CONFERENCE PROGRAM (5th Int'l Conference on Chemical Kinetics)

Sunday, 15th July

6:00 - 8:30 p.m -- Registration and Reception at the Holiday Inn Gaithersburg.

Oral Sessions

Monday, 16th July

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

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

8:45 a.m.
- Opening Remarks.

Session A: Modeling
NIST Red Auditorium
Chair: Russell Johnson III

9:05 --9:25 a.m.
- **A1. "A Model For Alkyl Nitrate Yields From The RO_2 + NO Reaction"**
  - *John R. Barker, Lawrence L. Lohr, Robert M. Shroll, Susan Reading, and Timothy J. Wallington*

9:30 --9:50 a.m.
- **A2. "Towards a Quantitative Modeling of the Reaction: H + O_2 ←→ HO_2 ←→ HO + O"**
  - *Jürgen Troe*

9:50 -- 10:10 a.m.
- **A3. "High Dimensional Model Representations"**
  - *Genyuan Li and Herschel Rabitz*

10:15 - 10:35 a.m.
- **A4. "On the Number of Observable Species and Observable Reactions in Liquid Phase Syntheses for Fine Chemicals and Pharmaceuticals - Advanced Chemometrics for System Identification"**
  - *Chen Li, Effendi Widjaja, Chew Wee, and Marc Garland*

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

11:00 - 11:45 a.m.

- **A5.** *Invited.* **"Towards Predictive Kinetics for Technologically Important Processes"**
    - *William H. Green, Jr.* (MIT Department of Chemical Engineering)

11:50 - 12:10 a.m.

- **A6. "Automated Elementary Reaction Mechanism Generation Incorporating Thermochemistry, Fall-off, and Chemical Activation Reactions of OH with Olefins"**
    - *Jeffrey M. Grenda and Joseph W. Bozzelli*

12:15 - 12:35 p.m.

- **A7. "Analysis of the Valid Parameter Ranges for a Computer-generated Chemical Kinetic Model"**
    - *Jing Song, George Stephanopoulos, William H. Green*

12:40 - 1:40 p.m.

- **Lunch**

Session B: Radical-Radical Reactions
NIST Red Auditorium
Chair: Jeffrey Manion

1:40 -- 2:20 p.m.

- **B1.** *Invited.* **"Radical-Radical Recombination Reactions"**
    - *Dr. Larry Harding* (Argonne Nat'l Lab.)

2:25 -- 2:45 p.m.

- **B2. "Implications of Unusual Pressure Dependence Observed in Various Radical Combination Reactions of CCl_3"**
    - *Klaus Luther, Kawon Oum and Jürgen Troe*

2:50 -- 3:10 p.m.

- **B3. "Determination Of The Branching Ratios In The Radical-Radical Reaction: CN($^2\Sigma^+$) + OH($^2\Pi$)"**
    - *B. K. Decker and R. Glen Macdonald*

3:15 -- 3:35 p.m.

- **B4. "A Kinetics and Product Study of the Reaction of CH_3 Radicals with O(^{3}P) Atoms using Time Resolved Time-of-Flight Mass Spectrometry"**
    - *Christopher Fockenberg*

3:40 -- 4:00 p.m.

- **B5. "CO VUV-Visible Emissions During Laser Photolysis of Ketene in the Presence of Excess O-atoms"**
    - *Ghanshyam L. Vaghjiani*

4:15 p.m.

- Buses leave NIST for the Holiday Inn Gaithersburg.
    - (Buses will be waiting at the entrance of the Administration building.*)*

4:25 -- 6:30 p.m.

- **Session C: Poster 1**
    - Refreshments will be served.

Tuesday 17th July

8:15 a.m.

- Buses leave the Holiday Inn Gaithersburg for NIST.
    - (**Note:** *Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.)*

Session D: Unimolecular and High Pressure Kinetics
NIST Red Auditorium
Chair: Jeffrey W. Hudgens

9:00 -- 9:20 a.m.

- **D1. "Pressure Dependence of the Product Branching for $O(^3P) + C_2H_4$ Reaction"**
    - *Jun-ichi Yoshida, Akira Miyoshi, Mitsuo Koshi, and Hiroyuki Matsui*

9:25 -- 9:45 a.m.

- **D2. "Rate Constants for $H + O_2 + M \rightarrow HO_2 + M$ in Seven Bath Gases"**
    - *J. V. Michael, M.-C. Su, J. W. Sutherland, J. J. Carroll, and A. F. Wagner*

9:50 -- 10:10 a.m.

