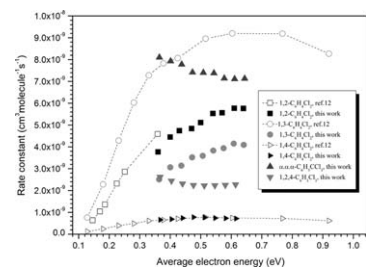


## 30–34

### Rate constants of electron attachment to chlorobenzenes measured by atmospheric pressure nitrogen corona discharge electron attachment ion mobility spectrometry

Hongtao Feng, Wenqi Niu, Haiyan Han, Chaoqun Huang, Hongmei Wang, Jan Matuska, Martin Sabo, Stefan Matejcik, Haihe Jiang, Yannan Chu

- ▶ The measurement principle of electron attachment rate constant was clearly described.
- ▶ The rate constants of electron attachment to the five chlorobenzene derivatives were reported.
- ▶ The discrepancy between the present work and the previous result in literature was discussed.



## 35–39

### Flowing afterglow studies of dissociative electron-ion recombination for a series of single ring compounds at room temperature

David Osborne Jr., Patrick A. Lawson, Nigel G. Adams

- ▶ Protonated five and six membered rings with heteroatoms N, O and S studied.
- ▶ Protonated six membered rings recombined ~2 times faster than five membered rings.
- ▶ Proton bound five membered ring dimers recombined more rapidly than six membered.
- ▶ 1,4 dioxane behaves differently from other five and six membered rings.

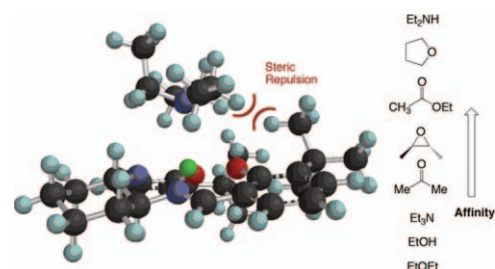
Species	Structure	Measured	Other
<b>6-Membered Ring Compounds</b>			
Benzene	<chem>c1ccccc1</chem>	6,800.07	~6,800.07
Toluene	<chem>Cc1ccccc1</chem>	6,800.07	~7,200.06
Pyridine	<chem>c1ccncc1</chem>	6,300.07	~6,800.07
Acetophenone	<chem>CC(=O)c1ccccc1</chem>	6,800.07	~6,700.07
Pyrimidine	<chem>C1=CN=CN=C1</chem>	5,300.06	~5,300.07
<b>5-Membered Ring Compounds</b>			
Cyclopentadiene	<chem>C1=CC=CC1</chem>	3,300.06	~3,300.06
Li-Dioxane	<chem>C1OCCOCC1</chem>	6,300.07	~6,300.06
Pyridole	<chem>C1=CC=NC=C1O</chem>	6,600.07	~6,600.07
N-Methylpyrrolidine	<chem>CN1CCCC1</chem>	3,800.07	~3,800.06
Furan	<chem>C1=CC=OC1</chem>	6,300.07	~5,200.07
Thiophene	<chem>C1=CC=SC1</chem>	17,000.0	N/A
<b>Other 5-Membered Ring Compounds</b>			
Pyridothione	<chem>C1=CC=NC=C1S</chem>	3,700.06	~3,800.07

## 40–44

### Gas-phase ligand binding to Jacobsen's manganese salen catalyst: Functional group and steric effects

William C. Clodfelter, Emileigh H. Wong, Kelly A. Hay, Scott Gronert

- ▶ Gas-phase binding affinities of 18 ligands to Jacobsen's catalyst.
- ▶ Identification of functional group patterns in the binding affinities.
- ▶ Identification of strong steric effects in the binding affinities.
- ▶ Major differences in binding to atomic cations, proton and lithium.

