

# Fourth International Conference on Chemical Kinetics

July 14-18, 1997

National Institute of Standards and Technology, Gaithersburg, MD 20899

Conference Organizers: Dr. Robert E. Huie, Conference Chair  
Dr. Jeffrey W. Hudgens  
Dr. Wing Tsang

Conference Web Site: [http://www.nist.gov/cstl/div838/kinet\\_conf.conference.html](http://www.nist.gov/cstl/div838/kinet_conf.conference.html)  
E-mail: [4th.kinetics.conf@nist.gov](mailto:4th.kinetics.conf@nist.gov)

The conference will feature nearly 190 oral and poster papers describing the latest results from internationally respected laboratories.

On Sunday, 13 July, the conference will hold a reception at the Gaithersburg Hilton Hotel between 6:30--8:30 p.m. We hope that you can attend. The conference will end on Friday near noon. Europe-bound travelers will have sufficient time to travel to airports (and pass security) for the early evening flights.

We also offer useful information at the conference World Wide Web-site:

[http://www.nist.gov/cstl/div838/kinet\\_conf/conference.html](http://www.nist.gov/cstl/div838/kinet_conf/conference.html)

Here, you will find:

**1) CONFERENCE PROGRAM AND ABSTRACTS.** We encourage authors to proof-read their abstracts. Please let us know of any significant corrections. You will also find helpful cross-links between the oral and poster papers of each topical session. If you do not have access to the web site, we can provide you with an advanced copy of the program.

**2) REGISTRATION DESK.** Using a secure (encrypted transmission) Web-form, you may pay the conference fee with a personal or corporate credit card. Alternately, you can use the registration form and register via fax or mail using a credit card, purchase order, or check. *We request that your register by June 30th using either one of the mentioned options.*

**Fax the form to:**

NIST Office of the Comptroller

FAX: 301-963-5972

*or*

**Mail the form to:**

NIST Office of the Comptroller

A807 Administration Building

Gaithersburg, MD 20899-0001 USA

**3) TRAVEL INFORMATION.** Through the Web-site, you may reserve a hotel room at most Gaithersburg hotels--including the Gaithersburg Hilton at the conference rate. You may make a reservation at the Hilton with the reservation form. Also include in the travel information section on the web site are:

- I)** A map of the NIST grounds and of the Metro system.
- II)** Maps and driving directions to NIST.
- III)** Links to the three regional airports including links for ground transportation between the airports and Gaithersburg.
- IV)** A list of taxicab companies in Gaithersburg.
- V)** A Hotel guide.
- VI)** Restaurant guides.
- VII)** Weather information.
- VIII)** Currency exchange rates.

# Program

## Sunday, 13th July

6:30 - 8:30 p.m. -- Registration and Reception at the Gaithersburg Hilton Hotel.

## Oral Sessions

## Monday, 14th July

7:45 a.m. -- Buses leave the Gaithersburg Hilton Hotel for NIST. (Note: Coffee and breakfast items are available in the NIST cafeteria adjacent the Green Auditorium.)

8:00 a.m. - Registration at the NIST.

8:30 a.m. - Opening Remarks.

Session A: Small Radical Kinetics 1

NIST Green Auditorium

Chair: Dr. Robert E. Huie

- 9:00 - 9:20 a.m.      **A1.** "Negative Activation Energies and Abnormally Fast Rates in Direct Metathesis Reactions"  
• Sidney W. Benson and Otto Dobis
- 9:25 - 9:45 a.m.      **A2.** "Kinetics Studies of the Reactions  $\text{Br} + \text{C}_2\text{H}_4 \rightleftharpoons \text{C}_2\text{H}_4\text{Br}$  and  $\text{Br} + \text{C}_2\text{H}_6 \rightleftharpoons \text{HBr} + \text{C}_2\text{H}_5$ "  
• J. M. Nicovich, V. M. Ferrell, and P. H. Wine
- 9:50 - 10:10 a.m.      **A3.** "Kinetic Study of  $\text{CH}_3$  Radical Reactions Over 1-100 bar Buffer Gas Pressure Range"  
• Lev N. Krasnoperov and Kashyap Mehta
- 10:15 - 10:35 a.m.      **A4.** "Thermochemistry of the R-O<sub>2</sub> Bond in Alkyl and Chloroalkyl Peroxy Radicals"  
• Vadim D. Knyazev, Akos Bencsura, and Irene R. Slagle
- 10:40 - 11:00 a.m.      **Break**
- 11:00 - 11:45 a.m.      **A5.** *Invited.* "Physical Factors Determining the Reactivity of Reagents in Free Radical Reactions of Abstraction and Addition"  
• E. T. Denisov

11:50 - 12:10 a.m. **A6.** "Trends in the Reactivity of Cl, OH and CF<sub>3</sub>O with Halogenated Alkanes"  
• Garrett Locke, John O'Reilly, John Wenger, Jack Treacy, and Howard Sidebottom

12:15 - 12:35 p.m. **A7.** "Infrared Absorption Probing of Cl-Atom Reactions with Hydrocarbons"  
• Jeffrey S. Pilgrim, John T. Farrell, and Craig A. Taatjes

12:40 - 1:40 p.m. **Lunch**

Session B: High Temperature Inorganic Radicals  
NIST Green Auditorium  
Chair: Jeffrey Manion

1:40 - 2:00 p.m. **B1.** "Kinetics of the O(3P) + N<sub>2</sub>O Reaction at Intermediate Temperatures"  
• Nancy E. Meagher, William R. Anderson, Abdellatif Goumri, and Arthur Fontijn

2:05 - 2:25 p.m. **B2.** "Kinetic Study of the Reaction of NH<sub>2</sub> with NO in the Temperature Range from 1400 to 2000 K"  
• H.-J. Römming and H. Gg. Wagner

2:30 - 2:50 p.m. **B3.** "The Riddle of the H + O<sub>2</sub> Reaction at High Temperatures"  
• Heshel Teitelbaum and Assa Lifshitz

2:55 - 3:15 p.m. **B4.** "Calculation of Reactive Cross Sections and Microscopic Rates from Kinetic Data"  
• Jan P. Hessler

3:20 - 3:40 p.m. **B5.** "Chemical Activation Analysis of the NH<sub>2</sub> + NO and CH<sub>3</sub> + NO Reactions"  
• Anthony M. Dean and Joseph W. Bozzelli

4:00 p.m. Buses leave NIST for the Gaithersburg Hilton Hotel.  
(Buses will be waiting at the entrance of the Administration building.)