- **D3. "Mode Specificity and Non-Exponential Unimolecular Decay of Vibrationally Highly Excited States of DCO** ($X\ ^2A'$)"
    - *F. Renth, F. Temps, and A. Tröllsch*

10:15 - 10:35 a.m.

- **D4. "Unimolecular Reactions of Alkoxy Radicals: Experiment and Theory"**
    - *H. Somnitz, A. Hoffmann, C. Lotz and R. Zellner*

10:40 - 11:00 a.m.

- **Break**

11:00 - 11:45 a.m.

- **D5.** *Invited.* **-- "Rotational Channel Switching in Unimolecular Decomposition Reactions: Experiments and Theory"**
    - *Horst Hippler* (U. Karlesruhe)

11:50 - 12:10 a.m.

- **D6. "Size-Selected Nanoparticle Chemistry: Kinetics of Soot Oxidation"**
    - K. Higgins, H.J. Jung, D. Kittelson, J.T. Roberts and M.R. Zachariah

12:15 - 12:35 a.m.

- **D7. "Small-Angle X-Ray Scattering Studies Of Soot Inception And Growth"**
    - *Jan P. Hessler, Soenke Seifert, Randall E. Winans,* and *Thomas H. Fletcher*

12:40 - 1:40 p.m.

- **Lunch**

Session E: Condensed Phase Kinetics
NIST Red Auditorium
Chair: Dr. Robert E. Huie

1:40 -- 2:00 p.m.

- **E1. "Real-time Observation of Intramolecular Vibrational Energy Redistribution and Intermolecular Vibrational Energy Transfer of Selectively Excited CH_2I_2 and C_3H_5I Molecules in Solution"**
    - *B. Abel*

2:05 -- 2:25 p.m.

- **E2. "Kinetics of Aqueous Phase Reactions of OH and SO_4^- Radicals with Organosulfur Compounds of Atmospheric Interest"**
    - *Zhu, J.M. Nicovich, and P.H. Wine*

2:30 -- 2:50 p.m.

- **E3. "Reaction Kinetics in Ionic Liquids. Pulse Radiolysis Studies"**
    - *Pedatsur Neta and David Behar*

2:55 -- 3:15 p.m.

- **E4. "Kinetics of the full oxidation of zinc powders to zinc oxide powders above the melting temperature of zinc metal"**
    - *R. Metz, C. Machado, R. Tenu, J.J. Counioux, and H. Delalu*

3:20 -- 3:40 p.m.

- **E5. "Reactivity of Higher Oxidation States of Iron (Fe(VI), Fe(V), and Fe(IV)) with Cyanide and Thiocyanate: A Stopped-Flow and Premix Pulse Radiolysis Study"**
    - *Virender K. Sharma and Christopher R. Burnett*

3:45 -- 4:05 p.m.

- **E6. "Molecular Dynamics and the Solvation of Isopropyl Alcohol from Ambient to Supercritical Conditions"**
    - *Raymond Mountain*

4:15 p.m.

- Buses leave NIST for the Holiday Inn Gaithersburg.

- (Buses will be waiting at the entrance of the Administration building.*)*

4:20 - 6:30 p.m.

- **Session F: Poster 2**
  - Refreshments will be served.

Wednesday 18th July

8:15 a.m.

- Buses leave the Holiday Inn Gaithersburg for NIST.
    - (**Note:** *Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.*)

Session G: Atmospheric Chemistry I
NIST Red Auditorium
Chair: Michael Kurylo III

9:00 -- 9:20 a.m.

- **G1. "Kinetic and Thermodynamic Pathway Analysis and Elementary Reaction Mechanism for Atmospheric Reactions of Aromatics: Benzene and Toluene"**
    - *Chiung-Ju Chen and Joseph W Bozzelli*

9:25 -- 9:45 a.m.

- **G2. "An Investigation of N_2O Production From Photolysis of $O_3/N_2/O_2$ Mixtures at 266 nm and 532 nm"**
    - *E. G. Estupiñán, R. E. Stickel, J.M. Nicovich, and P.H.Wine*

9:50 -- 10:10 a.m.

