

International Journal of Mass Spectrometry

International Journal of Mass Spectrometry 185/186/187 (1999) 1005-1017

Subject index

Ab initio

Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies, 577

Ab initio calculations

Coulomb repulsion in multiply charged ions: a computational study of the effective dielectric constants of organic spacer groups, 351

On the formation of the carbon dioxide anion radical CO_2^- in the gas phase, 25

Metastable states of dimethylsulfonium radical, (CH₃)₂SH: a neutralization-reionization mass spectrometric and ab initio computational study, 639

Structure and stability of the CF_3^{2+} dication, 701

A theoretical study of the isomerization and dissociation processes of the $HO-C=O^+$ ion: interstate crossing in the formation of $H-C=O^+ + O$, 291

Ab initio quantum chemistry

The unimolecular chemistry of protonated hydroxylamine, 231

Acidity of metal ion hydrates M(H₂O)²⁺

Formation, acidity and charge reduction of the hydrates of doubly charged ions M²⁺ (Be²⁺, Mg²⁺, Ca²⁺, Zn²⁺), 685 Acrylonitrile

Ion-molecule association in acrylonitrile, 663

Aldehydes

Mass spectrometric analysis of pentafluorobenzyl oxime derivatives of reactive biological aldehydes, 795

Alkali atoms

Application of the DM formalism to the calculation of electron-impact ionization cross sections of alkali atoms, 319

Alkali metal ions

Absolute alkali metal ion binding affinities of several azoles determined by threshold collision-induced dissociation, 359

Ionic clathrates from aqueous solutions detected with laser induced liquid beam ionization/desorption mass spectrometry, 271

Alkenes

Selected ion flow tube studies of the atomic oxygen radical cation reactions with ethylene and other alkenes, 477

Allyl ion

Flow tube and theoretical study of proton transfer reactions of $C_3H_5^+$ ions, 253

Amine isomers

Selected ion flow tube studies of the reactions of H_3O^+ , NO^+ , and O_2^+ with eleven amine structural isomers of $C_5H_{13}N$, 139

Amino acids

Complexes of L-histidine with Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺ studied by electrospray ionization mass spectrometry, 11

Ammonia

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

Analytical applications

The application of ultra-short light pulses for the analysis of quickly relaxing organic molecules by means of laser mass spectrometry, 307

Angle-resolved mass spectrometry

Gas phase copper(I) ion affinities of valine, lysine, and arginine based on the dissociation of Cu⁺-bound heterodimers at varying internal energies, 107

Anion

Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies, 577

Anion radicals

On the formation of the carbon dioxide anion radical CO_2^- in the gas phase, 25

Arginine

Gas phase copper(I) ion affinities of valine, lysine, and arginine based on the dissociation of Cu⁺-bound heterodimers at varying internal energies, 107

Autoionization

Photoionization mass spectrometry of chlorine oxides, 545

Azoles

Absolute alkali metal ion binding affinities of several azoles determined by threshold collision-induced dissociation, 359

Back bonding

Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation, 263

BCl₃ or boron trichloride

Reaction of C_{60}^{2+} with BCl₃: observation of fullerene cage shrinkage, 149

Beam scattering

A crossed beam scattering study of reactions in the system acetylene cation-acetylene: formation of C_2HD^+ in $C_2D_2^+ + C_2H_2$ and formation of $C_4H_3^+$ and $C_4H_2^+$ in $C_2H_2^+ + C_2H_2$ collisions, 195

Benzene cation dissociation

Dissociation rates of energy-selected benzene cations: comparison of experimental results from ion cyclotron resonance and cylindrical ion trap time-of-flight mass spectrometry, 517

Benzenium cation

Isomerization and dissociation processes of protonated benzene and protonated fulvene in the gas phase, 241

Bicyclo[3,1,0]-hexenyl cation

Isomerization and dissociation processes of protonated benzene and protonated fulvene in the gas phase, 241

Binding affinities

Absolute alkali metal ion binding affinities of several azoles determined by threshold collision-induced dissociation, 359

Binding energy

Binding energies of chromium cations with fluorobenzenes from radiative association kinetics, 913

Mass spectrometric study of unimolecular decompositions of endohedral fullerenes, 61

Oxidation of CO and reduction of CO_2 by gas phase Zr^+ , ZrO^+ , and ZrO_2^+ , 117

Biomolecular nucleophilic substitution

Orientational effects in the direct $Cl^- + CH_3Cl\ S_N2$ reaction at elevated collision energies: hard-ovoid line-of-centers collision model, 343

Branching ratio

Selected ion flow tube studies of the atomic oxygen radical cation reactions with ethylene and other alkenes, 477

C_{co}^{2+}

Reaction of C_{60}^{2+} with BCl₃: observation of fullerene cage shrinkage, 149

C_{60}

Transition-metal C_{60} bonding by guided ion beam scattering, 603

Ca⁺(CH₃OH),

Molecular dynamics simulation of gas phase ion cluster formation, 883

Calculated

Experimental and theoretical study of the double ionization of the sulphur hexafluoride molecule to singlet and triplet electronic states of its dication, 651

Carbene anion

Carbyne thermochemistry from energy-resolved collision-induced dissociation. The heats of formation of CH, CF, and CCl, 745

Carbenes

Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment, 925

Carbon cluster

Hydrogen atom elimination from polycyclic aromatic hydrocarbons with sustained off-resonance irradiation: a new approach to produce carbon/hydrogen cluster cations $C_nH_x^+$, 1

Carbon dioxide

On the formation of the carbon dioxide anion radical CO₂⁻⁻ in the gas phase, 25

Oxidation of CO and reduction of CO_2 by gas phase Zr^+ , ZrO^+ , and ZrO_2^+ , 117

Carbon tetrachloride

Dissociative charge transfer in reactions of CCl₄ and SF₆ with ions having recombination energies between 6.4 eV and 24.5 eV, 759

