

Poster List for Gaseous Ions: Structures, Energetics & Reactions

Sunday Evening – Monday Afternoon

GOKHAN ALTINAY - UNIVERSITY OF MASSACHUSETTS IN AMHERST

Vibrational Spectroscopy of Intermediates in Methane-Methanol Conversion by FeO⁺: IR Resonance
Enhanced Photodissociation Spectroscopy of [HO-Fe-CH₃]⁺(Ar)_n (n=0-2)

RICHARD BEARDSLEY - UNIVERSITY OF ARIZONA

Probing the Gas Phase Fragmentation of Noncovalent Protein Oligomers via Surface Induced Dissociation

ANNE-MARIE BOULANGER - UNIVERSITY OF OTTAWA

Entropy Effects in the Fragmentation of Methyl Substituted Hydrazine Compounds

RYAN CALVI - JILA/UNIVERSITY OF COLORADO

Negative Ion Photoelectron Spectroscopy of Copper Hydrides

BIPASHA DEB - TEXAS TECH UNIVERSITY

An Analytic Function to Represent Both Short-Range and Long-Range Intermolecular Potential For
Modeling Soft-Landing Experiments

NICOLE EYET - UNIVERSITY OF COLORADO AT BOULDER

Deuterium Kinetic Isotope Effects in Microsolvated Gas-Phase E2 Reactions

KANCHANA GUNAWARDHANA - UNIVERSITY OF MASSACHUSETTS

Photofragment spectroscopy of TiO⁺.CO₂

STEPHANIE VILLANO - UNIVERSITY OF COLORADO AT BOULDER

Thermochemical Studies of N-methylpyrazole and N-methylimidazole.

ZHIXIN TIAN - UNIVERSITY OF MINNESOTA

H/D exchange and equilibrium acidities of amino acids and peptides

WILLIAM TAYLOR - UNIVERSITY OF CENTRAL ARKANSAS

Reactions of Cu⁺(1S, 3D) with CF₃X (X=Cl, Br, I)

THOMAS MORTON - UNIVERSITY OF CALIFORNIA, RIVERSIDE

Differentiating Acyclic Diastereomers by MS/MS

JOHN MERLE - NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

COMPUTATIONAL PREDICTION OF PEPTIDE FRAGMENTATION MECHANISMS IN TANDEM
MASS SPECTROMETER

JOSE LOPEZ - TEXAS TECH UNIVERSITY

Ab initio Direct Dynamics Trajectory Studies of the Base-Mediated Decomposition of CH₃OOH. Non-
IRC Dynamics

SIMON KING - UNIVERSITY COLLEGE LONDON

Studies on Singly and Multiply Charged Ions of Hydrocarbons and Fluorocarbons using Ion-Coincidence Mass Spectrometry

MICHAEL VOLNY - UNIVERSITY OF WASHINGTON

Structure determination of gas-phase ions by Surface-Enhanced Raman Scattering after soft landing on dry metal surfaces

SUNG HWAN YOON - UNIVERSITY OF ARIZONA

Kinetics of Surface-Induced Dissociation (SID) of $N(CH_3)_4^+$ using Laser Desorption (LD) and Silicon Nanoparticle Assisted Laser Desorption/Ionization (SPALDI)

Monday Evening – Tuesday Afternoon

ANTHONY MIDEY - INSTITUTE FOR SCIENTIFIC RESEARCH

Reactions of O^- and O_2^- with $O_2(a)$ at 300 K

RICHARD MARTA - UNIVERSITY OF WATERLOO

Infrared Multiphoton Dissociation Spectra as a Probe of Ion Molecule Reaction Mechanism: Formation of the Protonated Water Dimer via Sequential Bimolecular Reactions with Tetrafluorodimethyl Ether

SVEND KNAK JENSEN - UNIVERSITY OF AARHUS

Excited states in $[OH^-, nH_2O]$ clusters

SCOTT ANDERSON - UNIVERSITY OF UTAH

Use of Direct Dynamics Quasiclassical trajectories in ion-molecule reaction systems