4:25 - 6:30 p.m. **Session C: Poster 1**

## Tuesday, 15th July

8:15 a.m. -- Buses leave the Gaithersburg Hilton Hotel for NIST. (Note: Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.)

### Session D: Unsaturated Radical Reactions

NIST Green Auditorium

Chair: Wing Tsang

- 9:00 - 9:20 a.m.     **D1.** "Reaction of the Propargyl Radical (C<sub>3</sub>H<sub>3</sub>) with NO"  
• J. D. DeSain, R. F. Curl and Graham P. Glass
- 9:25 - 9:45 a.m.     **D2.** "A Product Study of the C<sub>2</sub>H<sub>3</sub> + C<sub>2</sub>H<sub>3</sub> and C<sub>2</sub>H<sub>3</sub> + CH<sub>3</sub> Radical"  
• R. Peyton Thorn Jr., Walter A. Payne, Louis J. Steif, Fred L. Nesbitt, Xavier Chiller, and Dwight C. Tardy
- 9:50 - 10:10 a.m.    **D3.** "Spectroscopic and Kinetic Investigations of the Propargyl Radical Using Ultraviolet Cavity Ring-Down Spectroscopy"  
• Dean Atkinson and Jeffrey W. Hudgens
- 10:15 - 10:35 a.m.    **D4.** ""On the Role of Oligomerization in the Thermal Gas-Phase Reaction of Propene"  
• Laszlo Seres
- 10:40 - 11:00 a.m.    **Break**
- 11:00 - 11:45 a.m.    **D5.** Invited. "Kinetics of Phenyl Radical Reactions Studied by Assorted Spectrometric Methods"  
• M. C. Lin
- 11:50 - 12:10 a.m.    **D6.** "High Temperature Pyrolysis of Phenol"  
• C. Horn and P. Frank
- 12:15 - 12:35 a.m.    **D7.** "Kinetics and Thermochemical Studies of Reactions of the Phenoxy Radical"  
• F. Berho, M. T. Rayez, F. Caralp, R. Lesclaux, E. Ratajczak
- 12:40 - 1:40 p.m.     **Lunch**

Session E: Theory  
NIST Green Auditorium  
Chair: Anthony M. Dean

- 1:40 - 2:00 p.m.      **E1.** "Evaluation of Transition State Properties by Density Functional Theory"  
• Joseph L. Durant
- 2:05 - 2:25 p.m.      **E2.** "A Direct RRKM Theory Study of  $\text{CH}_3 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_6$ "  
• Stephen J. Klippenstein and Lawrence B. Harding
- 2:30 - 2:50 p.m.      **E3.** "Potential Energy Surfaces for Chemical Reactions"  
• Stephen P. Walch
- 2:55 - 3:15 p.m.      **E4.** "Prediction of High Pressure Rate Constants for Dissociation and Recombination Reactions"  
• Juergen Troe
- 3:20 - 3:40 p.m.      **E5.** "Spectroscopy of the Low Lying Triplet States of Ozone in the Near Infrared and Their Possible Role for its Kinetics"  
Ales Charvat, Sabine F. Deppe, and Bernd Abel
- 3:55 p.m.              Buses leave NIST for the Gaithersburg Hilton Hotel.  
(Buses will be waiting at the entrance of the Administration building.)
- 4:20 - 6:30 p.m.      **Session F: Poster 2**

## Wednesday, 16th July

8:15 a.m. -- Buses leave the Gaithersburg Hilton Hotel for NIST. (Note: Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.)

Session G: Solution Kinetics  
NIST Green Auditorium  
Chair: Pedatsur Neta

- 9:00 - 9:20 a.m.      **G1.** "Kinetics and Mechanisms for C1 Compounds in Supercritical Water"  
• Phillip E. Savage, Eric Brook, Naoko Akiya, Jianli Yu, and John R. Barker
- 9:25 - 9:45 a.m.      **G2.** "Effects of Cationic Micelles on Rate of Intramolecular General Base-Catalysed Ethanediolysis of Ionized Phenyl Salicylate (PS-)"  
• M. Niyaz Khan and Zainudin Arifin

9:50 - 10:10 a.m. **G3.** "Modulation of Reaction Rate Constant is a New Method of Chemical Kinetics"

- Michael M. Triebel and George E. Zorinants

10:15 - 10:35 a.m. **G4.** "Reactivity of Ferrate(VI) and Ferrate(V) with Cyanide in Alkaline Medium"

- Virender K. Sharma, Wayne Rivera, and Don O'Connor

10:40 - 11:00 a.m. **Break**

Session H: Low Temperature

NIST Green Auditorium

Chair: Tomas Baer

11:00 - 11:45 a.m. **H1.** Invited. "Low Temperature Rate Studies of Ions and Radicals in Supersonic Flows"

- Mark A. Smith

11:50 - 12:10 a.m. **H2.** "Laboratory Studies of Low Temperature Rate Coefficients"

- Ray J. Hoobler, Brain J. Opansky, and Stephen R. Leone

12:15 - 12:35 a.m. **H3.** "Gas Phase Kinetic Measurements of the HO<sub>2</sub> + NO, HO<sub>2</sub> + NO<sub>2</sub>, and HO<sub>2</sub> + O<sub>3</sub> Reactions at Stratospheric Temperatures and Pressures using a New Turbulent Flow Tube Reactor with Tunable Diode Laser/Astigmatic Multi-Pass Cell Detection"

- Peter W. Villalta, Mark S. Zahniser, David D. Nelson, John T. Jayne, and Charles E. Kolb

12:40 - 1:40 a.m. **Lunch**

Session I: Small Radical Kinetics 2

NIST Green Auditorium

Chair: Juergen Troe

1:40 - 2:00 p.m. **I1.** "HCl Yield from OH + ClO: RRKM Calculations and Stratospheric Model Sensitivities"

- Gregory P. Smith, Manvendra K. Dubey, and Mark McGrath

2:05 - 2:25 p.m. **I2.** "Kinetics Studies of the HO<sub>2</sub> + ClO Reaction"