Carbyne

Carbyne thermochemistry from energy-resolved collision-induced dissociation. The heats of formation of CH, CF, and CCl, 745

Catalytic hydrogenation

Reactions of electrosprayed rhodium phosphine complexes in the gas phase: modeling homogeneous catalytic hydrogenation, 871

CBS-QCVI/APNO

Conjugate base of a cyclic hydrazine: formation and energetics of N-diaziridyl anion, 179

2c-3e bonding

Experimental and theoretical investigation into the structural and thermodynamic properties of the mixed methyl halide association radical cations, 413

Charge separation

Near thermal energy collisions with fullerenes: a generally applicable soft ionization method for low IP molecules?, 497

Charge transfer

Dissociative charge transfer in reactions of ${\rm CCl_4}$ and ${\rm SF_6}$ with ions having recombination energies between 6.4 eV and 24.5 eV, 759

Selected ion flow tube studies of the reactions of H_3O^+ , NO^+ , and O_2^+ with eleven amine structural isomers of $C_5H_{13}N$, 139

Chemical ionization

Selected ion flow tube studies of the reactions of $\mathrm{H_3O^+}$, $\mathrm{NO^+}$, and $\mathrm{O_2^+}$ with eleven amine structural isomers of $\mathrm{C_5H_{13}N}$, 139

Ring versus oxygen protonation in metastable ion decompositions of protonated isopropyl phenyl ether, 393

Chirality

Chiral ions in the gas phase. 5. Acid-induced methanolysis of optically active styrene oxide, 425

Chiral recognition

Analysis of enantiomeric excess using mass spectrometry: fast atom bombardment/sector and electrospray ionization/Fourier transform mass spectrometric approaches, 977

Chiral recognition and the deprotonation reaction of gas-phase cytochrome c ions, 401

Chlorine oxides

Photoionization mass spectrometry of chlorine oxides, 545

Chromium ions

Binding energies of chromium cations with fluorobenzenes from radiative association kinetics, 913

Clathrates

Ionic clathrates from aqueous solutions detected with laser induced liquid beam ionization/desorption mass spectrometry, 271

Cluster

Nucleophilic displacement ($S_{\rm N}2$) reactions in binary van der Waals clusters induced by resonant electron capture, 463

Cluster anions

Formation of some transition metal oxide cluster anions and reactivity towards methanol in the gas phase, 825

Mass-spectrometric study of formation and stability of manganese and manganese oxide cluster anions, 673

Photodissociation of silver-coronene cluster cations, 617

Cluster assisted sigma bond activation

Activation of methane by ${\rm Ti}^+$: a cluster assisted mechanism for σ -bond activation, experiment, and theory, 989

Cluster ions

Molecular dynamics simulation of gas phase ion cluster formation, 883

Co⁺ + acetone

Bimolecular reaction dynamics of $Co^+(^3F_4)$ + acetone reaction in real time, 837

Collisional dynamics

A crossed beam scattering study of reactions in the system acetylene cation-acetylene: formation of C_2HD^+ in $C_2D_2^+ + C_2H_2$ and formation of $C_4H_3^+$ and $C_4H_2^+$ in $C_2H_2^+ + C_2H_2$ collisions, 195

Collision-assisted dissociation (CAD)

Collisional dissociation studies of Cu²⁺ (H₂O)_n using electrospray ionization mass spectrometry, 227

Collision-induced dissociation (CID)

Absolute alkali metal ion binding affinities of several azoles determined by threshold collision-induced dissociation, 359

Carbyne thermochemistry from energy-resolved collision-induced dissociation. The heats of formation of CH, CF, and CCl, 745

Complexes of L-histidine with Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺ studied by electrospray ionization mass spectrometry, 11

Hydrogen atom elimination from polycyclic aromatic hydrocarbons with sustained off-resonance irradiation: a new approach to produce carbon/hydrogen cluster cations $C_nH_r^+$, 1

The [Re, O₃]⁺ potential energy surface: Fourier transform ion cyclotron resonance collision induced dissociation studies and density functional calculations, 625

Molecular dynamics study of the collision-induced dissociation of the methyl nitrite cation, 847

Collision theory

Orientational effects in the direct ${\rm Cl}^- + {\rm CH_3Cl~S_N2}$ reaction at elevated collision energies: hard-ovoid line-of-centers collision model, 343

Condensed and gas phase comparison

Gas phase and condensed phase $S_{\rm N}{\rm i}$ reactions. The competitive five and six centre cyclisations of the 4,5-epoxypentoxide anion: a joint experimental and theoretical study, 327

CO oxidation

Oxidation of CO and reduction of CO_2 by gas phase Zr^+ , ZrO^+ , and ZrO_2^+ , 117

Copper (II)

Collisional dissociation studies of Cu^{2+} (H₂O)_n using electrospray ionization mass spectrometry, 227

Coulomb explosion

Coulomb repulsion in multiply charged ions: a computational study of the effective dielectric constants of organic spacer groups, 351

Cross sections

Application of the DM formalism to the calculation of electron-impact ionization cross sections of alkali atoms, 319

Cu⁺ affinity

Gas phase copper(I) ion affinities of valine, lysine, and arginine based on the dissociation of Cu⁺-bound heterodimers at varying internal energies, 107

DCO^{+}

Radiative lifetime measurements of the CO and CD stretching modes in DCO⁺, 131

Density functional calculations

The [Re, O₃]⁺ potential energy surface: Fourier transform ion cyclotron resonance collision induced dissociation studies and density functional calculations, 625

Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment, 925

Density functional theory (DFT)

Activation of methane by Ti^+ : a cluster assisted mechanism for σ -bond activation, experiment, and theory, 989 Computational approach to the proton affinities of Gly_n (n = 1-10), 935

Density functional theory (DFT) and G2 calculations Stepwise solvation of halides by alcohol molecules in the gas phase, 707