ANDRAS BODI - EOTVOS UNIVERSITY

Alkylamine and Alkyl Radical Heats of Formation by Photoelectron Photoion Coincidence Spectroscopy and Isodesmic Reaction Networks

RONGHU WU - UNIVERSITY OF WATERLOO

Cation-p Hydrogen Bond and Salt Bridge Interactions of Amino Acids in the Gas Phase

JACK SIMONS - UNIVERSITY OF UTAH

Mechanisms for ETC/ECD

CHUNHAI RUAN - WAYNE STATE UNIVERSITY

Metal Ion Binding Affinities and Activation of Phosphate Esters Studied by Threshold Collision-Induced Dissociation and Theory Calculations

PAUL MAYER - UNIVERSITY OF OTTAWA

Modelling Entropy in Unimolecular Dissociation Reactions

BEIKE JIA - UNIVERSITY OF NEVADA AT RENO

Threshold Collision Induced Dissociation Study of Hydrogen-bonded Dimers of Common Carboxylic Acids

MARILYN JACOX - NATL INSTITUTE OF STANDARDS & TECHNOLOGY

Infrared Spectrum of $NN...CO^+$ Trapped in Solid Neon

C.F CORREIA - ECOLE POLYTECHNIQUE

Structural characterization of protonated phosphorylated aminoacids

JESSE BEAUCHAMP - CALIFORNIA INSTITUTE OF TECHNOLOGY

A new ion source for biomolecules

HAO CHEN - PURDUE UNIVERSITY

Ambient Ion Thermal Dissociation: Activation of Peptide/Protein Ions and of Ion/Molecule Reactions at Atmospheric Pressure

JASON BOYLE - UNIVERSITY OF UTAH CHEMISTRY

Effects of vibration and vibrational angular momentum on the reaction of NO₂⁺ with acetylene.

YU HOU - UNIVERSITY OF CALIFORNIA, DAVIS

Development of the VUV Laser Pulsed Field Ionization-Photoion Technique for State-Selected Ion-Molecule Reaction Dynamics Studies

KAREN JOYCE - UNIVERSITY OF ARIZONA

Ion-Surface Collisions on Halogen Terminated Self-Assembled Monolayers (SAMs)

Tuesday Evening – Wednesday Afternoon

JASON GREEN - PURDUE UNIVERSITY

Thermal dehydration of gaseous ions: stochastic master equation dynamics and ion trap experiments

JUERGEN GROTEMEYER - UNIVERSITY OF KIEL

Investigation of Bio- and organic molecular Ions by MATI

TRAVIS FRIDGEN - MEMORIAL UNIVERSITY OF NEWFOUNDLAND

Infrared Spectra of Gas-Phase Amino Acid Proton-Bound Dimers

MARIE-PIERRE GAIGEOT - UNIVERSITE D'EVRY VAL D'ESSONNE, LAMBE

Car-Parrinello molecular dynamics simulations for modeling IR-MPD experiments of gaseous ions

GARY DOUBERLY - UNIVERSITY OF GEORGIA

Infrared spectroscopy of protonated molecular clusters isolated in the gas phase

KRIS ELDRIDGE - UNIVERSITY OF WATERLOO

Gas Phase Investigation of the Energetic Contributions of Methanol and Cation- π Interactions to the Conformations of Amino Acids

GEREON NIEDNER-SCHATTEBURG - TU KAISERSLAUTERN

Mode specific fragmentation of hydrated ammonium

JIANHUA REN - UNIVERSITY OF THE PACIFIC

Sequence and Conformational Effects on the Gas-Phase Acidities of Cysteine-Polyalanine Peptides

DOUGLAS RIDGE - UNIVERSITY OF DELAWARE

SID and Molecular Mechanics Studies of an Oxidized Peptide

AUDE SIMON - CESR

Photodissociation, spectroscopy and reactivity of iron-PAH complexes of astrophysical interest : experiments in a cold FTICR ion trap and DFT calculations.