- Barna Laszlo, Randall R. Friedl, Stanley P. Sander

2:30 - 2:50 p.m. **I3.** "Experimental and ab initio Theoretical Studies of the Reactions Between Fluorine Atoms and a Series of Halogenated Methanes"

- Florent Louis, Marie-Therese Rayez, Jean-Claude Rayez, and Jean-Pierre Sawerysyn

- 2:55 - 3:15 p.m. **I4.** "Wide-Temperature Range Studies of BO and BO<sub>2</sub> Reactions"  
 • David P. Belyung, George T. Dalakos, Qifeng Zhang, John-David R. Rocha, and Arthur Fontijn
- 3:20 - 3:40 p.m. **Break**
- 3:40 - 4:00 p.m. **I5.** "The High Pressure Range of the Reaction CH + CO"  
 • D. Fulle, H. Hippler and F. Striebel
- 4:05 - 4:25 p.m. **I6.** "The Reactions of Substituted Styrenes with O(3P) in the Gas Phase"  
 • M. Eichholtz, R. Oswald, and H. Gg. Wagner
- 4:30 - 4:50 p.m. **I7.** "Ultrasensitive Absorption Spectroscopy of Methane Flame"  
 • Sergey Cheskis, Igor Derzy, Vladimir A. Lozovsky
- 5:05 p.m. Buses leave NIST for the Gaithersburg Hilton Hotel.  
 (Buses will be waiting at the entrance of the Administration building.)
- 7:00 p.m. **Reception and Banquet, Gaithersburg Hilton Hotel**  
 Speaker: Prof. Sidney W. Benson

## Thursday, 17th July

8:15 a.m. -- Buses leave the Gaithersburg Hilton Hotel for NIST. (Note: Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.)

Session J: Applied Kinetics  
 NIST Green Auditorium  
 Chair: Joseph L. Durant

- 9:00 - 9:20 a.m. **J1.** "Fundamental Kinetic Modeling of Industrial Reactors"  
 • Max M. Tirtowidjojo
- 9:25 - 9:45 a.m. **J2.** "Pyrolysis of Indole, Quinoline and Isoquinoline. Application to Coal Combustion"  
 • Alexander Laskin and Assa Lifshitz
- 9:50 - 10:10 a.m. **J3.** "Computational Construction of Kinetic Models Using a Rate-Based Algorithm"  
 • Jeffrey M. Grenda, Roberta G. Susnow, David J. Klinke, Pawel Peczak, Anthony M. Dean, and William H. Green
- 10:15 - 10:35 a.m. **J4.** "Thermal Decomposition of Silane"  
 • A. A. Onischuk, V. P. Strunin, M. A. Ushakova, and V. N. Panfilov
- 10:40 - 11:00 a.m. **Break**



- 11:00 - 11:45 a.m. **J5.** "The Kinetics of Elementary Reactions of CF<sub>3</sub>Br and CF<sub>3</sub>I with H, OH, O and CH<sub>3</sub> Radicals: Experiments, Ab Initio Calculations and Implications for Combustion Chemistry"  
 • Jessie Yuan, Ashutosh Misra, Leah Wells, Samantha Hawkins, Aneal Krishnan, Ripal B. Nathuji, Paul Marshall, and Rajiv Berry
- 11:50 - 12:10 p.m. **J6.** "Experimental and Modeling Study of the Effect on CF<sub>3</sub>H, C<sub>2</sub>F<sub>6</sub> and CF<sub>3</sub>Br on the Ignition Delays of Methane-Oxygen-Argon Mixtures Behind Shock Waves"  
 • J. C. Bauge, P. A. Glaude, P. Pommier, F. Battin-Leclerc, G. Scacchi, G. M. Côme, F. Baronnet
- 12:15 - 12:35 p.m. **J7.** "Combustion Kinetics of Hydrofluorocarbons (HFCs)"  
 • G. P. Brownless, M. J. Pilling, and R. L. Powell
- 12:40 - 1:40 p.m. **Lunch**

Session K: Heterogeneous Chemistry  
 NIST Green Auditorium  
 Chair: Michael Kurylo

- 1:40 - 2:20 p.m. **K1.** Invited. "Some Reflections on Atmospheric Chemistry and Photochemistry on Ices"  
 • John R. Sodeau.
- 2:25 - 2:45 p.m. **K2.** "Real-Time Measurement of Residence Times of Gas Molecules on Solid Surfaces: Relevance for Heterogeneous Chemical Kinetics"  
 • Michel J. Rossi
- 2:50 - 3:10 p.m. **K3.** "Laboratory Study of Heterogeneous Sinks of Tropospheric HO<sub>2</sub>"  
 • A. V. Ivanov, R. G. Remorov, M. Yu. Gershenson Jr., Yu. S. Il'in, A. Yu. Zasytkin, V. M. Grigorieva, and Yu. M. Gershenson
- 3:15 - 3:35 p.m. **K4.** "Role and Fate of N<sub>2</sub>O<sub>5</sub> in Tropospheric Chemistry of Sea-Spray Aerosol: Precursor of the Nitronium Ion, ClNO<sub>2</sub>, BrNO<sub>2</sub>, Nitrophenols and N<sub>2</sub>O"  
 • W. Behnke, M. Elend, A. Frenzel, H.-U. Kruger, V. Scheer, R. Sikorski, and C. Zetzsch
- 3:40 -- 4:00 p.m. **K5.** "Laboratory Kinetic Studies of the Reaction System NO<sub>2</sub>/H<sub>2</sub>O/H<sub>2</sub>SO<sub>4</sub>"  
 • K. H. Becker, J. Kleffmann, R. Kurtenbach, and P. Wiesen
- 4:15 p.m. Buses leave NIST for the Gaithersburg Hilton Hotel.  
 (Buses will be waiting at the entrance of the Administration building.)