Deprotonation reaction

Chiral recognition and the deprotonation reaction of gas-phase cytochrome c ions, 401

Diaziridine

Conjugate base of a cyclic hydrazine: formation and energetics of *N*-diaziridyl anion, 179

Dications

Structure and stability of the CF_3^{2+} dication, 701

Dielectric constants

Coulomb repulsion in multiply charged ions: a computational study of the effective dielectric constants of organic spacer groups, 351

Dimethylsulfonium

Metastable states of dimethylsulfonium radical, $(CH_{3)2}SH$: a neutralization-reionization mass spectrometric and ab initio computational study, 639

Dissociation energy

Kinetic energy release for metastable fullerene ions, 813 Dissociation pathway

Dissociation pathways of sulfur dioxide clusters and mixed sulfur dioxide-water clusters, 905

Dissociative attachment

Thermally activated decay channels of superhot C_{60}^- : delayed electron emission and dissociative attachment studied by hyperthermal negative surface ionization, 773 Distonic anions

On the formation of the carbon dioxide anion radical CO_2^- in the gas phase, 25

Distonic ions

Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment, 925

Reactions of tert-butyl isocyanide with distonic radical cations, 91

Double-ionization energies

Experimental and theoretical study of the double ionization of the sulphur hexafluoride molecule to singlet and triplet electronic states of its dication, 651

Double-well potential model

Ion-molecule association in acrylonitrile, 663

Doubly charged rare gas ions

A Fourier transform ion cyclotron resonance study of two- and one-electron capture reactions between doubly charged rare gas ions and rare gas atoms, 281

Droplet fission

Theoretical prediction of charged droplet evaporation and fission in electrospray ionization, 97

Droplet

Theoretical prediction of charged droplet evaporation and fission in electrospray ionization, 97

Electron affinity (EA)

Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies, 577

Electron attachment

Nucleophilic displacement ($S_{\rm N}2$) reactions in binary van der Waals clusters induced by resonant electron capture, 463

Electron capture dissociation

Electron capture dissociation of multiply charged peptide cations, 787

Electron emission

Thermally activated decay channels of superhot C_{60}^- : delayed electron emission and dissociative attachment studied by hypethermal negative surface ionization, 773

Electronic correlation effects

A theoretical study of the isomerization and dissociation processes of the $HO-C = O^+$ ion: interstate crossing in the formation of $H-C = O^+ + O$, 291

Electronic structure calculations

Mg⁺NO and Mg⁺ON: potentially important ionospheric species, 961

Electron impact

Orthogonal electron impact source for a time-of-flight mass spectrometer with high mass resolving power, 221 Electron impact ionization

Application of the DM formalism to the calculation of electron-impact ionization cross sections of alkali atoms, 319

Electron transfer

Complexes of L-histidine with Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺ studied by electrospray ionization mass spectrometry, 11

Electroscopy

Electron capture dissociation of multiply charged peptide cations, 787

Electrospray

Collisional dissociation studies of $\mathrm{Cu^{2+}}\ (\mathrm{H_2O})_n$ using electrospray ionization mass spectrometry, 227

Influence of solvent composition and capillary temperature on the conformations of electrosprayed ions: unfold-

ing of compact ubiquitin conformers from pseudonative and denatured solutions, 37

Reactions of electrosprayed rhodium phosphine complexes in the gas phase: modeling homogeneous catalytic hydrogenation, 871

Electrospray ionization

Theoretical prediction of charged droplet evaporation and fission in electrospray ionization, 97

Enantiomer

Analysis of enantiomeric excess using mass spectrometry: fast atom bombardment/sector and electrospray ionization/Fourier transform mass spectrometric approaches, 977

Endohedral fullerenes

Ion mobility studies of metal-coated fullerenes, 507 Mass spectrometric study of unimolecular decompositions of endohedral fullerenes, 61

Energy

Vacuum ultraviolet single-photon and ultraviolet nonresonant two-photon pulsed field ionization photoelectron study of CH₃SCH₃, 533

Energy deposition

Molecular dynamics study of the collision-induced dissociation of the methyl nitrite cation, 847

Energy partitioning

Partitioning of kinetic energy to internal energy in the low energy collision-induced dissociations of proton-bound dimers of polypeptides, 75

Energy selection

Dissociation rates of energy-selected benzene cations: comparison of experimental results from ion cyclotron resonance and cylindrical ion trap time-of-flight mass spectrometry, 517

Entropy effects

Gas phase copper(I) ion affinities of valine, lysine, and arginine based on the dissociation of Cu⁺-bound heterodimers at varying internal energies, 107

4,5-Epoxypentoxide anion

Gas phase and condensed phase S_N i reactions. The competitive five and six centre cyclisations of the 4,5-epoxypentoxide anion: a joint experimental and theoretical study, 327

Exchange

Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation, 263

Excited states

Metastable states of dimethylsulfonium radical, $(CH_3)_2SH$: a neutralization-reionization mass spectrometric and ab initio computational study, 639

Field induced surface reactions

Field ionization behavior of cyclohexane on Au tips, 189

Field ion mass spectrometry

Field ionization behavior of cyclohexane on Au tips, 189 Field ion microscopy

Field ionization behavior of cyclohexane on Au tips, 189 Fine structure changing collisions

Laser excited N_2^+ in a 22-pole ion trap: experimental studies of rotational relaxation processes, 589

Flowing afterglow

Carbyne thermochemistry from energy-resolved collision-induced dissociation. The heats of formation of CH, CF, and CCl, 745

Gas phase chemistry of pyrene and related cations with molecules and atoms of interstellar interest, 949

Fluorobenzenes

Binding energies of chromium cations with fluorobenzenes from radiative association kinetics, 913

Fourier transform

Gas-phase bovine ubiquitin cation conformations resolved by gas-phase hydrogen/deuterium exchange rate and extent, 565