- **G3. "UV Absorption Spectrum of Hydroxycyclohexadienyl Radical, C_6H_8OH, and Thermochemistry of the Oxidation Reaction $C_6H_8OH + O_2 <=> C_6H_8(OH)OO$**
    - *Sergey Y. Grebenkin and Lev N. Krasnoperov*

10:15 - 10:35 a.m.

- **G4. "Conversion Of Acetaldehyde Vapor To Ultrafine Aerosols Initiated By Photochemical Reactions"**
    - *G. I. Skubnevskaya, S. N. Dubtsov , G. G. Dultseva and E. N. Dultsev*

10:40 - 11:00 a.m.

- **Break**

Session H: Atmospheric Chemistry II
NIST Red Auditorium
Chair: Michael Kurylo III

11:00 - 11:45 a.m.

- **H1.** *Invited.* **"The Chemical Kinetics of Heterogeneous Reactions in Atmospheric Chemistry"**
    - *Michel J. Rossi (EPFL, Lausanne, Switzerland)*

11:50 - 12:10 a.m.

- **H2. "Kinetic Mechanisms of HO_2 and NO_3 Uptake on Solid NaCl"**
    - *Yu. M. Gershenzon, R. G. Remorov, M. Yu. Gershenzon, Jr., D. V. Shestakov, E. A. Aparina, V. V. Zelenov, L. T. Molina, M. J. Molina*

12:15 - 12:35 a.m.

- **H3. "Time and Particle Size Resolved Kinetics of Photochemical Aerosol Formation by Laser Photolysis – Laser Scattering Imaging"**
    - *Sergei N. Dubtsov, Evgeni N. Chesnokov and Lev N. Krasnoperov*

12:40 - 1:40 a.m.

- **Lunch**

Session I: Hideo Okabe Celebration Session: Small Radical Kinetics & Photochemistry

NIST Red Auditorium

Chair: Louis J. Stief

1:40 -- 1:50 p.m.

- **An Appreciation of the Career of Hideo Okabe**

1:50 -- 1:55 p.m.

- **Presentation of Book of Letters**
    - *Louis J. Stief and Joshua B. Halpern*

1:55 -- 2:25 p.m.

- **I1. "Velocity Imaging Studies of the photolysis of CS_2 in the VUV region"**
    - *Dadong Xu, Jianhua Huang, and William M. Jackson*

2:30 -- 2:50 p.m.

- **I2. "Kinetics of the Reaction Between Propargyl Radical and Acetylene"**
    - *Vadim D. Knyazev and Irene R. Slagle*

2:55 -- 3:15 p.m.

- **I3. "Low-temperature Kinetics of Reactions of C_2H and OH Radicals with Selected Hydrocarbons: Implications to Chemistry of the Outer Planets"**
    - *Andrei B. Vakhtin, Dwayne E. Heard, Ian W. M. Smith, and Stephen R. Leone*

3:20 -- 3:40 p.m.

- **Break**

3:40 -- 4:00 p.m.

- **I4. "The Kinetics of the Reactions of H atoms with Halogenated Ethylenes"**
    - *Xiaohua Hu, A. Goumri and Paul Marshall*

4:05 -- 4:25 p.m.

- **I5. "Time-Resolved Infrared Probing of HO_2 Formation in Alkyl + O_2 Reactions"**
    - *John D. DeSain, Eileen P. Clifford, and Craig A. Taatjes*

4:30 -- 4:50 p.m.

- **I6. The Vinyl Radical (A^2A' <-- X^2A'') Spectrum Between 530 and 415 nm: Vibrational and rotational spectra of C_2H_3 and C_2D_3"**
    - *Joshua B. Halpern, Katina Patrick, Charles. D. Pibel, Mohamed Bouadani, Milena Shahu, Andrew. McIlroy, Craig A. Taatjes*

5:05 p.m.

- Buses leave NIST for the Holiday Inn Gaithersburg.
    - (Buses will be waiting at the entrance of the Administration building.*)*

7:00 p.m.

- **Reception and Banquet,** Holiday Inn Gaithersburg
    - **Speaker:** *Dr. Chuck Kolb, "Is the Future Rate Limited?"*

Thursday 19th July

8:15 a.m.

- Buses leave the Holiday Inn Gaithersburg for NIST.
    - (**Note:** *Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.)*

Session J: Ion and Plasma Processes
NIST Red Auditorium
Chair: Karl Irikura

9:00 -- 9:20 a.m.

