

## Contents

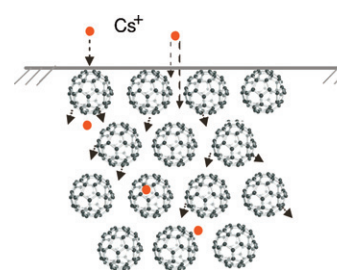
### Regular Articles

1–6

#### Mass spectrometric identification of $C_{60}$ 's fragmentation regimes under energetic $Cs^+$ bombardment

Sumaira Zeeshan, Sumera Javeed, Shoaib Ahmad

► Three fragmentation regimes are identified for  $Cs^+$  bombarded fullerite as a function of  $Cs^+$  energy. ►  $C_2$  dominates all the fragments at all energies. ► Upper threshold energy of  $C_{60}$  to fragment by emission of  $C_2$  is 210 eV. ► The cumulative effect of the  $Cs^+$  induced fragmentation results in the conversion of fullerite into amorphous carbon.

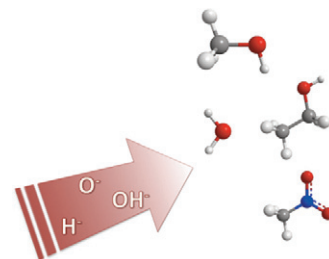


7–16

#### Mass spectrometry of anions and cations produced in 1–4 keV $H^-$ , $O^-$ , and $OH^-$ collisions with nitromethane, water, ethanol, and methanol

D. Almeida, R. Antunes, G. Martins, G. Garcia, R.W. McCullough, S. Eden, P. Limão-Vieira

► 1–4 keV anions ( $H^-$ ,  $O^-$ , and  $OH^-$ ) interactions with gas-phase molecules. ► Negative and positive ion formation. ► Dipole-bound states. ► Charge transfer to shape resonance.

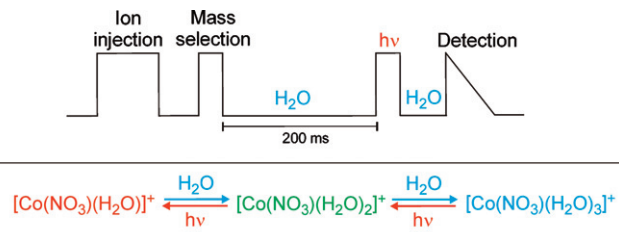


17–23

#### Microhydrated cobalt-nitrate cations $[Co(NO_3)(H_2O)_n]^+$ ( $n = 2, 3$ ) studied by infrared spectroscopy in the gas phase

Christopher J. Shaffer, Detlef Schröder

► IRMPD spectra of mass-selected  $[Co(NO_3)(H_2O)_2]^+$  and  $[Co(NO_3)(H_2O)_3]^+$ . ► Computed structures and IR spectra of  $[Co(NO_3)(H_2O)_n]^+$  cations. ► Kinetic modeling of association/ dissociation equilibria in an ion-trap mass spectrometer.

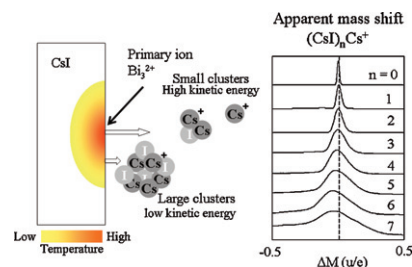


## 24–30

### Mass shift in the mass spectra of TOF-SIMS and the analysis of kinetic energies of the ions

Taisuke Nakanaga, Hidekazu Nagai, Naoaki Saito, Yukio Fujiwara, Hidehiko Nonaka

► Apparent mass shifts of the CsI cluster ions were observed in the corrected mass spectrum of CsI measured by TOF-SIMS. ► The kinetic energies of the secondary ions have been determined using post acceleration electrodes. ► The unimolecular dissociation of the cluster ion strongly depends on the relative stability of the cluster ions.

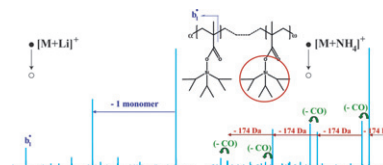


## 31–39

### Fragmentation pathways of methacrylic homopolymers with labile trialkylsilyl ester side-groups—A mass spectrometric investigation of the RAFT process

Laurence Charles, Marlène Lejars, André Margailan, Christine Bressy

► CID of poly(triisopropylsilyl methacrylate) has been established. ► The adducted cation was shown to determine the dissociation routes. ► Accurate characterization of end-groups allowed a deeper insight in the RAFT process.