Fourier transform ion cyclotron resonance

Binding energies of chromium cations with fluorobenzenes from radiative association kinetics, 913

Dissociation rates of energy-selected benzene cations: comparison of experimental results from ion cyclotron resonance and cylindrical ion trap time-of-flight mass spectrometry, 517

Electron capture dissociation of multiply charged peptide cations, 787

Formation of some transition metal oxide cluster anions and reactivity towards methanol in the gas phase, 825

A Fourier transform ion cyclotron resonance study of two- and one-electron capture reactions between doubly charged rare gas ions and rare gas atoms, 281

Fragmentation

Reaction of C_{60}^{2+} with BCl₃: observation of fullerene cage shrinkage, 149

Fullerenes

Ion mobility studies of metal-coated fullerenes, 507 Kinetic energy release for metastable fullerene ions, 813 Reaction of C_{60}^{2+} with BCl_3 : observation of fullerene cage

shrinkage, 149 Thermally activated decay channels of superhot C_{60}^- : delayed electron emission and dissociative attachment studied by hypethermal negative surface ionization, 773 Transition-metal C_{60} bonding by guided ion beam scat-

tering, 603

Gas basicity

Gas-phase reactivity of HS₂H⁺⁺ and S₂⁺⁺: an investigation of the gas basicity and proton affinity of HS₂, 727

Gas phase

Chiral recognition and the deprotonation reaction of gas-phase cytochrome c ions, 401

Complexes of L-histidine with Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺ studied by electrospray ionization mass spectrometry, 11

Gas-phase ion chemistry

Chiral ions in the gas phase. 5. Acid-induced methanolysis of optically active styrene oxide, 425

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

Gas phase ion-molecule reactions

Gas-phase bovine ubiquitin cation conformations resolved by gas-phase hydrogen/deuterium exchange rate and extent, 565

G2(MP2) molecular orbital calculation

Isomerization and dissociation processes of protonated benzene and protonated fulvene in the gas phase, 241 G2 theory

Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation, 263

Guided ion beams

Absolute alkali metal ion binding affinities of several azoles determined by threshold collision-induced dissociation, 359

Oxidation of CO and reduction of CO_2 by gas phase Zr^+ , ZrO^+ , and ZrO_2^+ , 117

Halide alcohol clusters

Stepwise solvation of halides by alcohol molecules in the gas phase, 707

$H-Co_2^+$

A theoretical study of the isomerization and dissociation processes of the $HO-C = O^+$ ion: interstate crossing in the formation of $H-C = O^+ + O$, 291

$HO-C=O^+$

A theoretical study of the isomerization and dissociation processes of the $HO-C = O^+$ ion: interstate crossing in the formation of $H-C = O^+ + O$, 291

Homogeneous catalysis

Reactions of electrosprayed rhodium phosphine complexes in the gas phase: modeling homogeneous catalytic hydrogenation, 871

HS² radical

Gas-phase reactivity of HS_2H^+ and S_2^+ : an investigation of the gas basicity and proton affinity of HS_2^- , 727

Hydration

Collisional dissociation studies of Cu^{2+} (H₂O)_n using electrospray ionization mass spectrometry, 227

Hydration of metal ions M2+

Formation, acidity and charge reduction of the hydrates of doubly charged ions M^{2+} (Be²⁺, Mg^{2+} , Ca^{2+} , Zn^{2+}), 685

Hydrazine

Conjugate base of a cyclic hydrazine: formation and energetics of *N*-diaziridyl anion, 179

Hydrogen-deuterium exchange

Gas-phase bovine ubiquitin cation conformations resolved by gas-phase hydrogen/deuterium exchange rate and extent, 565

Hydrogen elimination

Hydrogen atom elimination from polycyclic aromatic hydrocarbons with sustained off-resonance irradiation: a new approach to produce carbon/hydrogen cluster cations $C_nH_v^+$, 1

Hypervalent radicals

Metastable states of dimethylsulfonium radical, (CH₃)₂SH: a neutralization-reionization mass spectrometric and ab initio computational study, 639

Intermediate complex formation

A crossed beam scattering study of reactions in the system acetylene cation-acetylene: formation of C_2HD^+ in $C_2D_2^+ + C_2H_2$ and formation of $C_4H_3^+$ and $C_4H_2^+$ in $C_2H_2^+ + C_2H_2$ collisions, 195

Internal energy content

Radiative lifetime measurements of the CO and CD stretching modes in DCO⁺, 131

Interstate crossing

A theoretical study of the isomerization and dissociation processes of the HO-C=O⁺ ion: interstate crossing in the formation of H-C=O⁺ + O, 291

Interstellar chemistry

Gas phase chemistry of pyrene and related cations with molecules and atoms of interstellar interest, 949

Gas-phase reactivity of HS₂H⁺⁺ and S₂⁺⁻: an investigation of the gas basicity and proton affinity of HS₂, 727

Intramolecular H-atom transfer

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

Ion activation

Molecular dynamics study of the collision-induced dissociation of the methyl nitrite cation, 847

Ion-association reactions

Ion-molecule association in acrylonitrile, 663

Ion cyclotron resonance (ICR)

Conjugate base of a cyclic hydrazine: formation and energetics of *N*-diaziridyl anion, 179

Gas-phase bovine ubiquitin cation conformations resolved by gas-phase hydrogen/deuterium exchange rate and extent, 565

Ion-molecule association in acrylonitrile, 663

Ion formation

Is the incorporation of analytes into matrix crystals a prerequisite for matrix-assisted laser desorption/ionization mass spectrometry? A study of five positional isomers of dihydroxybenzoic acid, 859

Ion fragmentation

The application of ultra-short light pulses for the analysis of quickly relaxing organic molecules by means of laser mass spectrometry, 307

Ionization

Near thermal energy collisions with fullerenes: a generally applicable soft ionization method for low IP molecules?, 497