- **J1. "A Combined Theoretical and Experimental Study of the Structure, Thermochemistry, and Reactivity Trends of Sulfur Oxyfluoride Neutrals and Anions"**
    - *Susan T. Arnold, Thomas M. Miller, A. A. Viggiano*

9:25 -- 9:45 a.m.

- **J2. "Kinetics of Destruction of Organophosphorous Compounds in Corona Discharge"**
    - *Oleg P. Korobeinichev, Anatoly A. Chernov, Vladimir V. Sokolov*

9:50 -- 10:10 a.m.

- **J3. "Mechanisms of Thermal Decomposition of Silane and Disilane and Formation of Small Si Clusters, Si_nH_x (n=3-10, x=0-2), in the Gas Phase"**
    - *Steven D. Chambreau, Liming Wang, and Jingsong Zhang*

10:15 - 10:35 a.m.

- **J4. "REMPI-LIF studies of ion-molecule association reactions"**
    - *Michael J. Frost and Christopher R. J. Sharpe*

10:40 - 11:00 a.m.

- **Break**

11:00 - 11:20 a.m.

- **J5. "Ion Molecule Chemistry at High Temperature: Derivation of Rotational and Vibrational Energy Dependencies"**
    - *A. A. Viggiano*

11:25 - 11:45 a.m.

- **J6. "Ion-molecule Reactions of State Selected HCl^+ and HBr^+ Ions"**
  - *Helmar Waiczies, Marcus Malow, Klaus Brembs, and Karl-Michael Weitzel*

11:50 - 12:10 a.m.

- **J7. "Kinetic and Mechanism of Hydrocarbons Transformation in Dielectric Barrier Corona Discharge"**
  - *Lev N. Krasnoperov and Larisa G. Krishtopa*

12:15 - 12:35

- **J8. "Bond Dissociation Energies of the Polyynes: $D_0(HC_{2n}–H)$ is smaller than $D_0(HCC–H)$ for $n > 2$"**
  - *Kent M. Ervin and Yang Shi*

12:40 - 1:40 p.m.

- **Lunch**

Session K: Combustion Chemistry
NIST Red Auditorium
Chair: Wing Tsang

1:40 -- 2:20 p.m.

- **K1.** *Invited.* **"Stochastic Models for High Temperature Combustion Reactions"**
  - *Dr. Jim Miller (Sandia Lab.)*

2:25 -- 2:45 p.m.

- **K2. "Surprising Kinetic Behavior in NO–Butane–Air "Reburning"**
  - *Hans-Heinrich Carstensen and Anthony M. Dean*

2:50 -- 3:10 p.m.

- **K3. "Thermochemical Properties, Reaction Paths and Kinetic Parameters for Vinylidene Insertion Reactions Important to Molecular Weight Growth"**
  - *Leonhard Rutz and Henning Bockhorn, and Joseph W. Bozzelli*

3:15 -- 3:35 p.m.

- **K4. "A Theoretical Study of the Reactions on the C_2H_3O Potential Energy Surfaces: Kinetics of C_2H_2+OH → Products and the Unimolecular Dissociation of the Vinoxy Radical"**
  - *Scott G. Davis, Hai Wang, and Wing Tsang*

3:40 -- 4:00 p.m.

- **K5. "Investigation On The Decay Of Benzene And The Recombination Reaction H + Phenyl At High Temperatures"**
    - *S. Scherer, P. Vöhringer, Marina Braun-Unkhoff, P. Frank, Th. Just*

4:15 p.m.

- Buses leave NIST for the Holiday Inn Gaithersburg.
    - (Buses will be waiting at the entrance of the Administration building.*)*

4:40 -- 6:30 p.m.

- **Session L: Poster 3**
    - Refreshments will be served.

Friday 20th July

8:15 a.m.

- Buses leave the Holiday Inn Gaithersburg for NIST.
    - (**Note:** *Coffee and breakfast items are available in the NIST cafeteria adjacent to the Green Auditorium.)*

Session M: Theory
NIST Red Auditorium
Chair: Anne Chaka

9:00 -- 9:20 a.m.

- **M1.** "***Ab Initio* Studies of the Kinetics of the Reactions of OH Radicals with a Series of Haloalkanes"**
    - *Florent Louis, Carlos A. Gonzalez, Michael J. Kurylo, and Robert E. Huie*

9:25 -- 9:45 a.m.