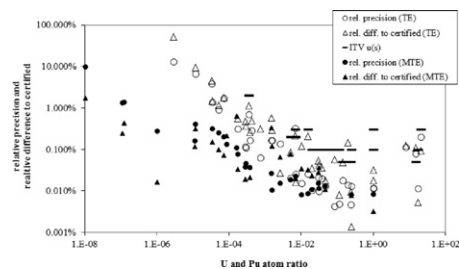


## 40–50

### Uranium and plutonium analysis of nuclear material samples by multi-collector thermal ionisation mass spectrometry: Quality control, measurement uncertainty, and metrological traceability

S. Bürger, S.D. Balsley, S. Baumann, J. Berger, S.F. Boulyga, J.A. Cunningham, S. Kappel, A. Koepf, J. Poths

► A gain of up to an order of magnitude in precision in actinide isotope ratio measurements is observed when comparing the latest with the previous generation of MC-TIMS instruments. ► Uranium isotope ratio analysis is demonstrated utilizing a dynamic range of at least eight orders of magnitude. ► The agreement between the certified values of the two major uranium reference material series, IRMM's and NBL's, highlights the quality of both independently produced series.

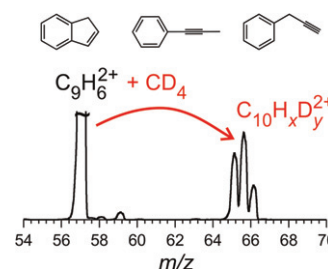


## 51–55

### Reactivity of $C_9H_n^{2+}$ dications with methane

Jana Vachelová, Jana Roithová

► Dications  $C_9H_x^{2+}$  react with methane to yield  $C_{10}$  coupling products. ► The coupling reaction proceeds via a long-lived intermediate. ► The reactivities of analogous dications generated upon electron ionization from different neutral precursors are very similar.

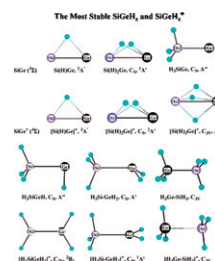


56–63

## Structures and energetics of $\text{SiGeH}_z^{0,+1}$ , $\text{Ge}_2\text{H}_z^{0,+1}$ , and $\text{Si}_2\text{H}_z^{0,+1}$ : A systematic theoretical study

Liming Wang, Jingsong Zhang

► Structures of  $\text{SiGeH}_z$  and cations are examined by quantum chemistry calculations. ► Adiabatic ionization energies are predicted at G4 level. ► Appearance energies of ion fragments from  $\text{SiGeH}_6$  are predicted. ► Results are compared with those for  $\text{Si}_2\text{H}_z$  and  $\text{Ge}_2\text{H}_z$ . ► Photoionization of  $\text{SiGeH}_6$  is discussed with the potential energy surface of  $\text{SiGeH}_6^+$ .

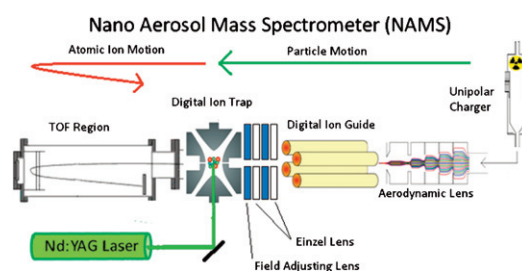


64–71

## Trapping charged nanoparticles in the nano aerosol mass spectrometer (NAMS)

M. Ross Pennington, Murray V. Johnston

► The nano aerosol mass spectrometer (NAMS) analyzes individual airborne particles in the 10–30 nm size range. ► Inside the NAMS, charged nanoparticles are captured by a digital ion trap (DIT). Particle trapping is optimized through proper design of a field adjusting lens (FAL) assembly upstream of the DIT. ► A new FAL assembly increases the particle analysis rate of NAMS by an order of magnitude over the previous design.



## Erratum

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## Erratum to “Numerical investigation of stability regions in a cylindrical ion trap” [Int. J. Mass Spectrom. 308 (1) (2011) 109–113]

Houshyar Noshad, Behjat-Sadat Kariman