Vacuum ultraviolet single-photon and ultraviolet nonresonant two-photon pulsed field ionization photoelectron study of CH_3SCH_3 , 533

Ionization energy

Ethene loss kinetics of methyl butanoate ions studied by threshold photoelectron-photoion coincidence: the enol ion of methyl acetate heat of formation, 165

Ion mobility

Influence of solvent composition and capillary temperature on the conformations of electrosprayed ions: unfolding of compact ubiquitin conformers from pseudonative and denatured solutions, 37

Ion mobility studies of metal-coated fullerenes, 507

Ion-molecule dynamics

Bimolecular reaction dynamics of $Co^+(^3F_4)$ + acetone reaction in real time, 837

Ion-molecule reactions

A crossed beam scattering study of reactions in the system acetylene cation-acetylene: formation of C_2HD^+ in $C_2D_2^+ + C_2H_2$ and formation of $C_4H_3^+$ and $C_4H_2^+$ in $C_2H_2^{+-} + C_2H_2$ collisions, 195

Experimental and theoretical investigation into the structural and thermodynamic properties of the mixed methyl halide association radical cations, 413

Gas phase chemistry of pyrene and related cations with molecules and atoms of interstellar interest, 949

Gas-phase reactivity of HS_2H^{++} and S_2^{+-} : an investigation of the gas basicity and proton affinity of HS_2 , 727

Nucleophilic displacement ($S_{\rm N}2$) reactions in binary van der Waals clusters induced by resonant electron capture, 463

Reactions of tert-butyl isocyanide with distonic radical cations, 91

Selected ion flow tube studies of the atomic oxygen radical cation reactions with ethylene and other alkenes, 477

Selected ion flow tube studies of the reactions of H_3O^+ , NO^+ , and O_2^+ with eleven amine structural isomers of $C_5H_{13}N$, 139

Ionospheric species

Mg⁺NO and Mg⁺ON: potentially important ionospheric species, 961

Ion source

Orthogonal electron impact source for a time-of-flight mass spectrometer with high mass resolving power, 221 Ion temperatures

Thermal dissociation in the quadrupole ion trap: ions derived from leucine enkephalin, 207

Ion traps

Laser excited N_2^+ in a 22-pole ion trap: experimental studies of rotational relaxation processes, 589

Ion vibrational relaxation

Vibratonal relaxation of NO⁺ (ν) in collisions with CH₄: experimental and theoretical studies, 559

Isocyanides

Reactions of tert-butyl isocyanide with distonic radical cations, 91

Isomeric structures

Flow tube and theoretical study of proton transfer reactions of $C_3H_5^+$ ions, 253

Isotopic exchange

Ring versus oxygen protonation in metastable ion decompositions of protonated isopropyl phenyl ether, 393

Jahn-Teller effect

Structure and stability of the CF₃²⁺ dication, 701

Keto-enol tautomerization

Ethene loss kinetics of methyl butanoate ions studied by threshold photoelectron-photoion coincidence: the enol ion of methyl acetate heat of formation, 165

Kinetic energy release distributions (KERDs)

Mass spectrometric study of unimolecular decompositions of endohedral fullerenes, 61

Kinetic energy release (KER)

Dissociation of N_2O^+ ions from the valence states reached by one-photon photoionization, 437

Ethene loss kinetics of methyl butanoate ions studied by threshold photoelectron-photoion coincidence: the enol ion of methyl acetate heat of formation, 165

Experimental and theoretical investigation into the structural and thermodynamic properties of the mixed methyl halide association radical cations, 413

Kinetic energy release for metastable fullerene ions, 813 Unimolecular reaction dynamics from kinetic energy release distributions. IV. Dissociation of the pyridine ion, 155

Kinetic method

Partitioning of kinetic energy to internal energy in the low energy collision-induced dissociations of proton-bound dimers of polypeptides, 75

Kinetics

Selected ion flow tube studies of the atomic oxygen radical cation reactions with ethylene and other alkenes, 477

Landau-Zener

Near thermal energy collisions with fullerenes: a generally applicable soft ionization method for low IP molecules?, 497

Laser desorption

The application of ultra-short light pulses for the analysis of quickly relaxing organic molecules by means of laser mass spectrometry, 307

Ionic clathrates from aqueous solutions detected with laser induced liquid beam ionization/desorption mass spectrometry, 271

Laser desorption ionization

Formation of some transition metal oxide cluster anions and reactivity towards methanol in the gas phase, 825

Laser induced charge transfer

Laser excited N_2^+ in a 22-pole ion trap: experimental studies of rotational relaxation processes, 589

Laser mass spectrometry

The application of ultra-short light pulses for the analysis of quickly relaxing organic molecules by means of laser mass spectrometry, 307

Leucine enkephalin

Thermal dissociation in the quadrupole ion trap: ions derived from leucine enkephalin, 207

Ligand exchange

Solvent displacement in transition metal complexes, 49 Lysine

Gas phase copper(I) ion affinities of valine, lysine, and arginine based on the dissociation of Cu⁺-bound heterodimers at varying internal energies, 107

Manganese

Mass-spectrometric study of formation and stability of manganese and manganese oxide cluster anions, 673 Mass-analyzed ion kinetic energy (MIKE)

Kinetic energy release for metastable fullerene ions, 813 Ring versus oxygen protonation in metastable ion decompositions of protonated isopropyl phenyl ether, 393

Mass spectrometric determination

Analysis of enantiomeric excess using mass spectrometry: fast atom bombardment/sector and electrospray ionization/Fourier transform mass spectrometric approaches, 977

Mass spectrometry

On the formation of the carbon dioxide anion radical CO_2^- in the gas phase, 25

Gas-phase bovine ubiquitin cation conformations resolved by gas-phase hydrogen/deuterium exchange rate and extent, 565

Ionic clathrates from aqueous solutions detected with laser induced liquid beam ionization/desorption mass spectrometry, 271