- **M2. "Thermodynamic and Kinetic Analysis using *ab initio* Calculations on Formyl Methyl Radical + O_2 Reaction System"**
    - *Jongwoo Lee and Joseph W. Bozzelli*

9:50 -- 10:10 a.m.

- **M3. "Molecular Hydrogen Elimination from 2,5-dihydrofuran, 2,3- dihydrofuran and 2-methyl-2,5-dihydrofuran. Quantum chemical and Kinetics Calculations"**
    - *Faina Dubnikova and Assa Lifshitz*

10:15 - 10:35 a.m.

- **M4. "Quasiclassical Trajectory Studies of the Kinetics and Dynamics of the OH + H_2 --> H + H_2O and the Reverse Reaction"**
    - *Matthew J. Lakin, Diego Troya, György Póta, György Lendvay, Miguel González, and George C. Schatz*

10:40 - 11:00 a.m.

- **Break**

11:00 - 11:20 a.m.

- **M5. "*Ab Initio* Study of the Effect of H_2O on the Self-Reaction of HO_2*"**
    - *Rongshun Zhu and M. C. Lin*

11:25 - 11:45 a.m.

- **M6. "A Theoretical Comparison of the Reactions of OH and $O(^3P_J)$ with H_2O_2"**
    - *Juan P. Senosiain, Charles B. Musgrave, David M. Golden*

11:50 - 12:10 a.m.

- **M7. "Comparison of Quantum and Quasiclassical Calculations of Gateway Frequencies for Collisional Energy Transfer in Polyatomic Molecules"**
    - *Victor Bernshtein and Izhack Oref*

12:15 - 1:15 p.m.

- **Lunch**

1:30 p.m.

- Buses leave NIST for the Holiday Inn Gaithersburg.
    - (Buses will be waiting at the entrance of the Administration building.*)*

Session C: Poster Session 1

Monday, 4:30 - 6:30 p.m. -- Gaithersburg Holiday Inn

- **C1.** "**First-principles prediction of the rate constants for OH + NO_x (x=1, 2) reactions"**
    - *Rongshun Zhu and M. C. Lin*
- **C2.** "**Complete Mapping of Aqueous Medium Chain Oxidation of S(IV) to S(VI) In Presence of O_2"**
    - *Tomi Nath Das*
- **C3.** "**Pulse Radiolysis Study on the Antioxidant Activity of Bacuchiol: Kinetic Aspects"**
    - *S. Adhikari, Ravi joshi, B. S. Patro, S. Chattopadhyay, T.K. Ghanty, and T. Mukherjee*
- **C4. "Quantum Monte Carlo Studies of Thermodynamics and Electronic States of Ozone"**
    - *John A. W. Harkless*
- **C5. "Thermodynamic properties (Enthalpies, Entropies and Heat Capacities) and Reactions of vinyl hydroperoxides, peroxy radicals and phenyl hydroperoxides"**
    - *Nadia Sebbar, Henning Bockhorn, and Joseph W. Bozzelli*
- **C6. "Applications of Bayesian Parameter Estimation and Uncertainty Analysis Methods to Complex Reaction Mechanisms"**
    - *Bharthwaj Anantharaman, Jose Ortega, William H. Green Jr., and Gregory J. McRae*
- **C7. "Simulation of Chemical Mechanisms Using REACT for Windows"**
    - *Michael J. Manka*
- **C8.** "**Validation of Noisy Single-Exponential-Decay Data**"
    - *Abel Fernandez and Arthur Fontijn*
- **C9. "A Predictive Correlation Between Rate Coefficients, Electron Affinities and Energetics of Radical-Radical Combination Reactions"**
    - *Askar Fahr, Parviz Hassanzadeh, and Dwight C. Tardy*

