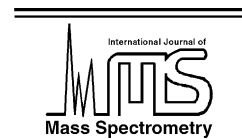




ELSEVIER

International Journal of Mass Spectrometry 217 (2002) 275–277



www.elsevier.com/locate/ijms

Subject index Volume 217

Ab initio

Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153

Ab initio calculations

Self-catalysis in the gas-phase: enolization of the acetone radical cation, 97

Acid-catalyzed cyclization

Thermochemistry and unimolecular reactivity of protonated α,ω -aminoalcohols in the gas phase, 195

Adduct

Adduct formation between phthalate esters and Li^+ in the gas phase: a thermochemical study by FT-ICR mass spectrometry, 75

O-alkyl benzaldoximes

Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153

Alkyl transfer transition states

Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C_5 – C_7 ketones in the gas phase, 257

Allylic cations

Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C_5 – C_7 ketones in the gas phase, 257

Ammonia loss

Evidence for the formation of acyclic ions from the radical cations and cyclic ions from the protonated molecules of α,ω -diamines upon loss of ammonia, 55

Aniline

Ionized aniline and its distonic radical cation isomers, 45

Associative ion–molecule reactions

Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation, 1

Basicity

Adduct formation between phthalate esters and Li^+ in the gas phase: a thermochemical study by FT-ICR mass spectrometry, 75

Benzaldehyde

Distonic isomers of ionized benzaldehyde, 65

Binding energies

The ions $\text{CH}_6\text{O}^{\bullet+}$ and CH_7O^+ , 179

Carbon

Silicon- versus carbon-containing ions: 1,3- CH_3^+ transfers, 245

Carbon cluster

Small carbon clusters (C_n^0 , C_n^+ , C_n^-) from acyclic and cyclic precursors. Neutralization–reionization and theory, 81

C–H bond activation

Regio- and diastereoselective C–H bond activation of valeramide and 3-methyl valeramide by bare Fe^+ ions, 169

CH_3^+ transfers

Silicon- versus carbon-containing ions: 1,3- CH_3^+ transfers, 245

Chemical ionization

Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C_5 – C_7 ketones in the gas phase, 257

Collisionally activated decomposition

Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C_5 – C_7 ketones in the gas phase, 257

Collisionally activated dissociation

Small carbon clusters (C_n^0 , C_n^+ , C_n^-) from acyclic and cyclic precursors. Neutralization–reionization and theory, 81

Collision-induced dissociation

Evidence for the formation of acyclic ions from the radical cations and cyclic ions from the protonated molecules of α,ω -diamines upon loss of ammonia, 55

Reactions of low-energy pentenyl methyl ether radical cations $\text{C}_2\text{H}_5\text{CH}=\text{CHCH}_2\text{OCH}_3^{\bullet+}$, $\text{CH}_2=\text{CHCH}(\text{C}_2\text{H}_5)\text{OCH}_3^{\bullet+}$ and $\text{CH}_2=\text{C}(\text{C}_2\text{H}_5)\text{CH}_2\text{OCH}_3^{\bullet+}$, 109

Convergency

A theoretical study of the interaction between Ni^+ and small oxygen- and nitrogen-containing bases, 119

Cyclization reactions

Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131

Cyclopropylcarbanyl cations

Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C_5 – C_7 ketones in the gas phase, 257

Density functional theory

Why are smaller fragments preferentially lost from radical cations at low energies and larger ones at high energies?. An experimental and theoretical study, 23

A theoretical study of the interaction between Ni^+ and small oxygen- and nitrogen-containing bases, 119

Density-functional calculations

Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation, 1

- Deuterated derivatives
 Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153
- Deuterium labelling
 Reactions of low-energy pentenyl methyl ether radical cations $C_2H_5CH=CHCH_2OCH_3^{\bullet+}$, $CH_2=CHCH(C_2H_5)OCH_3^{\bullet+}$ and $CH_2=C(C_2H_5)CH_2OCH_3^{\bullet+}$, 109
- DFT molecular orbital calculations
 B3LYP DFT molecular orbital approach, an efficient method to evaluate the thermochemical properties of MALDI matrices, 231
- α,ω -Diamines
 Evidence for the formation of acyclic ions from the radical cations and cyclic ions from the protonated molecules of α,ω -diamines upon loss of ammonia, 55
- Dimer radical cation
 Self-catalysis in the gas-phase: enolization of the acetone radical cation, 97
- Distonic ion
 Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153
- Distonic ions
 Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation, 1
 Distonic isomers of ionized benzaldehyde, 65
 Reactions of low-energy pentenyl methyl ether radical cations $C_2H_5CH=CHCH_2OCH_3^{\bullet+}$, $CH_2=CHCH(C_2H_5)OCH_3^{\bullet+}$ and $CH_2=C(C_2H_5)CH_2OCH_3^{\bullet+}$, 109
- Distonic radical cations
 Ionized aniline and its distonic radical cation isomers, 45
- Electron affinity
 B3LYP DFT molecular orbital approach, an efficient method to evaluate the thermochemical properties of MALDI matrices, 231
- Enolization
 Self-catalysis in the gas-phase: enolization of the acetone radical cation, 97
- Fe⁺ chemistry
 Regio- and diastereoselective C–H bond activation of valeramide and 3-methyl valeramide by bare Fe⁺ ions, 169
- Fragmentation mechanism
 Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153
- Fragmentation reactions
 Fragmentation reactions of protonated peptides containing phenylalanine: a linear free energy correlation in the fragmentation of H–Gly–Xxx–Phe–OH, 185
- FT-ICR
 Adduct formation between phthalate esters and Li⁺ in the gas phase: a thermochemical study by FT-ICR mass spectrometry, 75
- H/D exchange
 Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131
- Hydride transfer
 Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131
- Hydride transfer transition states
 Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C₅–C₇ ketones in the gas phase, 257
- Hydroxypyridine
 Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation, 1
- Ion structures
 Evidence for the formation of acyclic ions from the radical cations and cyclic ions from the protonated molecules of α,ω -diamines upon loss of ammonia, 55
- Ion/molecule complexes
 Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131
- Ion/molecule reactions
 Evidence for the formation of acyclic ions from the radical cations and cyclic ions from the protonated molecules of α,ω -diamines upon loss of ammonia, 55
- Ion/neutral complexes
 The ions CH₆O^{•+} and CH₇O⁺, 179
- Ionization energy
 B3LYP DFT molecular orbital approach, an efficient method to evaluate the thermochemical properties of MALDI matrices, 231
- Lithium cation
 Adduct formation between phthalate esters and Li⁺ in the gas phase: a thermochemical study by FT-ICR mass spectrometry, 75
- MALDI matrices
 B3LYP DFT molecular orbital approach, an efficient method to evaluate the thermochemical properties of MALDI matrices, 231
- Mass spectrometry
 B3LYP DFT molecular orbital approach, an efficient method to evaluate the thermochemical properties of MALDI matrices, 231
- Metastable ion
 Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153
- Metastable ion decomposition
 Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C₅–C₇ ketones in the gas phase, 257
- Metastable ions
 Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131
- MIKE spectra
 Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C₅–C₇ ketones in the gas phase, 257
- Neutralisation–reionisation mass spectrometry
 Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation, 1