The [Re, O₃]⁺ potential energy surface: Fourier transform ion cyclotron resonance collision induced dissociation studies and density functional calculations, 625

Mass spectrometric analysis of pentafluorobenzyl oxime derivatives of reactive biological aldehydes, 795

Mass-spectrometric study of formation and stability of manganese and manganese oxide cluster anions, 673

The unimolecular chemistry of protonated hydroxylamine, 231

Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS)

Is the incorporation of analytes into matrix crystals a prerequisite for matrix-assisted laser desorption/ionization mass spectrometry? A study of five positional isomers of dihydroxybenzoic acid, 859

Matrix effects

Is the incorporation of analytes into matrix crystals a prerequisite for matrix-assisted laser desorption/ionization mass spectrometry? A study of five positional isomers of dihydroxybenzoic acid, 859

Maximum entropy method

Unimolecular reaction dynamics from kinetic energy release distributions. IV. Dissociation of the pyridine ion, 155

Measured

Experimental and theoretical study of the double ionization of the sulphur hexafluoride molecule to singlet and triplet electronic states of its dication, 651

Mechanism

Ring versus oxygen protonation in metastable ion decompositions of protonated isopropyl phenyl ether, 393

Metal clusters

Near thermal energy collisions with fullerenes: a generally applicable soft ionization method for low IP molecules?, 497

Metal-coated fullerene

Ion mobility studies of metal-coated fullerenes, 507 Metal complexes

Solvent displacement in transition metal complexes, 49 Metal ion hydrates, preparation, and stabilities

Formation, acidity and charge reduction of the hydrates of doubly charged ions M^{2+} (Be²⁺, Mg^{2+} , Ca^{2+} , Zn^{2+}), 685

Metal ion solvation

Molecular dynamics simulation of gas phase ion cluster formation, 883

Metal oxides

Mass-spectrometric study of formation and stability of manganese and manganese oxide cluster anions, 673

Metastable decay

Kinetic energy release for metastable fullerene ions, 813 Metastable dissociation

Competitive elimination of methane and ethylene from trimethylsilyl-substituted silylenium ions, 449

Metastable negative ions

Thermally activated decay channels of superhot C_{60}^- : delayed electron emission and dissociative attachment studied by hyperthermal negative surface ionization, 773 Methane activation

Activation of methane by Ti⁺: a cluster assisted mechanism for σ -bond activation, experiment, and theory, 989 Methanolysis

Chiral ions in the gas phase. 5. Acid-induced methanolysis of optically active styrene oxide, 425

Methyl halides

Experimental and theoretical investigation into the structural and thermodynamic properties of the mixed methyl halide association radical cations, 413

Molecular orbital calculations

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

Monitor ion technique

Radiative lifetime measurements of the CO and CD stretching modes in DCO⁺, 131

MS/MS

Experimental and theoretical investigation into the structural and thermodynamic properties of the mixed methyl halide association radical cations, 413

Multiply charged ions

Coulomb repulsion in multiply charged ions: a computational study of the effective dielectric constants of organic spacer groups, 351

Negative ions

Nucleophilic displacement (S_N2) reactions in binary van der Waals clusters induced by resonant electron capture, 463

Neutralization-reionization

Metastable states of dimethylsulfonium radical, (CH₃)₂SH: a neutralization-reionization mass spectrometric and ab initio computational study, 639

Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment, 925

N₂O⁺ dissociation

Dissociation of N_2O^+ ions from the valence states reached by one-photon photoionization, 437

$NO^+(\nu)$

Vibratonal relaxation of NO $^+$ (ν) in collisions with CH $_4$: experimental and theoretical studies, 559

O2 ligand

The [Re, O₃]⁺ potential energy surface: Fourier transform ion cyclotron resonance collision induced dissociation studies and density functional calculations, 625

Optical purity

Analysis of enantiomeric excess using mass spectrometry: fast atom bombardment/sector and electrospray ionization/Fourier transform mass spectrometric approaches, 977

Organic substances

The application of ultra-short light pulses for the analysis of quickly relaxing organic molecules by means of laser mass spectrometry, 307

Organosilicon

Competitive elimination of methane and ethylene from trimethylsilyl-substituted silylenium ions, 449

Paul trap

Dissociation rates of energy-selected benzene cations: comparison of experimental results from ion cyclotron resonance and cylindrical ion trap time-of-flight mass spectrometry, 517

Pentafluorobenzyl oxime

Mass spectrometric analysis of pentafluorobenzyl oxime derivatives of reactive biological aldehydes, 795

Peptide dissociation

Partitioning of kinetic energy to internal energy in the low energy collision-induced dissociations of proton-bound dimers of polypeptides, 75

Peptides

Electron capture dissociation of multiply charged peptide cations, 787

Phase space

Unimolecular reaction dynamics from kinetic energy release distributions. IV. Dissociation of the pyridine ion, 155

Photodissociation

Photodissociation of silver-coronene cluster cations, 617 Photoelectron

Vacuum ultraviolet single-photon and ultraviolet nonresonant two-photon pulsed field ionization photoelectron study of CH₃SCH₃, 533

Photoelectron-photoion coincidence (PEPICO)

Dissociation of N_2O^+ ions from the valence states reached by one-photon photoionization, 437

Photoelectron spectroscopy

Dissociative charge transfer in reactions of CCl_4 and SF_6 with ions having recombination energies between 6.4 eV and 24.5 eV, 759

Photoelectron spectrum

Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies, 577

Photoionization

Vacuum ultraviolet single-photon and ultraviolet nonresonant two-photon pulsed field ionization photoelectron study of CH₃SCH₃, 533

Photoionization mass spectrometry

Photoionization mass spectrometry of chlorine oxides, 545

π interactions

Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation, 263

Polycyclic aromatic hydrocarbons (PAH)

Gas phase chemistry of pyrene and related cations with molecules and atoms of interstellar interest, 949