- **C20. "Kinetics of the Reaction Al + SF_6 in the Temperature Range 499 To 813 K"**
    - *James K. Parker, Nancy L. Garland, and Herbert H. Nelson*
- **C21. "Association Reaction Kinetics of Iron and Cobalt Atoms with Sulfur Dioxide: Experimental, RRKM, and DFT Studies"**
    - *Roy E. McClean*
- **C22. "Kinetic Study of the Reactions of Gas Phase Pd(a^1S_0), Ag($5s\ ^2S_{1/2}$), Au($6s\ ^2S_{1/2}$), Cd($5s^2\ ^1S_0$) and Hg($6s^2\ ^1S_0$) Atoms with Nitrous Oxide**
    - *Mark L. Campbell*
- **C23. "Kinetics Study of Si(^3P) + SiH_4 Reaction"**
    - *M. Koi, S. Ide, A. Tezaki, K. Yoshida, K. Tonokura, and M. Koshi*
- **C24. "Temperature Dependence of the Acid Dissociation Constant of the Hydroxyl Radical"**
    - *G. A. Poskrebyshev, P. Neta, and R. E. Huie*
- **C25. "Isodesmic Reactions and Thermochemistry of Free Radicals"**
    - *Dmitri Ponomarev and Vjacheslav Takhistov*
- **C26. "Computational Study of the Mechanism and Product Yields in the Reaction System $C_2H_3 + CH_3 <=> C_3H_6 <=> H + C_3H_5$"**
    - *Stanislav I. Stoliarov, Vadim D. Knyazev, and Irene R. Slagle*
- **C27. "Computational Study of the HCCO + NO Reaction: *Ab Initio* MO/vRRKM Calculation of the Total Rate Constant and Product Branching Ratios"**
    - *L. V. Moskaleva, D. Paschenko, and M. C. Lin*
- **C28. "Kinetics of the Ca + CH_3Br Reaction Between 303 And 878 K"**
    - *G. Gilis and C. Vinckier*
- **C29. "The Reaction of NH_2 with O_2 in the Presence of H_2O"**
    - *Russell D. Johnson III and Robert E. Huie*

- **C30. "*Ab Initio* Calculations of Reactions Relevant to the Formation of Atomic Metal Layers in the Mesopause"**
    - *Rubén Delgado, Yasuyuki Ishikawa, Jonathan S. Friedman, and Brad R. Weiner*
- **C31. "Linear Free Energy Relationship in a Pseudozero Order Reaction"**
    - *K. Nagajyothi, P.S. Raghavan, and R. Gopalan*
- **C32. "Study the Enzyme Catalytic Decomposition Reaction of Terephthalic Acid by Rhodopseudomonas"**
    - *Qiang Wang , Yi Shou-zhi, and Yong Wang*
- **C33. "Kinetics of the Thermal Isomerization of 1,1,2-trimethyl- and 1,1,2,2-tetramethyl-Cyclopropane"**
    - *Bansi L. Kalra, Janet Cho, Debra Mish, David K. Lewis, Jessica Schlier, Steven M. Hughes, Kevin Wilkinson, and Sara Wilkinson*
- **C34. "Kinetic Study of the Hydroxyl Radical Reaction with H_2 from 200K to 480K"**
    - *Gregory Poskrebyshev, Sergey Kozlov, Vladimir Orkin , Robert Huie, and Michael Kurylo*
- **C35. "A Virtual Data Engine for Gas Phase Chemistry"**
    - *Wing Tsang*
- **C36. "Thermochemical and Kinetics Analysis of the 2-hydroperoxy Ethyl Radical ($H_2C.CH_2OOH$) + O_2 Reaction in the Ethyl Radical + O_2 Oxidation System"**
    - *C. Seng and J. W. Bozzelli*
- **C37. Combined Screening And Exploration Of Pressure-Dependent Reaction Networks: H + Cycloalkenes"**
    - *David M. Matheu, Preeti Aghalayam, William H. Green, and Jeffery M. Grenda*
- **C38. "Rate Coefficients and Mechanistic Analysis for Reaction of OH with Vinyl Chloride between 292 and 730 K"**
    - *Takahiro Yamada, Masud Siraj, Philip H. Taylor, Jingping Peng, Xiaohua Hu, and Paul Marshall*