4:40 - 6:30 p.m.      **Session L: Poster 3**

Friday, 18th July

8:15 a.m. -- Buses leave the Gaithersburg Hilton Hotel for NIST. (Note: Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.) **Conferees are encouraged to bring their luggage to the meeting and store them in the Red Coat Room.**

Session M: Small Radical Kinetics 3  
NIST Green Auditorium  
Chair: Jeffrey W. Hudgens

- 9:00 - 9:20 a.m.      **M1.** "The Reactions of C<sub>2</sub>H<sub>5</sub> Radicals with O, O<sub>3</sub>, NO<sub>3</sub>, and NO<sub>2</sub>: Decomposition Pathways of the Intermediarily Formed C<sub>2</sub>H<sub>5</sub>O Radicals"  
• K. Hoyermann, M. Olzmann, J. Seeba, and B. Viskolcz
- 9:25 - 9:45 a.m.      **M2.** "Photodissociation Dynamics of Methyl Iodide Clusters"  
• L. Poth, E. M. Snyder, S. Sato, D. Folmer, Q. Zhong, J. V. Ford, A. W. Castleman, Jr.
- 9:50 - 10:10 a.m.      **M3.** "Dimethyl-ether Radical + O<sub>2</sub> and the Respective Adduct Radical + O<sub>2</sub> Reactions."  
• Takahiro Yamada, Joseph W. Bozzelli, and Tsan Lay
- 10:15 - 10:35 a.m.      **M4.** "Isomerization and Dissociation in Competition: The two-Component Dissociation Rates of Energy Selected Ions"  
• Oleg A. Mazzyar, Paul M. Mayer, Jeffrey W. Keister, and Tomas Baer
- 10:40 - 11:00 a.m.      **Break**
- 11:00 - 11:20 a.m.      **M5.** "Pressure and Temperature Analysis of the C<sub>2</sub>H<sub>5</sub> and H<sub>2</sub>C CH<sub>2</sub>OOH + O<sub>2</sub> Reactions"  
• Joseph W. Bozzelli, Anthony M. Dean, Chad Sheng, and Tsan Lay
- 11:25 - 11:45 a.m.      **M6.** "Thermal Decomposition and Isomerization Processes of Alkyl and Allyl Radicals"  
• A. Miyoshi, N. Yamauchi, T. Harada, K. Kosaka, M. Koshi, and H. Matsui
- 11:50 - 12:10 a.m.      **M7.** "Kinetics and Atmospheric Implications of Peroxy Radical Cross Reactions Involving the CH<sub>3</sub>C(O)O<sub>2</sub> Radical"  
• E. Villenave, R. Lesclaux, S. Seefeld, W. R. Stockwell

## Session C, Poster Session 1

**Monday, 4:25 - 6:30 p.m. -- Gaithersburg Hilton Hotel**

**C1.** "Experiments and Theory on the Thermal Decomposition of  $\text{CHCl}_3$  and the Thermal Reactions of  $\text{CCl}_2$ "

- S. S. Kumaran, M.-C. Su, K. P. Lim, J. V. Michael, S. J. Klippenstein, J. DiFelice, P. S. Mudipalli, J. H. Kiefer, David A. Dixon, Kirk A. Peterson

**C2.** "H-Atom Elimination in the Unimolecular Decomposition of Alkyl Radicals"

- Vadim D. Knyazev, Akos Bencsura, and Irene R. Slagle

**C3.** "Measurements of the Rates of Dissociation of t-Butyl Hydroperoxide, Propane, and Methylidimide"

- Paul J. Ogren, Peng Wang, and Jan P. Hessler

**C4.** "Chemical Kinetics of Rich Methane – Air Low Pressure Flames"

- Andrew McIlroy

**C5.** "The Pyrolysis and Oxidation of N-Butane & Iso-Butane: A Flow Tube Reactor Molecular Beam Mass Spectrometry Study"

- Mark D. Weisel, Albert Y. Chang, Xian Zhong, and Anthony M. Dean

**C6.** "Pressure Dependent Reaction Mechanism for C1 and C2 Combustion Systems: 0.001-100 Atm, 300-2500 K"

- Joseph W. Bozzelli, Wen-Chiung Ing, Takahiro Yamada, Chad Sheng, Anthony M. Dean

**C7.** "Ab Initio MO Calculations of CO Adsorption on the Si(100)-2x1 Surface"

- F. T. Bacalzo, D. Musaev, and M. C. Lin

**C8.** "Correlation Between Rate Constants and Energetics of Radical-Radical Reactions"

- Askar Fahr and Parvize Hassanzadeh

**C9.** "Radiolytic Formation of Metal Clusters In Aqueous and Micro Emulsion Solutions"

- S. K. Kapoor, S. Adhikari, M. M. Kumar, C. Gopinathan and J. P. Mittal

**C10.** "Methylcyclopropane Isomerization Kinetics at 990 – 1154 K"

- Janet Y. Cho, Bansi L. Karla and David K. Lewis

**C11.** "Ab initio Study of 1,5 H Atom Transfer Reactions in Free Radicals"

- Bela Viskolcz

**C12.** "Study of Basic Mechanisms of Nucleation and Cloud/Aerosol Interactions with Taking Into Account Heterogeneous Physical-Chemical Processes"

- V. G. Bondarenko and V. Ye. Smorodin

**C13.** "Heterogeneous Accommodation and Reaction Kinetics for NH<sub>3</sub> Uptake on Aqueous and Concentrated Sulfuric Acid Droplets"

- Q. Shi, E. Swartz, and P. Davidovits

**C14.** "A Low Temperature FT-RAIRS Study of the Production of ClNO and HNO<sub>3</sub> from the Photolysis of N<sub>2</sub>O<sub>4</sub>/HCl/H<sub>2</sub>O films"

- Tristan B. Roddis, Neil A. Williams and John R. Sodeau

**C15.** "XO + XO Reactions – Kinetics, Mechanism and Thermochemistry"

- R. A. Cox and D. M. Rowley

**C16.** "Reaction in Mixture of CF<sub>4</sub> and H<sub>2</sub> Initiated by Small Amount of CF<sub>3</sub>Cl in a Shock Tube"

- Yushong He, Jiping Cui, and Bingcheng Fan

**C17.** "Kinetic Studies of the Reactions of CF<sub>3</sub>O<sub>2</sub> with I and Cl"

- C. E. Canosa-Mas, A. Vipond, and R. P. Wayne

**C18.** "Kinetic and Transition State Analysis on the Neopentyl Reaction with Oxygen"

- Ru Wei and Joseph W. Bozzelli

**C19.** "Electron Transfer Reactions Anions of Nitrobenzene and Perfluoronitrobenzene in Aqueous Solution. Does Inner Sphere Mechanism Plays a Role?"