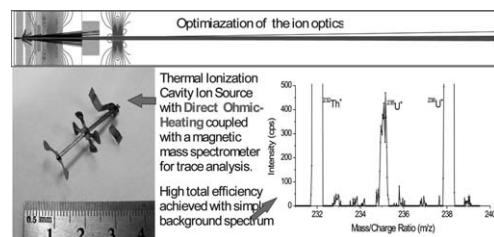


## 45–49

### A new, ohmic-heating based thermal ionization cavity source for mass spectrometry

Zhai Li-hua, Deng Hu, Wei Guan-yi, Li Zhi-ming, Wang Chang-hai, Li Xue-song, Zhou Guo-qing, Su Yong-yang, Zhang Zi-bin

- ▶ A New, ohmic-heating based thermal ionization cavity source for mass spectrometry is developed.
- ▶ High total efficiency achieved for uranium and plutonium.
- ▶ The Extraction and transmission of ions improved with special design and simulation.

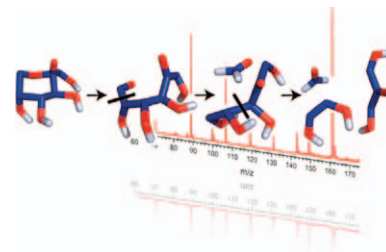


50–57

### Fast and metastable fragmentation of deprotonated D-fructose – A combined experimental and computational study

Helga D. Flosadottir, Ilko Bald, Oddur Ingólfsson

- ▶ Metastable ( $\approx 8 \mu\text{s}$ ) and prompt fragmentation ( $< 200 \text{ ns}$ ) of deprotonated D-fructose is compared.
- ▶ Prompt fragmentation proceeds selectively with charge retention on the anomeric center.
- ▶ In metastable fragmentation charge retention on C6 contributes significantly.
- ▶ Classical dynamics simulations can predict metastable fragmentation of deprotonated D-fructose.
- ▶ Simulations reveal that the site of initial deprotonation determines the decay pathway.

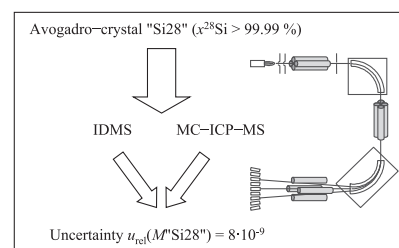


58–68

### Novel concept for the mass spectrometric determination of absolute isotopic abundances with improved measurement uncertainty: Part 3—Molar mass of silicon highly enriched in $^{28}\text{Si}$

Axel Pramann, Olaf Rienitz, Detlef Schiel, Bernd Güttler, Staf Valkiers

- ▶ Measurement of the molar mass of silicon highly enriched in  $^{28}\text{Si}$ .
- ▶ Molar mass enables new determination of Avogadro constant with lowest uncertainty so far.
- ▶ Extended experimental proof of applicability of MC-ICP-MS and IDMS for molar mass determination.
- ▶ Measurement uncertainty of the molar mass according to GUM.



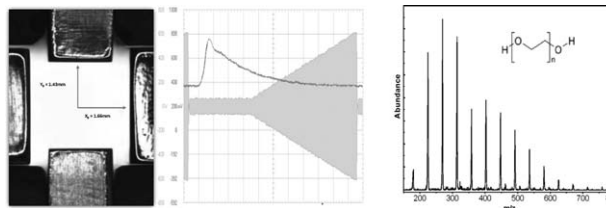
## Short communication

69–73

### Performance of a low voltage ion trap

Paul Hendricks, Jason Duncan, Robert J. Noll, Zheng Ouyang, R. Graham Cooks

- ▶ Design and fabrication of a miniaturized rectilinear ion trap mass analyzer.
- ▶ Mass analyzer performance characterization for mass resolution, mass range, operating pressure, and operating voltage.
- ▶ Demonstration of tandem MS capabilities.



## Corrigendum

74–75

### Corrigendum to ‘Tandem Fourier transform mass spectrometry of block and random copolymers’ [Int. J. Mass Spectrom. 301 (2011) 184–194]

Sasa M. Miladinovic, Cynthia J. Kaeser, Matthias M. Knust, Charles L. Wilkins