International Journal of Mass Spectrometry 299 (2011) iii–v

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

journal homepage: www.elsevier.com/locate/ijms

Contents

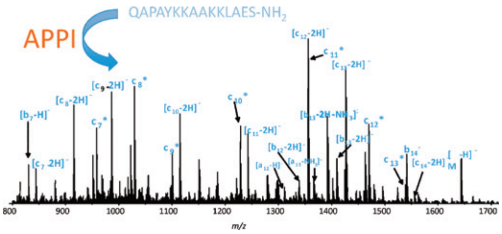
Regular articles

1–4

Atmospheric pressure photoionization of peptides

A. Bagag, A. Giuliani and O. Laprévote

► Peptide. ► Positive & Negative ion mode APPI. ► Positive & Negative *c*-fragment ions.

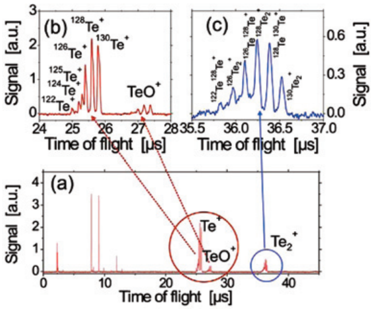


5–8

Time-of-flight mass spectroscopy of femtosecond and nanosecond laser ablated TeO_2 crystals

S. Beke, T. Kobayashi, K. Sugioka, K. Midorikawa and J. Bonse

► Single-pulse fs and ns-laser ablation of single-crystalline TeO_2. ► Significant differences observed regarding the laser-induced species in the plasma plume. ► Singly charged positive Te ions in the form of six isotopes were detected predominantly in the ablation plume in case of both ns and fs-laser irradiations. ► The Te ion peak intensities in the TOFMS strongly depended on the applied laser pulse energy.

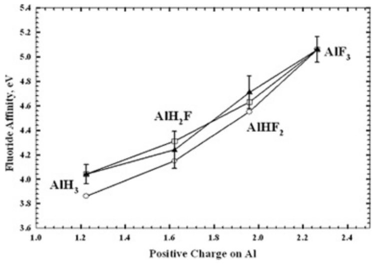


9–12

Fluoride affinities of fluorinated alanes

J.K.P. Williams and P.G. Wenthold

► Fluorinated aluminate anions ($AlH_mF_{4-m}^-$) can be formed in the gas phase by ionization of diethylmethylamine-alane with molecular fluorine. ► Energy-resolved collision-induced dissociation is used to measure fluoride affinities of the alanes. ► The measured fluoride affinities agree with predictions obtained from coupled-cluster calculations with very large basis sets. ► Fluoride affinities reflect the extent of positive charge character on the aluminum in the alanes.



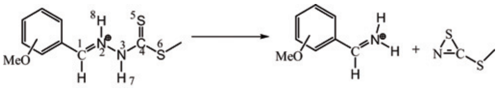
Elsevier B.V.
doi:10.1016/S1387-3806(10)00449-5

13–19

Recognizing *ortho*-, *meta*- or *para*-positional isomers of S-methyl methoxylphenylmethylenehydrazine dithiocarboxylates by ESI-MS^2: The positional effect of the methoxyl substituent

K. Jiang, G. Bian, Y. Pan and G. Lai

The *ortho*, *meta* or *para* methoxyl-substituted isomers were differentiated by ESI tandem MS according to the different abundance of the fragment ion (*m/z* 136), due to the different positional effect on the (NSC)SCH$_3$ elimination.

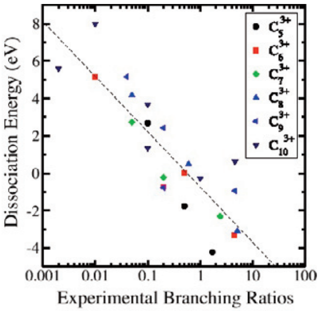


20–26

Theoretical study of the stability of small triply charged carbon clusters C_n^{3+} (n = 3–12)

G. Sánchez-Sanz, S. Díaz-Tendero, F. Martín and M. Alcamí

► Smaller C_n^{3+} clusters are metastable. ► The lowest dissociation channel always corresponds to evaporation of a singly charged-carbon atom. ► The third ionization potential of the corresponding neutral species decreases with cluster size.