- Lian C. T. Shoute and Jai P. Mittal

**C20.** "The Analysis of Acetylene + O<sub>2</sub> Reaction Based on Semi-Empirical and Ab Initio Data"

- Chad Sheng, Joseph W. Bozzelli

**C21.** "The Low Temperature Kinetic Behavior of the Bimolecular Reaction OH + HBr (76–242 K)"

- Dean B. Atkinson, Veronica I. Jaramillo, and Mark A. Smith

**C22.** "Temperature Coefficients of Rates of Ethyl Radical Reaction with HBr and Br. The Heat of Formation of Ethyl Radical"

- Otto Dobbis and Sidney W. Benson

**C23.** "FTIR and Mass Spectrometric Measurements of the Rate Constant for the C<sub>6</sub>H<sub>5</sub> + H<sub>2</sub> Reaction"

- J. Park, I. V. Dyakov, and M. C. Lin

- C24.** "Characterization the Products from F + t-butanol with Photoionization Mass Spectrometry: Hydrogen Migrations,  $\beta$  Scissions, Enolization"
- Dwight C. Tardy, Szu-Cherng Kuo, Zhengyu Zhang, and R. Bruce Klemm
- C25.** "Sequential Two Photon Absorption by NO<sub>2</sub> in the Presence of H<sub>2</sub> as a Source of OH in Pulsed Photolysis Kinetic Studies: Reaction of OH with Aliphatic Amines and with C<sub>2</sub>H<sub>6</sub>, i-C<sub>3</sub>H<sub>7</sub>I and n-C<sub>3</sub>H<sub>7</sub>I"
- Shaun A. Carl and John N. Crowley
- C26.** Kinetics of the Reaction of Oxygen Atoms with CHCl<sub>2</sub>
- Stanislav I. Stoliarov, Akos Bencsura, Vadim D. Knyazev, and Irene R. Slagle
- C27.** "Kinetics of the Gas-phase Reactions of the NO<sub>3</sub> Radical with Selected Monoterpenes over the Temperature Range 296-430 K, Using L.I.F. Detection"
- E. Martinez, B. Cabanas, A. Aranda and P. Martin
- C28.** "Fluoroalkene Photochemistry or How We Measured the Rate Constant for the Reaction Between OH and HFC-245cb"
- Vladimir Orkin, Robert E. Huie, and Michael J. Kurylo
- C29.** "Iron Cluster Thermal Decomposition and Ionization"
- P. A. Vlasov, I. S. Zaslanko, Yu.K. Karasevich, and V. N. Smirnov
- C30.** "Structure of H<sub>2</sub>/O<sub>2</sub>/Ar Flames Doped with DMMP and TMP Studied by Molecular Beam Mass-Spectrometry and Modelling. TMP and DMMP Destruction Chemistry in Flames"
- O. P. Korobeinichev, V. M. Shvartsberg, S. B. Ilin, A. A. Chernov, V. V. Mokrushin, and Tatyana A. Bolshova
- C31.** "Atmospheric Studies Using Cluster Ions: An Investigation Into the Reactivity of Iodine Ion Species"
- Ronald S. MacTaylor, John J. Gilligan, and A. W. Castleman, Jr.
- C32.** "Kinetic Study of NO<sub>x</sub> Destruction in Air and Nitrogen by Dielectric Barrier Corona Discharge"
- Larisa G. Krishtopa and Lev N. Krasnoperov
- C33.** Fundamental Processes Undergone by Ba[6s5d(3D1,2,3)] Generated Following Pulsed Dye-Laser Excitation at  $\lambda = 553/5$  m, {Ba[6s6p(1P1)]  $\leftrightarrow$  Ba[6s2(1S0)]} in the Presence of Noble Gases
- J. W. Adams, D. Husain, Jie Lei, F. Castano, and Maria N. Sanchez Rayo
- C34.** "The Association Reaction of Ruthenium with Nitric Oxide in the Gas Phase"
- Roy E. McClean, Mark L. Campbell, and Michelle D. Vorce

**C35.** "Kinetics of Oxidation in System Titanium-Oxygen at a Temperature Range of 400oC – 500oC"

- Magdalena Momirlan

**C36.** "Influence of the Ketene Photolysis Wavelength on Measured 1CH<sub>2</sub> (n 1A1) Rate Constants"

- Hans-Heinrich Carstensen

**C37.** "A Direct Measurement of O(1D<sub>2</sub>) Quantum Yields and Translational Energies from the Photodissociation of Ozone"

- Stephen M. Ball, Wolfgang Denzer, Gus Hancock, John C. Pinot de Moira, and Phil L. Tyley

**C38.** "The Semi-Empirical Estimation of D fH<sub>0</sub> 298(SO<sub>x</sub>-) (x = 2 , 5) for Aqueous Solutions"

- Gregory A. Poskrebyshev

**C39.** "Why is the Human Visual System Sensitive Only to Light of Wavelengths from about 760 to 380 nm? –An Answer from Thermochemistry and Kinetics"

- Yu-Ran Luo

**C40.** "Reduction Potential of the tert-Butylperoxyl Radical in Aqueous Solutions"

- T. N. Das, T. Dhanasekaran, Z. B. Alfassi, and P. Neta

**C41.** "Shock Tube Study of Monomethylamine Thermal Decomposition"

- M. Votsmeier, D. F. Davidson and R. K. Hanson

**C42.** Low Barrier Isomerization Reactions in Free Jet Expansions: Axial-Equatorial Interconversion Rates in Methyl and Ethyl Cyclohexanones

- Tomas Baer, Alan R. Potts, and Wing Tsang

**C43.** "Estimation Method for OH Abstraction Rate Constants"

- W. B. DeMore

**C44.** "Rate Measurements of the Self-Reaction of Ethyl and Ethylperoxy Radicals and the Reaction, O<sub>2</sub> + C<sub>2</sub>H<sub>5</sub> ® C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>, using Ultraviolet Cavity Ring-Down Spectroscopy"

- Dean B. Atkinson and Jeffrey W. Hudgens

**C45.** "Numerical Modeling of an Artificial Claciation and the Formation of Improved Visibility Areas in Fog. Recommendations for Conducting Fog Dispersal at Airports"