Hydrogen atom elimination from polycyclic aromatic hydrocarbons with sustained off-resonance irradiation: a new approach to produce carbon/hydrogen cluster cations $C_uH_u^+$, 1

Polyether

Solvent displacement in transition metal complexes, 49 Polyglycine

Computational approach to the proton affinities of Gly_n (n = 1-10), 935

Propane

Kinetic energy release for metastable fullerene ions, 813 2-Propenyl ion

Flow tube and theoretical study of proton transfer reactions of $C_3H_5^+$ ions, 253

Protein

Gas-phase bovine ubiquitin cation conformations resolved by gas-phase hydrogen/deuterium exchange rate and extent, 565

Proton affinity

Computational approach to the proton affinities of Gly_n (n = 1-10), 935

Gas-phase reactivity of HS₂H⁺⁺ and S₂⁺⁺: an investigation of the gas basicity and proton affinity of HS₂, 727

The unimolecular chemistry of protonated hydroxylamine, 231

Protonated benzene

Isomerization and dissociation processes of protonated benzene and protonated fulvene in the gas phase, 241

Protonated fulvene

Isomerization and dissociation processes of protonated benzene and protonated fulvene in the gas phase, 241

Proton-bound dimers

Partitioning of kinetic energy to internal energy in the low energy collision-induced dissociations of proton-bound dimers of polypeptides, 75

Proton transfer

Flow tube and theoretical study of proton transfer reactions of $C_3H_5^+$ ions, 253

Selected ion flow tube studies of the reactions of H_3O^+ , NO^+ , and O_2^+ with eleven amine structural isomers of $C_5H_{13}N$, 139

Proton transfer, intramolecular, in metal ion hydrates

Formation, acidity and charge reduction of the hydrates of doubly charged ions M^{2+} (Be²⁺, Mg^{2+} , Ca^{2+} , Zn^{2+}), 685

Pulsed-ionization high pressure mass spectrometry

Stepwise solvation of halides by alcohol molecules in the gas phase, 707

Pyridine ion

Unimolecular reaction dynamics from kinetic energy release distributions. IV. Dissociation of the pyridine ion, 155

Quadrupole ion trap

Thermal dissociation in the quadrupole ion trap: ions derived from leucine enkephalin, 207

Radiative association

Binding energies of chromium cations with fluorobenzenes from radiative association kinetics, 913

Radiative lifetimes

Radiative lifetime measurements of the CO and CD stretching modes in DCO⁺, 131

Rare gas ion/atom reactions

A Fourier transform ion cyclotron resonance study of two- and one-electron capture reactions between doubly charged rare gas ions and rare gas atoms, 281

Rate coefficients

A Fourier transform ion cyclotron resonance study of two- and one-electron capture reactions between doubly charged rare gas ions and rare gas atoms, 281

Laser excited N₂⁺ in a 22-pole ion trap: experimental studies of rotational relaxation processes, 589

Rate constant

Molecular dynamics study of the collision-induced dissociation of the methyl nitrite cation, 847

Rayleigh limit

Theoretical prediction of charged droplet evaporation and fission in electrospray ionization, 97

Reaction dynamics

Molecular dynamics study of the collision-induced dissociation of the methyl nitrite cation, 847

Reactivity

Formation of some transition metal oxide cluster anions and reactivity towards methanol in the gas phase, 825 Mass-spectrometric study of formation and stability of manganese and manganese oxide cluster anions, 673

Rhenium

The [Re, O₃]⁺ potential energy surface: Fourier transform ion cyclotron resonance collision induced dissociation studies and density functional calculations, 625

Rhodium phosphine complexes

Reactions of electrosprayed rhodium phosphine complexes in the gas phase: modeling homogeneous catalytic hydrogenation, 871

Ring-opening reaction

Chiral ions in the gas phase. 5. Acid-induced methanolysis of optically active styrene oxide, 425

Rotational relaxation

Laser excited N_2^+ in a 22-pole ion trap: experimental studies of rotational relaxation processes, 589

Scattering

Molecular dynamics study of the collision-induced dissociation of the methyl nitrite cation, 847

Transition-metal C_{60} bonding by guided ion beam scattering, 603

Selected ion flow drift tube

Vibratonal relaxation of NO⁺ (ν) in collisions with CH₄: experimental and theoretical studies, 559

Selected ion flow tube (SIFT)

Dissociative charge transfer in reactions of CCl_4 and SF_6 with ions having recombination energies between 6.4 eV and 24.5 eV, 759

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

Flow tube and theoretical study of proton transfer reactions of $C_3H_5^+$ ions, 253

Ion-molecule association in acrylonitrile, 663

Selected ion flow tube studies of the atomic oxygen radical cation reactions with ethylene and other alkenes, 477

Selected ion flow tube studies of the reactions of ${\rm H_3O^+}$, ${\rm NO^+}$, and ${\rm O_2^+}$ with eleven amine structural iosomers of ${\rm C_5H_{13}N}$, 139

SF_6

Experimental and theoretical study of the double ionization of the sulphur hexafluoride molecule to singlet and triplet electronic states of its dication, 651

Silicon fluoride cations

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular

H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

S_Ni reactions

Gas phase and condensed phase $S_{\rm N}i$ reactions. The competitive five and six centre cyclisations of the 4,5-epoxypentoxide anion: a joint experimental and theoretical study, 327

S_N2 reactions

Nucleophilic displacement (S_N 2) reactions in binary van der Waals clusters induced by resonant electron capture, 463

Orientational effects in the direct Cl⁻ + CH₃Cl S_N2 reaction at elevated collision energies: hard-ovoid line-of-centers collision model, 343

SO2 clusters

Dissociation pathways of sulfur dioxide clusters and mixed sulfur dioxide-water clusters, 905

SO₂-H₂O clusters

Dissociation pathways of sulfur dioxide clusters and mixed sulfur dioxide-water clusters, 905