Neutralization–reionization

Small carbon clusters (C_n^0 , C_n^+ , C_n^-) from acyclic and cyclic precursors. Neutralization–reionization and theory, 81

 Ni^+ binding energies

A theoretical study of the interaction between Ni^+ and small oxygen- and nitrogen-containing bases, 119

Phenylalanine residues

Fragmentation reactions of protonated peptides containing phenylalanine: a linear free energy correlation in the fragmentation of H–Gly–Xxx–Phe–OH, 185

Photoionization mass spectrometry

Why are smaller fragments preferentially lost from radical cations at low energies and larger ones at high energies? An experimental and theoretical study, 23

Phthalate

Adduct formation between phthalate esters and Li^+ in the gas phase: a thermochemical study by FT-ICR mass spectrometry, 75

Proton affinities

Ionized aniline and its distonic radical cation isomers, 45

Proton affinity

B3LYP DFT molecular orbital approach, an efficient method to evaluate the thermochemical properties of MALDI matrices, 231

Proton transfer

Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131

Proton transfer catalysis

Self-catalysis in the gas-phase: enolization of the acetone radical cation, 97

Protonated α,ω -aminoalcohols

Thermochemistry and unimolecular reactivity of protonated α,ω -aminoalcohols in the gas phase, 195

Protonated ketones

Carbocation rearrangements of trimethylsilyl adducts of saturated acyclic C_5 – C_7 ketones in the gas phase, 257

Protonated peptides

Fragmentation reactions of protonated peptides containing phenylalanine: a linear free energy correlation in the fragmentation of H–Gly–Xxx–Phe–OH, 185

Quantum chemical calculations

Ionized aniline and its distonic radical cation isomers, 45

Quantum mechanical calculations

Distonic isomers of ionized benzaldehyde, 65

Rearrangement

Reactions of low-energy pentenyl methyl ether radical cations $C_2H_5CH=CHCH_2OCH_3^{\bullet+}$, $CH_2=CHCH(C_2H_5)OCH_3^{\bullet+}$ and $CH_2=C(C_2H_5)CH_2OCH_3^{\bullet+}$, 109

Functional group migration in benzaldoxime-*O-n*-propyl ether radical cation, 153

RRKM theory

Why are smaller fragments preferentially lost from radical cations at low energies and larger ones at high energies? An experimental and theoretical study, 23

Silicon

Silicon- versus carbon-containing ions: 1,3- CH_3^+ transfers, 245

Size effects

Why are smaller fragments preferentially lost from radical cations at low energies and larger ones at high energies? An experimental and theoretical study, 23

Spin contamination

A theoretical study of the interaction between Ni^+ and small oxygen- and nitrogen-containing bases, 119

Stereochemistry

Regio- and diastereoselective C–H bond activation of valeramide and 3-methyl valeramide by bare Fe^+ ions, 169

Structures

The ions $CH_6O^{\bullet+}$ and CH_7O^+ , 179

Surface crossing

Self-catalysis in the gas-phase: enolization of the acetone radical cation, 97

Tandem mass spectrometer

Ionized aniline and its distonic radical cation isomers, 45

Tandem mass spectrometry

Distonic isomers of ionized benzaldehyde, 65

Self-catalysis in the gas-phase: enolization of the acetone radical cation, 97

tert-Butylbenzenes

Large hydrocarbon ion/molecule complexes formed during the unimolecular fragmentation of protonated *tert*-butyl-substituted tri- and tetrabenzylmethane, 131

Transition states

Why are smaller fragments preferentially lost from radical cations at low energies and larger ones at high energies? An experimental and theoretical study, 23