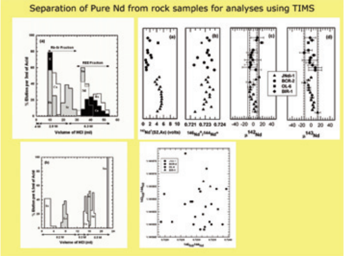


27–34

Precise thermal ionization mass spectrometric measurements of ^{142}Nd/^{144}Nd and ^{143}Nd/^{144}Nd isotopic ratios of Nd separated from geological standards by chromatographic methods

A. Ali and G. Srinivasan

► Chromatographic technique for separation of Nd from rock powders is established. ► The separated Nd was analyzed using TIMS for its isotopic composition. ► TIMS was tested for reliability using mono-element Nd reference standard. ► The ^{143}Nd/^{144}Nd values for standards had an external precision of ≤±15 ppm. ► The external reproducibility for ^{142}Nd/^{144}Nd is sufficient to resolve 20ppm anomalies.



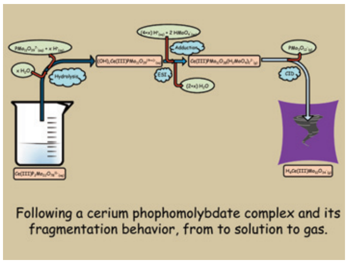
Separation of Pure Nd from rock samples for analyses using TIMS

35–46

Electrospray ionization mass spectrometry of a cerium(III) phosphomolybdate complex: Condensed and gas-phase cluster chemistry

T.H. Bray, R. Copping, D.K. Shuh and J.K. Gibson

► Cerium phosphomolybdate complexes have been transferred from solution to the gas phase by ESI. ► Compositions of large gas-phase complexes were established by successive CID. ► ^{31}P NMR demonstrates a direct correlation between solution and ESI speciation. ► Degradation and aggregation of complexes in dilute solutions is observed. ► The trivalent cerium oxidation state is established via substitution of ^{1}H$^+$ by ^{7}Li$^+$ counterions.



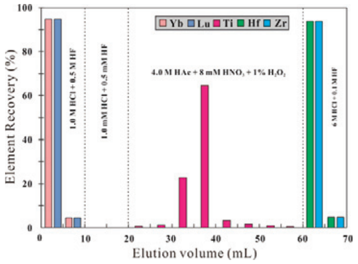
Following a cerium phophomolybdate complex and its fragmentation behavior, from to solution to gas.

47–52

A straightforward protocol for Hf purification by single step anion-exchange chromatography and isotopic analysis by MC-ICP-MS applied to geological reference materials and zircon standards

Y.-H. Yang, F.-Y. Wu, S.A. Wilde and L.-W. Xie

► To establish a rapid, straightforward protocol, based on conventional anion chromatography, which will enable the separation of Zr and Hf fractions from other interference (Yb, Lu) and matrix elements (Ti) so as to achieve a one-step chemical purification method and thus provide a viable alterative to complicated multiple-stage ion exchange chromatographic methods.

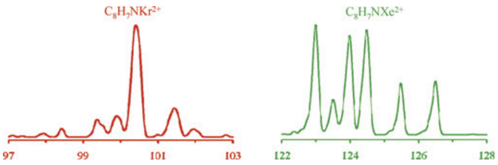


53–58

Influence of the structure of medium-sized aromatic precursors on the reactivity of their dications towards rare gases

E.-L. Zins and D. Schröder

► Several aromatic dication syield organoxenon species. ► Few organokrypton species also accessbile. ► Bond formation with rare gases as termolecular processes.

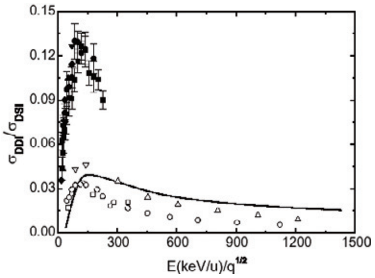


59–63

Relative cross-sections of charge transfer and ionization processes between multiply-charged ions and He at low and intermediate energies

B.W. Ding and D.Y. Yu

► We have considered a classical method, in which it is assumed that two electrons of target are removed one by one and the capture occurs prior to the ionization. ► This method has been applied to the evaluation of the cross-sections for single capture, double capture, single ionization, double ionization and transfer ionizationin collisions of multiply-charged ions A^{q+} (q = 2–5) with helium at low-to- intermediate velocities. ► The relative cross-sections are compared with the available experimental data. ► It is found that our results present a general good agreement with the experiments. ► It should also be emphasized that the present calculations are very simple and time saving.



64–70

Fast side-chain losses in keV ion-induced dissociation of protonated peptides

S. Bari, R. Hoekstra and T. Schlathölter

► Experimental study on keV ion-induced dissociation protonated peptides leucine enkephalin, bradykinin, LHRH and substance P. ► Ion-peptide interaction governed by resonant electron capture from the peptide and excitation due to electronic stopping. ► Immonium ions and side-chain fragments dominate the mass spectrum. ► KID seems to induce prompt cleavage of a side-chain linkage. ► Neutral side-chain cations are observed.