- V. G. Bondarenko

**C46.** "Isotopic Fractionation of Stratospheric Nitrous Oxide via Photolysis"

- Yuk L. Yung and Charles E. Miller

- C47.** "Theoretical and Experimental Studies of  $\text{HH} + \text{CN} \rightarrow \text{HCN}(v_1, v_2, v_3) + \text{H}$ "
- Albert F. Wagner, R. G. Macdonald, G. A. Bethardy, George C. Schatz and Marc A. ter Horst

## **Session F: Poster Session 2**

**Tuesday, 4:20 - 6:30 p.m. -- Gaithersburg Hilton Hotel**

- F1.** "Thermochemical Kinetic Analysis on the Reaction of Tertiary Butyl Radical with Oxygen and an Elementary Reaction Mechanism for Tertiary Butyl Oxidation"
- Chiung-Ju Chen and Joseph W. Bozzelli
- F2.** "Kinetics of the Thermal Isomerizations of Vinylcycloalkanes and Cycloalkenes"
- Bansi L. Kalra, David K. Lewis and John E. Baldwin
- F3.** "Gas-Phase Thermal Decomposition of Volatile Metal-Bearing Compounds Behind Shock Waves"
- I. S. Zaslonko and V. N. Smirnov
- F4.** "The Pyrolysis of Acetone"
- Philip D. Pacey and S. Hosein Mousavipour
- F5.** "The Role of Successive Reactions During Ignition Process and Flame Propagation in Chlorine Containing Systems"
- I.R. Begishev and A. K. Belikov
- F6.** "Kinetic Aspects of Fire-suppression by Propellant-Generated Aerosols"
- A. N. Baratov, I. S. Zaslonko, and V. N. Smirnov
- F7.** "Hydrogen Flame Inhibition by  $\text{CF}_3\text{I}$ "
- Andrew McIlroy
- F8.** "Detailed Chemical Structure of Fuel Rich Methane Flames with Comparison to Kinetic Model Predictions"
- L. I. Yeh and F. Luo
- F9.** "A Detailed Chemical Kinetic Model for Ethanol Oxidation"
- Nick M. Marinov
- F10.** "Semiempirical Estimation of Activation Energies and Rate Constants of Ozone Reactions with Hydrocarbons and Antioxidants"
- Taissa G. Denisova and Evguenii T. Denisov
- F11.** "Theoretical Studies of Radical-Radical Reactions:  $\text{H} + \text{HCO}$ ,  $\text{H} + \text{H}_2\text{CCH}$  and  $\text{H} + \text{H}_2\text{CCH}_3$ "
- Lawrence B. Harding and Stephen J. Klippenstein

- F12.** "Computer Experiments for Two-Temperature Chemical Kinetics"  
• A. L. Sergeivkaya and S. A. Losev
- F13.** "Ab Initio Kinetics of the Thermal Dehydrohalogenation of Alkyl Halides"  
• Karl K. Irikura and Wing Tsang
- F14.** "The Dependence of OH Concentration on the Intensity of Atmosphere – Surface Exchange with Nitrogen Species"  
• Alexander V. Keiko (G. I. Skubnevskaya)
- F15.** "The Conversion of Solid Inorganic Compounds Under the Effect of Gas Phase Chain Reactions"  
• Adolph A. Mantashyan
- F16.** "Kinetics of Aerosol Formation of Carbonyl-Containing Compounds Under Photolysis in the Air or Argon Flow"  
• Skubnevskaya G. I., Dubtsov S. N., Dultsev E. N., and Dultseva G. G.
- F17.** "Gas Phase Kinetics of the HO<sub>2</sub> + BrO Reaction"  
• J. M Cronkhite, R. E. Stickel, J. M. Nicovich, and P. H. Wine
- F18.** "Kinetic and Photochemical Studies of Gas Phase Iodine Oxide Chemistry of Atmospheric Importance"  
• David M. Rowley, William J. Bloss, Juliane Mossinger, R. Anthony Cox and Roderic L. Jones
- F19.** "Bromine Nitrate Photochemistry and Reaction Kinetics"  
• R. Soller, J. M. Nicovich, and P. H. Wine
- F20.** "HCl Yield from OH + ClO: RRKM Calculations and Stratospheric Model Sensitivities"  
• Gregory P. Smith, Manvendra K. Dubey, and Mark McGrath
- F21.** "Ethylene + OH and the Respective Adduct Radical + O<sub>2</sub> Reactions"  
• Takahiro Yamada, Joseph W. Bozzelli, and Tsan Lay
- F22.** "Reaction of •NH<sub>2</sub> with O<sub>2</sub> in Aqueous Solutions and Mechanism of Formation of Peroxynitrite"  
• B. Laszlo, Z. B. Alfassi, P. Neta, and R. E. Huie
- F23.**
- F24.** "Evanescent Wave Cavity Ring-down Spectroscopy as a Probe of Surface Processes"  
• Andrew Pipino, Jeffrey W. Hudgens, and Robert E. Huie



- F25.** "Absolute Rate Constant and Product Branching Ratios for the Reaction between F and C<sub>2</sub>H<sub>4</sub> at T=200 –298 K"  
• Fred L. Nesbitt, R. Peyton Thorn, Jr., and Walter A. Payne
- F26.** "Reactions of N(2D) with Alkane Hydrocarbons to Produce NH(X 3Sigma -)"  
• Hironobu Umemoto
- F27.** "Mechanistic and Kinetic Study of the Reaction of Hydroxyl Radicals with Dimethylsulfoxide"  
• Shawn P. Urbanski, Robert E. Stickel and Paul H. Wine
- F28.** "On the Energetics, Kinetics, and Product Distributions in the Reactions of Ozone with Ethene and 2,3-Dimethyl-2-butene"  
• M. Olzmann, E. Kraka, D. Cremer, R. Gutbrod, R. N. Schindler, and S. Andersson
- F29.** "Ozonolysis of Alkenes in the Troposphere"  
• Charlotte McGill, Andrew Rickard, and George Marston
- F30.** "Kinetics Studies of Some Halogenated Organic Compounds of Tropospheric Interest"  
• C. E. Canosa-Mas, T. J. Dillon, K. Thompson, R. P. Wayne
- F31.** "Rate Constants for Reactions of OH with CH<sub>2</sub>Cl<sub>2</sub> and CH<sub>2</sub>ClBr between 277 and 370 K"  
• Vladimir L Orkin, Eric Villenave, Robert E. Huie, and Michael J. Kurylo
- F32.** "Kinetic Study of the CH<sub>2</sub>ClO Radical Reaction with O<sub>2</sub> and the Unimolecular Elimination of HCl"  
• Robert W. Carr and Fuxiang Wu
- F33.** "High Temperature Kinetics of Ion-Molecule Reactions"  
• Robert A. Morris, A. A. Viggiano, I. Dotan, Peter M. Hierl
- F34.** "Studies of the Kinetics of VB Group Metals (Vanadium, Niobium, Tantalum) Interactions with Atomic and Molecular Oxygen"  
• S. A. Raspopov, A. G. Gusakov, A. G. Voropayev, and M. L. Zheludkevich
- F35.** "Kinetics and Mechanisms for the Pyrolysis of the Chlorinated Silanes"  
• Mark T. Swihart and Robert W. Carr
- F36.** "Quenching of the First Electronic Excited State of Carbene CCl<sub>2</sub> (A(0,7,0)) by Simple Molecules"  
• I. Merelas, M. N. Sanchez Rayo, F. Castano and D. Husain
- F37.** "Photochemical Kinetics of the O/O<sub>2</sub>/O<sub>3</sub> System: Recombination, Vibrational Deactivation, Excited Electronic States, and Instrument Response"  
• Jack G. Green and John R. Barker

