

**22nd ASILOMAR CONFERENCE on
MASS SPECTROMETRY**

**Sponsored by
American Society for Mass Spectrometry**

FUNDAMENTALS OF GAS PHASE ION CHEMISTRY: EXPERIMENT & THEORY

**Friday, October 20 - Tuesday, October 24, 2006
The Asilomar Conference Center, Pacific Grove, CA**

Program Chairs

Thomas Morton, University of California, Riverside
Frantisek Turecek, University of Washington

FRIDAY, OCTOBER 20

3:00 pm **Check-in**, *Asilomar Main Lobby*

5:00 pm **Registration** , *Asilomar Main Lobby*

6:00 - 7:00 pm **Asilomar dinner for on-site lodgers**, *Crocker Dining Hall.*
Asilomar meal ticket required.

Friday evening presenters should arrive at Fred Farr by 6:30 pm to set up their presentations.

7:00 – 10:00 pm **Session I**, *Fred Farr*
Each talk is followed by 10 minutes of discussion

7:00 – 7:30 pm **F. Turecek & T. H. Morton**
Welcome and introductory remarks

7:30 – 8:15 pm **Carl Lineberger**, University of Colorado, Boulder, CO
Plenary Lecture: *Photodissociation Dynamics of Partially Solvated Anions: Experiment and Theory in Concert*

8:30 – 9:00 pm **Nigel Adams**, University of Georgia, Athens, GA
Flow Tube Studies of Sources and Reactions of Pre-Life Molecules in Interstellar Clouds and the Titan Ionosphere

9:10 – 10:00 pm **Informal Poster Viewing and Reception**, *Kiln*

SATURDAY, OCTOBER 21

7:30 – 9:00 am **Asilomar Breakfast** for on-site lodgers, *Crocker Dining Hall*.
Asilomar meal ticket required.

Saturday morning presenters should arrive at 8:30 am to set up their presentations.

9:00 am – 12:15 pm **Session II, Fred Farr**
Steven Kass, session chair
Each talk is followed by 10 minutes of discussion

- 9:00 – 9:30 am **Steven Klippenstein**, Argonne National Lab, Argonne, IL
Applications of Theory: Identification of Combustion Species, of Metal Ligand Complexes, and Ion-Molecule Kinetics
- 9:40 – 10:10 am **Scott Anderson**, University of Utah, Salt Lake City, UT
What's Really Going on Here: Use of Mode-Selective Reactions and Direct Dynamics Trajectory Theory to Probe Ion-Molecule Reaction Mechanisms
- 10:20 – 10:35 am **Poster presentations, 5 min ea.**
1. **Georges Favre**, SEA Saclay, France
Theoretical Study of Collision Cross Sections of Zirconium Oxides with Collision Gas added to Oxygen in the Collision - Reaction Cell of an ICP-MS
 2. **James Kercher**, University of North Carolina, Chapel Hill
Dissociation Dynamics of Sequential Ionic Reactions: Heats of Formation of Tri-, Di- and Monoethyl Phosphine
 3. **Hao Chen**, Purdue University
Advances in the Exploration of Ion/Molecule Reactions at Atmospheric Pressure
- 10:35 – 10:50 am** **Coffee Break**
- 10:50 – 11:20 am **John Traeger**, La Trobe University, Victoria, Australia
Extending the Absolute Proton Affinity Scale by Photoionization Mass Spectrometry
- 11:30 am – 12:00 pm **Dan Neumark**, University of California, Berkeley, CA
Spectroscopy and Dynamics of Hydrated Anionic Species
- 12:10 - 2:00 pm** **Asilomar lunch**, *Crocker Dining Hall*. *Asilomar meal ticket required.*

SATURDAY AFTERNOON

Saturday afternoon presenters should arrive at 1:30 pm to set up their presentations.