Solvating collisions

Molecular dynamics simulation of gas phase ion cluster formation, 883

Solvation

Ionic clathrates from aqueous solutions detected with laser induced liquid beam ionization/desorption mass spectrometry, 271

Solvent displacement in transition metal complexes, 49 Solvation dynamics

Molecular dynamics simulation of gas phase ion cluster formation, 883

Solvent

Influence of solvent composition and capillary temperature on the conformations of electrosprayed ions: unfolding of compact ubiquitin conformers from pseudonative and denatured solutions, 37

Spin-orbit coupling

The unimolecular chemistry of protonated hydroxylamine, 231

Steady state kinetics

Ring versus oxygen protonation in metastable ion decompositions of protonated isopropyl phenyl ether, 393

Structure

Computational approach to the proton affinities of Gly_n (n = 1-10), 935

Dissociation pathways of sulfur dioxide clusters and mixed sulfur dioxide-water clusters, 905

Structures and stabilities

Experimental and theoretical studies of gas-phase reactions of SiF_x^+ (x = 1-3) with ammonia: intramolecular H-atom transfer reactions with SiF_3^+ and $F_2Si(NH_2)^+$, 381

Styrene oxide

Chiral ions in the gas phase. 5. Acid-induced methanolysis of optically active styrene oxide, 425

Sulfur hexafluoride

Dissociative charge transfer in reactions of ${\rm CCl_4}$ and ${\rm SF_6}$ with ions having recombination energies between 6.4 eV and 24.5 eV, 759

Surface ionization

Thermally activated decay channels of superhot C_{60}^- : delayed electron emission and dissociative attachment studied by hyperthermal negative surface ionization, 773 Sustained off-resonance irradiation (SORI)

Hydrogen atom elimination from polycyclic aromatic hydrocarbons with sustained off-resonance irradiation: a new approach to produce carbon/hydrogen cluster cations $C_nH_x^+$, 1

Symmetry

Structure and stability of the CF₃²⁺ dication, 701

Tautomerization

Absolute alkali metal ion binding affinities of several azoles determined by threshold collision-induced dissociation, 359

Temperature

Influence of solvent composition and capillary temperature on the conformations of electrosprayed ions: unfolding of compact ubiquitin conformers from pseudonative and denatured solutions, 37

Theoretical calculation

Application of the DM formalism to the calculation of electron-impact ionization cross sections of alkali atoms, 319

Theory

Competitive elimination of methane and ethylene from trimethylsilyl-substituted silylenium ions, 449

Theoretical prediction of charged droplet evaporation and fission in electrospray ionization, 97

Thermal dissociation

Thermal dissociation in the quadrupole ion trap: ions derived from leucine enkephalin, 207

Thermochemistry

Carbyne thermochemistry from energy-resolved collision-induced dissociation. The heats of formation of CH, CF, and CCl, 745

Conjugate base of a cyclic hydrazine: formation and energetics of N-diaziridyl anion, 179

Photoionization mass spectrometry of chlorine oxides, 545

Stepwise solvation of halides by alcohol molecules in the gas phase, 707

Three-membered heterocyclic ions

Exchange reactions of chloriranium and chlorirenium ions: a G2 investigation, 263

Time-of-flight mass spectrometry

Bimolecular reaction dynamics of $Co^+(^3F_4)$ + acetone reaction in real time, 837

Orthogonal electron impact source for a time-of-flight mass spectrometer with high mass resolving power, 221 Photodissociation of silver-coronene cluster cations, 617 Titanium

Activation of methane by ${\rm Ti}^+$: a cluster assisted mechanism for σ -bond activation, experiment, and theory, 989 Trace gas analysis

Selected ion flow tube studies of the reactions of H_3O^+ , NO^+ , and O_2^+ with eleven amine structural isomers of $C_sH_{13}N$, 139

Transition metal

Activation of methane by Ti⁺: a cluster assisted mechanism for σ -bond activation, experiment, and theory, 989 Transition metal atom chemistry

Bimolecular reaction dynamics of $Co^+(^3F_4)$ + acetone reaction in real time, 837

Transition metal complexes

Complexes of L-histidine with Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺ studied by electrospray ionization mass spectrometry, 11

Transition-metal ions

Transition-metal C_{60} bonding by guided ion beam scattering, 603

Transition metal oxide anions

Formation of some transition metal oxide cluster anions and reactivity towards methanol in the gas phase, 825

Two-electron capture

A Fourier transform ion cyclotron resonance study of two- and one-electron capture reactions between doubly charged rare gas ions and rare gas atoms, 281

Ubiquitin

Influence of solvent composition and capillary temperature on the conformations of electrosprayed ions: unfolding of compact ubiquitin conformers from pseudonative and denatured solutions, 37

Ultra-short laser pulses

The application of ultra-short light pulses for the analysis of quickly relaxing organic molecules by means of laser mass spectrometry, 307

Unimolecular chemistry

The unimolecular chemistry of protonated hydroxylamine, 231

Unimolecular reaction

Competitive elimination of methane and ethylene from trimethylsilyl-substituted silylenium ions, 449

Validity of statistical theory

Unimolecular reaction dynamics from kinetic energy release distributions. IV. Dissociation of the pyridine ion, 155

Vibrational spectrum

Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies, 577

Ylides

Pyrazine diradicals, carbenes, ylides, and distonic ions probed by theory and experiment, 925

Zicronium oxide ions

Oxidation of CO and reduction of CO_2 by gas phase Zr^+ , ZrO^+ , and ZrO_2^+ , 117

Zirconium ions

Oxidation of CO and reduction of $\rm CO_2$ by gas phase $\rm Zr^+$, $\rm ZrO^+$, and $\rm ZrO_2^+$, 117

Zwitterion

Computational approach to the proton affinities of Gly_n (n = 1-10), 935