**F38.** "Absorption Spectra and Reactivity of Vinylperoxyl and Arylperoxyl Radicals in Aqueous Solutions"

- Z. B. Alfassi, G. I. Khaikin, and P. Neta

**F39.** "Oxidation of SO<sub>2</sub> in Sulfuric Acid Solutions"

- J. Boniface, O. V. Rattigan, E. Swartz, and P. Davidovits

**F40.** "Laser Flash Photolysis Measurements of Several Reactions Involving Aqueous Cl, Cl<sup>-</sup>, and Cl<sub>2</sub><sup>-</sup>"

- Zhen-Chuan Bao and John R. Barker

**F41.** "Effect of Substituents on the Nature of OH Radical Reaction with Organic Sulfur Compounds: A Pulse Radiolysis Study"

- Hari Mohan and Jai P. Mittal

**F42.** "Experimental and Theoretical Studies of the Unimolecular Decomposition of Nitrosobenzene: High-Pressure Rate Constants and the C-N Bond Strength"

- J. Park, I. V. Dyakov, A. M. Mebel and M. C. Lin

**F43.** "Enthalpies of Formation and Group Additivity of Alkyl Peroxides"

- Tsan H. Lay and Joseph W. Bozzelli

**F44.** "The Carbon Atom Exchange Reaction  $13\text{CH} + 12\text{CO} \rightleftharpoons 12\text{CH} + 13\text{CO}$ "

- J. L. Durant and C. A. Taatjes

**F45.** "Reaction Kinetics of O-atoms and OH Radicals with Diamine Rocket Propellants"

- Ghanshyam L. Vaghjiani

**F46.** "Pathway and Kinetic Analysis on the Propyl Radical + O<sub>2</sub> Reaction System"

- Joseph W. Bozzelli and William J. Pitz

### **Session L: Poster Session 3**

**Thursday, 4:40 - 6:30 p.m. -- Gaithersburg Hilton Hotel**

**L1.** "Kinetics and Mechanism of a New Class of the Reversible Topochemical Reactions – Disproportionation of Acidic Phosphoric Salts"

- V. V. Samuskevich, O. A. Lukyanenko, L. N. Samuskevich

**L2.** "Stereochemistry of the Thermal Decompositions and Isomerizations of Deuterated Cyclohexenes and Vinylcyclobutane; Evidence of Nonconcerted Thermal Decomposition of Cyclohexene"

- David K. Lewis

- L3.** "High Temperature Pyrolysis and Oxidation of Cyclopentadiene"  
• K. Roy and P. Frank
- L4.** "Thermal Decomposition of Diethylmethylphosphonate and Ethymethylphosphonate"  
• Wing Tsang, James A. Walker, and Jeffrey A. Manion
- L5.** "Heterogeneous Reactions in the Process of Fluoroolefin/Oxygen Self-Ignition"  
• I. R. Begishev
- L6.** "Oxidation Chemistry of Dimethyl Ether Related to its Properties as a Diesel Fuel"  
• E. W. Kaiser and T. J. Wallington
- L7.** "The Peculiarities of Hydrocarbon Oxidation in a "Wall-less" Reactor Under the Laser Heating"  
• Adolph A. Mantashyan
- L8.** "Kinetic Modeling Study on MTBE Oxidation"  
• Ru Wei and Joseph W. Bozzelli
- L9.** "SOOT Particles Growth Kinetics During Hydrocarbon Pyrolysis Behind Shock Waves"  
• Karasevitch Yu., K., H. Gg. Wagner, I. S. Zaslono, and Zhil'tzova I. V.
- L10.** "Kinetic Evaluations of High Molecular Weight Aromatic Formation in Rich Premixed Ethylene Flames"  
• Andrea D'Anna and Angela Violi
- L11.** "Predicted Rates for H-Abstraction via Density Functional Theory"  
• Roberta G. Susnow, Anthony M. Dean and William H. Green, Jr.
- L12.** "The Influence of Hindered Rotations on Recombination Kinetics"  
• Albert F. Wagner, David M. Wardlaw, Struan H. Robertson
- L13.** "Transition State Structures and Properties of Hydrogen Transfer Reactions of Hydrocarbons: Ab Initio Benchmark Calculations"  
• J. A. Litwinowicz, S. Jurisevic, L. Rendak, M. Zalar, D. W. Ewing, and Michael J. Manka
- L14.** "Simulation of a Physical-Chemical Transformation of Gas-Aerosol Components of Engine Exhaust from Aircraft. Potential Environment Contamination and Climatic Trends"  
• V. G. Bondarenko
- L15.** "Numerical Modeling of Chemical Kinetics and Transport of Pollutants in the Atmosphere of Industrial Regions"  
• V. V. Penenko and E. A. Tsvetova, G. I. Skubnevskaya, G. G. Dultseva, and A. V. Keiko

**L16.** "Shockwave Study of the Reaction of Toluene with Molecular Oxygen in the Temperature Range between 1200 and 1400 K"