- 2:00 – 5:30 pm** **Session III, Fred Farr**
Wolfgang Schoeller, session chair
Each talk is followed by 10 minutes of discussion
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- 2:00 – 2:30 pm **Wes Borden**, University of North Texas, Denton, TX
The Synergism between Calculations and Experiments in Studying the Gas-Phase Ion Chemistry of Some Organic Molecules
- 2:40 – 3:10 pm **Einar Uggerud**, University of Oslo, Oslo, Norway
The relationship between Computational Modeling and Experiment in Gas Phase Ion Chemistry
- 3:20- 3:50 pm **Bela Paizs**, University of Heidelberg, Heidelberg, Germany
Fragmentation Pathways of Protonated Peptides
- 4:00 – 4:15 pm **Poster presentations**, 5 min ea.
4. **Stephen Coy**, Sionex Corporation
Collision-Induced Fragmentation and Dissociation of Ions Probed by Planar-Differential-Mobility Spectrometry (DMS) and by Pre-filtered Mass Spectrometry (DMS-MS)
5. **Patrick James**, University of Melbourne
Collision Induced Dissociation of Diacylglycerophosphocholine Divalent Metal Clusters: Competition between Carboxylate and Phosphate Abstraction
6. **Bálint Sztáray**, Eötvös Loránd University, Hungary
Manganese–Chalcocarbonyl Bond Strengths from Threshold Photoelectron Photoion Coincidence Spectroscopy
- 4:15 – 5:50 pm** **Poster Viewing**
- 6:00 - 7:00 pm** **Asilomar dinner for on-site lodgers, Crocker Dining Hall.**
Asilomar meal ticket required.

SATURDAY EVENING

Saturday evening presenters should arrive at 6:30 pm to set up their presentations.

7:00 – 8:35 pm Session IV, *Fred Farr*
Paul Wenthold, session chair
Each talk is followed by 10 minutes of discussion

7:00 – 7:45 pm **Jack Beauchamp**, California Institute of Technology, Pasadena, CA
Plenary Lecture: *Mass Spectrometric Investigations of Protein Oxidation with FRIPS and FIDI: Reactions of Free Radicals and Ozone with Model Peptides in the Gas Phase and at Liquid-Gas Interfaces*

7:55 – 8:25 pm **Scott McLuckey**, Purdue University, West Lafayette, IN
Gas-Phase Bio-Ion/Ion Reactions: Electron Transfer, Proton Transfer, and Metal Ion Transfer

SUNDAY, OCTOBER 22

7:30 – 9:00 am **Asilomar Breakfast** for on-site lodgers, *Crocker Dining Hall*.
Asilomar meal ticket required.

Sunday morning presenters should arrive at 8:30 am to set up their presentations.

9:00 am – 12:00 pm Session V, *Fred Farr*
Ryan Julian, Session Chair
Each talk is followed by 10 minutes of discussion

- 9:00 – 9:30 am **Vicki Wysocki**, University of Arizona, Tucson, AZ
Surface-induced Dissociation of Non-covalent Complexes
- 9:40 – 10:10 am **John Klassen**, University of Alberta, Edmonton, Alberta, Canada
Structure and Stability of Noncovalent Protein Complexes in Solution and the Gas Phase Studied by NanoES-FT-ICR/MS
- 10:20 – 10:35 am **Coffee Break**
- 10:35 – 11:05 am **Maurizio Speranza**, La Sapienza, University of Rome, Italy,
Dissymmetry in the Gas Phase
- 10:45 – 11:15 am **Preben Hvelplund**, University of Aarhus, Denmark
What Fate is in Store for Large Molecular Ions after Capture of Quasi-free Electrons
- 12:00 - 2:00 pm** **Asilomar lunch**, *Crocker Dining Hall*. *Asilomar meal ticket required.*

AFTERNOON FREE!

SUNDAY EVENING

Sunday evening presenters should arrive at 6:30 pm to set up their presentations.

7:00 – 9:40 pm **Session VI, Fred Farr**
Frank Turecek, session chair
Each talk is followed by 10 minutes of discussion

- 7:00 – 7:30 pm **Steen Hammerum**, University of Copenhagen, Denmark
Alkyl Radicals as Hydrogen Bond Acceptors
- 7:40 – 8:10 pm **Zdenek Herman, J.**, Heyrovsky Institute of Physical Chemistry,
Prague, Czech Republic
*Dynamics of Chemical and Charge Transfer Reactions of
Molecular Dications from Cross-Beam Scattering Experiments*
- 8:20 – 8:50 pm **Julia Laskin**, Pacific Northwest National Lab, Richland, WA
*The Energetics and Dynamics of Dissociation of Odd-Electron
Peptide Ions*
- 9:00 – 9:30 pm **Paul Mayer**, University of Ottawa, Ottawa, Ontario, Canada
Modelling Entropy in Unimolecular Dissociation Reactions

MONDAY, OCTOBER 23

7:30 – 9:00 am **Asilomar Breakfast** for on-site lodgers, *Crocker Dining Hall*.
Asilomar meal ticket required.