HELOISE SOLDI-LOSE - TECHNISCHE UNIVERSITAT BERLIN

Gas-Phase Chemistry of the *i*-Propyloxycarboxyl Cation

WILLIAM STEVENS - UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
RRKM modeling of halobenzene ion dissociations - kinetics from 10^3 to 10^7 sec⁻¹

LOURDERAJ UPAKARASAMY - TEXAS TECH UNIVERSITY
Direct Dynamics Simulations using Hesssian-Based Predictor-Corrector Integration Algorithms

RIDHA MABROUKI - VCU
Gas Phase Hydration and Deprotonation of the Cyclic C₃H₃⁺ Cation. Solvation by Acetonitrile, and Comparison with the Benzene Radical Cation

ZSOLT GENDELICZKI - EOTVOS LORAND UNIVERSITY BUDAPEST
Photoelectron Spectroscopy, Dissociation Dynamics, and bond energies of gas-phase Co(CO)₂NO(tBuNC)⁺ Ions

PETER ARMENTROUT - UNIVERSITY OF UTAH
The deamidation of cationized asparagine

MATTHEW FURZECOTT - UNIVERSITY OF WATERLOO
Probing the Effect of Fluorination on Strong Hydrogen Bonding in 2,4-Pentanedione Proton-Bound Dimers

Wednesday Evening – Thursday Afternoon

TOMAS BAER - UNIVERSITY OF NC, CHAPEL HILL
Temperature Dependent Breakdown Diagrams of n-butyl iodide by TPEPICO

MATTHEW BUSH - UNIVERSITY OF CALIFORNIA, BERKELEY
Infrared Spectroscopy of Biomolecular and Hydrated Ions

RYAN JULIAN - UNIVERSITY OF CALIFORNIA, RIVERSIDE
Synthesis of 2-Quinuclidonium by Eliminating Water: Experimental Quantification of the High Basicity of Extremely Twisted Amides

DINA JUSTES - PURDUE UNIVERSITY
Reactive DESI: A Different Milieu for Ion-Molecule Reactions

PHILIPPE MAITRE - CNRS & UNIVERSITY PARIS SUD 11
Infrared Spectroscopy of reactive intermediates associated to organometallic catalysts

ELAINE MARZLUFF - GRINNELL COLLEGE
Gas Phase Hydrogen Deuterium Exchange of Small Protonated Peptides: Side Chain Effects

JOSHUA MAZE - INDIANA UNIVERSITY
Opposite Polarity Droplets from Electrospray

ROBERT NIECKARZ - UNIVERSITY OF WATERLOO
Thermochemical Properties of Deprotonated Glycine/ROH (R = H, CH₃, C₂H₅) Clusters in the Gas Phase

J MARK PARNIS - TRENT UNIVERSITY
Matrix-isolation studies of the tautomerization of ketone and aldehyde cations

NALAKA RANNULU - WAYNE STATE UNIVERSITY

Influence of Solvents (Water, Methanol, Acetone, and Acetonitrile) on the Binding of Copper Ions to Imidazole and Pyridine

NICHOLAS SASSIN - UNIVERSITY OF NEVADA, RENO
Photodissociation and fluorescence of rhodamine ions in a 3D ion trap

ZACHARY SCOTT - UNIVERSITY OF ARIZONA
Variable temperature 22-pole RF ion trap for studies of ion-neutral reaction kinetics

ARPAD SOMOGYI - UNIVERSITY OF ARIZONA
Combination of CID and SID Ion Activation Methods with H/D Exchange to Probe Gas-Phase Intramolecular Rearrangements of Protonated Peptides

KIHYUNG SONG - KOREA NATIONAL UNIVERSITY OF EDUCATION
An Ab Initio Direct Dynamics Simulation of Protonated Glycine Surface Induced Dissociation

PAUL SPEIR - BRUKER DALTONICS, INC.
Rapid de-novo Terminal Domain Assignment of CAD Fragments from Intact Proteins

RICCARDO SPEZIA - UNIVERSITE D'EVRY VAL D'ESSONNE
Cobalt interacting with biomimetic cysteine-rich molecules in gas phase and in solution using DFT-based molecular dynamics

DIETHARD BOHME - YORK UNIVERSITY
A Novel Electrospray Selected-Ion Flow Tube Tandem Mass Spectrometer Suited for Biophysical Chemistry.