



## Contents

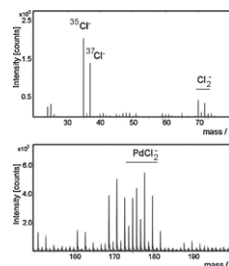
### Regular articles

#### 1–6

#### ToF-SIMS studies of the regeneration of Pd/TiO<sub>2</sub> catalyst used in hydrodechlorination process

Jacek Grams, Jacek Góralski, Paulina Kwintal

This work is focused on the application of time-of-flight secondary ion mass spectrometry (ToF-SIMS) to the surface studies of deactivation-regeneration process of Pd/TiO<sub>2</sub> catalyst used in the hydrodechlorination of CCl<sub>4</sub>.

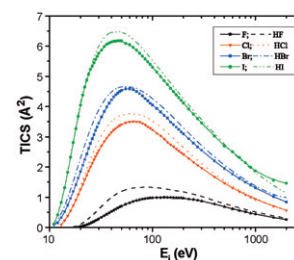


#### 7–13

#### Electron impact total ionization cross sections for halogens and their hydrides

Minaxi Vinodkumar, Rucha Dave, Harshad Bhutadia, Bobby K. Antony

Calculation for electron impact total ionization cross sections on halogen atoms (F, Cl, Br and I) and their hydrides (HF, HCl, HBr and HI) are performed employing Spherical Complex Optical Potential and Complex Optical Potential ionization contribution formalisms for energies ranging from above threshold to 2000 eV. The results are compared with other data wherever available. It is found that the present result gives a better account of the ionization cross sections.

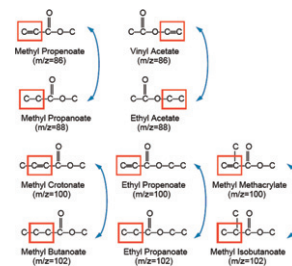


#### 14–22

#### Absolute cross-sections for dissociative photoionization of some small esters

Juan Wang, Bin Yang, Terrill A. Cool, Nils Hansen

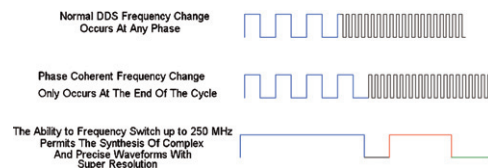
The first measurements of absolute cross-sections for near-threshold molecular and dissociative photoionization are presented for 11 small esters (methyl formate, ethyl formate, vinyl acetate, methyl propanoate, ethyl propanoate, methyl butanoate, methyl isobutanoate, methyl propenoate, ethyl propenoate, methyl crotonate, and methyl methacrylate).



## 23–31

### A novel phase-coherent programmable clock for high-precision arbitrary waveform generation applied to digital ion trap mass spectrometry

Hideya Koizumi, Bruce Jatko, William H. Andrews Jr., William B. Whitten, Peter T.A. Reilly

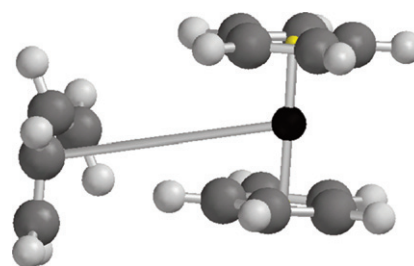


## 32–37

### Reactive MALDI mass spectrometry of saturated hydrocarbons: A theoretical study

William E. Wallace, Hans Lewandowski, Robert J. Meier

Density functional calculations have shown that the product of the reactive MALDI of alkanes and polyolefins is a weakly bound cobaltocene–alkadiene ion–molecule complex.

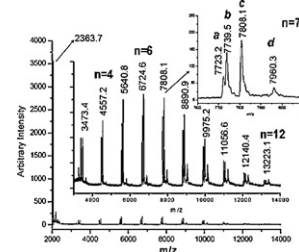


## 38–47

### ESI and MALDI mass spectrometry of large POSS oligomers

Stanley E. Anderson, Arpad Somogyi, Timothy S. Haddad, E. Bryan Coughlin, Gunjan Gadodia, David F. Marten, Julie Ray, Michael T. Bowers

We report MALDI-TOF mass spectra and assignments of major peaks for polyhedral oligomeric silsesquioxane (POSS) propylmethacrylate and styryl oligomers, obtained in a new matrix, 4,4'-dihydroxyoctafluoroazobenzene.

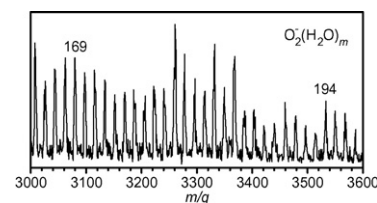


## 48–52

### On the formation of water-containing negatively charged clusters from atmospheric pressure corona discharge in air

Preben Hvelplund, Umesh Kadhane, Steen Brøndsted Nielsen, Subhasis Panja, Kristian Støchkel

Large anionic clusters with 200 water molecules are formed in a corona discharge of air using an STM needle held at  $-1$  kV.

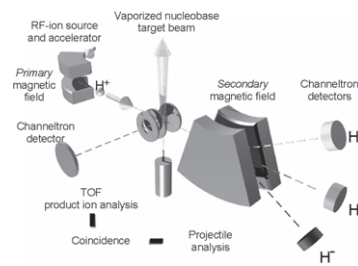


53–63

**Mass spectrometry (fragmentation ratios) of DNA base molecules following 80 keV proton impact with separation of direct ionization and electron capture processes**

J. Tabet, S. Eden, S. Feil, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, T.D. Märk

The first fragmentation ratios are presented for the ionization of gas-phase DNA bases by 80 keV ( $1.8 v_0$  in Bohr velocity units) proton impact. Event-by-event determination of the projectile charge state post-collision enables branching ratios to be determined for electron capture (EC) by the projectile and for direct ionization (DI) of the target molecule (without projectile neutralization). Results are compared with similar experiments on uracil [Tabet et al., Phys. Rev. A 81 (2010) 012711] and water [Gobet et al., Phys. Rev. A 70 (2004) 062716]. In all cases, whereas both processes (EC and DI) produce the same fragment ion groups, greater fragmentation ratios are observed for EC than for DI. Moreover the fragmentation ratio is greater for thymine than for adenine, cytosine, and uracil.



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