Monday morning presenters should arrive at 8:30 to set up their presentations.

9:00 am – 12:00 pm **Session VII, Fred Farr**
Tom Morton, session chair
Each talk is followed by 10 minutes of discussion

- 9:00 – 9:30 am **Steven Kass**, University of Minnesota, Minneapolis, MN
Hydrogen-Deuterium Exchange Reactions of Negative Ions
- 9:40 – 10:10 am **Dietmar Kuck**, University of Bielefeld, Germany
*Ion/neutral Complexes Generated During Unimolecular
Fragmentation: Regioselectivity of Intra-complex Hydride
Abstraction*
- 10:20 – 10:35 am **Coffee Break**
- 10:35 – 11:05 am **Paul Wenthold**, Purdue University, West Lafayette, IN
Studies of the Electron Promoted Cope Cyclization
- 11:15 – 11:45 am **Richard O'Hair**, University of Melbourne, Victoria, Australia
*The 3D Quadrupole Ion Trap Mass Spectrometer as a Complete
Chemical Laboratory for Fundamental Gas Phase Studies of Metal
Mediated Chemistry*
- 11:55 am – 12:05 pm **Poster presentations**, 5 min ea.
7. **Tony Ly**, UC Riverside
*Probing Protein Structures by Selective Formation of 18-Crown-6
Ether Adducts using ESI-MS*
8. **Katherine Stumpo**, Texas A&M University
*Fragmentation of Cu-Adducted Peptides by MALDI TOFMS using
Gold Nanoparticle Matrices*
- 12:05 - 2:00 pm** **Asilomar lunch**, *Crocker Dining Hall*. *Asilomar meal ticket
required.*

MONDAY AFTERNOON

Monday afternoon presenters should arrive at 1:30 pm to set up their presentations.

2:00- 5:00 pm	Session VIII, Fred Farr John Trager, session chair <i>Each talk is followed by 10 minutes of discussion</i>
2:00 – 2:30 pm	Nick Polfer , The FOM Institute, Amsterdam, The Netherlands <i>Insights into Biological Mass Spectrometry with IR Spectroscopy</i>
2:40 – 3:10 pm	Douglas Ridge , University of Delaware, Newark, DE <i>Deducing Structure of Gas Phase Polymer and Metal Cluster Ions: FTMS, Spectroscopic and Computational Studies</i>
3:20 – 3:50 pm	Detlef Schroder , Technical University Berlin and IOCB, Prague, Czech Republic <i>Multiply Charged Ions</i>
4:00 – 4:30 pm	Poster presentations , 5 min ea. 9. Sara Gaucher , Sandia National Lab <i>Tandem Mass Spectrometry of Non-Tryptic Peptides</i> 10. Sen Li , Purdue University <i>Reactions of Charged Phenyl Radicals with Dipeptides in the Gas Phase</i> 11. Hiroshi Yamaoka , Osaka Prefecture University, Japan <i>Single/Double/Triple Hydrogen Transferred Unimolecular Dissociation for N-acyllactams and their Related Systems during Metastable Time Window using a Four Sector Tandem Mass Spectrometer: Comparison with the Corresponding Thiocarbonyl Analogues</i> 12. Takemiche Nakamura , RIKEN, Japan <i>A Proposal for Extension of Biemann's Nomenclature: Peptide Backbone Fragmentation with Odd Electron Species</i>
4:30 – 5:50 pm	Poster Viewing
6:00 – 7:30 pm	Banquet, Seascope Please go directly to the Seascope entrance, to the right (ocean side) of main entrance to Crocker Hall. Please bring your ticket.
7:40 – 9:00 pm	Session IX, Fred Farr Doug Ridge, session chair <i>Each talk is followed by 10 minutes of discussion</i>
7:40 – 8:10 pm	Richard Vachet , University of Massachusetts, Amherst <i>Using Ion Chemistry to Probe Metal Complex Structures</i>
8:20 – 8:50 pm	Xue-Bin Wang , Washington State University, Richland, WA <i>Probing the Electronic Structure of Solution Anions in the Gas Phase using Photoelectron Spectroscopy</i>

TUESDAY, OCTOBER 24

7:30 – 9:00 am **Asilomar Breakfast** for on-site lodgers, *Crocker Dining Hall*.
Asilomar meal ticket required.

Depart at leisure