- R. Eng, C. Fittschen, P. Hibomvski, H. Hippler, and A.-N. Unterreiner

**L17.** "Modeling Study of Methane and Butane Photo-oxidation and Application to Regional Scale Air Pollution in Eastern Europe and Western Siberia"

- A. E. Aloyan, V. O. Arutyunyan, G. I. Skubenskaya, and G. G. Dultseva

**L18.** "Absolute Rate Constant for the Reaction between IO and O(3P) at T = 298K"

- Walter A. Payne, R. Peyton Thorn, Jr., Louis J. Stief, and Fred L. Nesbitt

**L19.** "Study of Iodine Oxides Ozone Chemistry Using Flash Photolysis and Time Resolved Absorption Spectroscopy"

- Peter Spietz, Stefan Himmelmann, and Uldis Gross

**L20.** "Deuterium Kinetic Isotope Effects in the Reactions of CH<sub>2</sub>· with Methane and Acetylene and C<sub>2</sub>H<sub>2</sub><sup>+</sup> with O<sub>2</sub>"

- Holger S. Thiesemann and Craig A. Taatjes

**L21.** "Thermochemical Kinetic Analysis on the Reaction of Allylic Isobutenyl Radical with O<sub>2</sub>: An Elementary Reaction Mechanism for Isobutene Oxidation"

- Chung-Ju Chen and Joseph W. Bozzelli

**L22.** "The Rate Constants for the Self-Combination Reactions of CF<sub>3</sub>, C<sub>2</sub>F<sub>5</sub>, and n-C<sub>3</sub>F<sub>7</sub> Radicals"

- A. B. Vakhtin

**L23.** "The Many Facets of Activation Energies"

- Jay E. Taylor

**L24.** "Halogenated Peroxyl Radical Induced Oxidation of β-Carotene in a Quaternary Micro Emulsion"

- S. Adhikari, S. K. Kapoor and C. Gopinathan

**L25.** "On the Reaction of Sulfate Radicals in Water"

- Barna Laszlo and Robert E. Huie

**L26.** "Products of the O(3P) + C<sub>3</sub>H<sub>6</sub> Reaction and Branching Fraction for Formation of CH<sub>3</sub>"

- R. Bruce Klemm, Szu-Cherng Kuo, Stuart K. Ross, and R. Peyton Thorn, Jr.

**L27.** "Kinetic Studies of Cl Atom Reactions with C<sub>3</sub>H<sub>n</sub> (n=4,6) between 300-850 K"

- John T. Farrell, Jeffrey S. Pilgrim, and Craig A. Taatjes

**L28.** "Kinetic and Transition State Analysis for alpha- and beta-Addition of Hydroxyl Radical to Chloroethylene"

- Li Zhu and Joseph W. Bozzelli

**L29.** "Kinetic Study of the Reactions of Chlorine Atoms with 2,3-butadione, Cyclohexanone and Cyclopentanone"

- A. Guschin, T. J. Wallington, and M. D. Hurley

**L30.** "Formation of Negative Ions by Attachment of Electrons to Radicals – Its Bearing on Radiation Chemistry"

- Masao Inoue

**L31.** "Simultaneous Oxidation of NO and Hydrocarbons in a Non-Thermal Plasma"

- William J. Pitz, Bernie M. Penetrante and Mark C. Hsiao

**L32.** "Rate Constants of Dissociative Electron Recombination with H<sub>2</sub><sup>+</sup> and D<sub>2</sub><sup>+</sup> Molecular Ions"

- Golubkov M. G., Golubkov G. V., Ivanov G. K.

**L33.** "Kinetics of the Termolecular Insertion Reaction of Rh(a<sub>4</sub>F<sub>9</sub>/2) with CH<sub>4</sub>"

- Mark L. Campbell

**L34.** "Kinetic Behaviour of the Titanium Alloys to 6Al 4V and to 6Al 5Zr 0.5Mo 0.25Si in Air and Oxygen at a Temperature Range of 400oC – 600oC"

- Magdalena Momirlan and Pincovschi Eugen

**L35.** "Ozone Yields from Oxygen Photolysis at 193 nm"

- Huei Tarnng Liou

**L36.** "Dissociation Dynamics of Hydrochloride Dimer Radical Cation"

- Q. Zhong, L. Poth, J. V. Ford, A. W. Castleman, Jr.

**L37.** "Non-Linear Phenomenon in Magnetic Field Sensible Recombination of Radicals in Luminol Chemiluminescent Reaction in Aqueous Solution"

- George E. Zorinians and Michael M. Triebel

**L38.** "Iron-Catalyzed Oxidation of Bisulfite Aqueous Solution as a Branching Reaction"

- Alexander N. Yermakov and Anatol P. Purnal

**L39.** "An Ab Initio Study of Bond Strengths in Party Chlorinated Saturated Small Hydrocarbons"

- J. A. Seetula

**L40.** "Reaction Kinetics of O(3P) with Unsaturated Cyano Compounds"

- Hari P. Upadhyaya, Prakash D. Naik, Avinash V. Sapre and Jai P. Mittal

**L41.** "Simulation Studies of Kinetics of Silane Combustion"

- V. Babushok, W. Tsang, D. R. Burgess, Jr., and M. R. Zachariah

- L42.** "The Reactions of CH<sub>3</sub> with O<sub>2</sub>"
- C.-C. Hsu, A. S. Rodgers, and M. C. Lin
- L43.** "Two-Color Kinetic Absorption Measurements of HO<sub>2</sub> + RO<sub>2</sub> Reaction Rates"
- Charles E. Miller and Stanley P. Sander
- L44.** "Ab Initio Determination of Molecular Thermochemistry: Extrapolation of Reaction Energies"
- Timothy J. Lee
- L45.** "Evidence for a Marcus Inverted Region in Biomolecular Electron Transfer Between C<sub>76</sub>/C<sub>78</sub> and Arene Radical Cations"
- Dirk M. Guldi and Klaus-Dieter Asmus
- L46.** "Chemical Kinetic Factors Involved in the Antioxidant Activity of Methoxy Phenols"
- K. Indira Priyadarsini and S. N. Guha
- L47.** "The Pyrolysis of Acetylene at Low Conversions"
- Stevan T. Dimitrijevic, Shelia Paterson, and Philip D. Pacey

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