Session F: Poster Session 2

Tuesday, 4:30 - 6:30 p.m. -- Gaithersburg Holiday Inn

- **F1. "Kinetics and Mechanism of the Benzene + OH Reaction in the Gas-Phase as a Function of NO_x Concentrations"**
    - *Björn Klotz, Takashi Imamura, Nobuaki Washida, Rainer Volkamer, Ulrich Platt, Klaus Wirtz, Ian Barnes, and Karl Heinz Becker*
- **F2. "Theoretical Study of H + C_5H_5/C_5H_6 Reactions and the Decomposition of C_5H_6"**
    - *L. V. Moskaleva and M. C. Lin*
- **F3. "Reduction, Aggregation and Emission of Silver Clusters in Isopropanol-Cyclohexane Mixtures"**
    - *Medha Rele, Sudhir Kapoor, and Tulsi Mukherjee*
- **F4. "Kinetics of Reaction between OH Radical and Unsaturated Alcohols : Allyl(H_2C=$CHCH_2OH$) and Propargyl (HC≡CCH_2OH) Alcohol"**
    - *Hari P. Upadhyaya, Awadhesh Kumar, P. D. Naik, A. V. Sapre, and J. P. Mittal*
- **F5. "Fitting Vibrational Energy Parameters to Falloff Experiments: CH_3 + CH_3 + He (0.6-2 Torr, 200-298 K)"**
    - *Dwight C. Tardy, Regina J. Cody, Walter A. Payne, R. Peyton Thorn, Fred L. Nesbitt, Mark A. Iannone, and Louis J. Stief*
- **F6. "Peroxynitrite Induced Oxidation Reactions of Two Phenolic Antioxidants"**
    - *K. Indira Priyadarsini*
- **F7. "Mechanisms of Flame Inhibition by Tin and Manganese Containing Additives"**
    - *V. I. Babushok, V. D. Knyazev, and G. T. Linteris*
- **F8. "Detailed Kinetic Study of the Growth of Polycyclic Aromatic Hydrocarbons: Phenyl + Benzene and 1-Naphthyl + Benzene"**
    - *Oleg A. Mazyar, Henning Richter, Jack B. Howard, and William H. Green, Jr.*
- **F9. "Chloroform Pyrolysis and Oxidation"**
    - *Joseph W. Bozzelli, Li Zhu, Tsan H. Lay, and Yang-Soo Won*

- **F10. "Addition Reaction of Chlorine and Propargyl Chloride Studied by Cavity Ring-down Spectroscopy and by *ab initio* Calculations"**
    - *Jeffrey W. Hudgens, Dean B. Atkinson, and Carlos Gonzalez*
- **F11. "Experimental and Modeling Studies of Laminar Flame Speeds for C_4 Hydrocarbons at Elevated Temperature and Pressure"**
    - *John T. Farrell and Robert J. Johnston*
- **F12. "Numerical Study on the Decay of Cyclopentadiene and the Association Reaction H + Cyclopentadienylradical at High Temperatures: Comparison with Measured Data"**
    - *K. Roy, Marina Braun-Unkhoff, P. Frank, and Th. Just*
- **F13. "Thermal Decomposition of Diketene: Theory and Experiment"**
    - *Binh Bui, Ti Jo Tsay, M. C. Lin and C. F. Melius*
- **F14. "Combustion of Acetylene, Ethylene and Benzene in Fuel-Rich Premixed Low-Pressure Flames"**
    - *Henning Richter, Raman Sumathi, William H. Green and Jack B. Howard*
- **F15. "The Kinetics of ADN Vapor Decomposition in Relation to ADN Combustion Chemistry"**
    - *Andrey G. Shmakov, Oleg P. Korobeinichev, Tatayna A. Bolshova, and Alexander A. Paletsky*
- **F16. "A Detailed Experimental and Theoretical Study on the Thermal Decomposition of Methoxy Radicals"**
    - *H. Hippler, F. Striebel, and B. Viskolcz*
- **F17. "Modelling Of Nonlinear Vibrational Relaxation Of Large Molecules In Shock Waves With A Nonlinear, Temperature Varying Master Equation"**
    - *Michael J. Davis, and John H. Kiefer*
- **F18. "Photoionization Mass Spectrometric Study of the Dissociative Ionization of Ethyl Radical: Heat of Formation of Vinyl Radical"**
    - *R. Bruce Klemm, Szu-Cherng Kuo, R. Peyton Thorn, Jr., and Louis J. Stief*
- **F19. "The Binding Energies of Small Ar, CO and N_2 Cluster Ions"**
    - *Joachim Mähnert and Karl-Michael Weitzel*

- **F20. "The Kinetics of Pyrolysis of Vinyl Bromide"**
    - *Patricia Ann Laws, Bradley D. Hayley, Lori M. Anthony, and John M. Roscoe*
- **F21. "On the Mechanism of SO_2 Oxidation by Methylperoxy Radicals. An *Ab Initio* Study"**
    - *Ruben S. Asatryan, Aram G. Davtyan, and Adolph A. Mantashyan*
- **F22. "A Pulsed Laser Photolysis-Pulsed Laser Induced Fluorescence Study of the Kinetics of the Gas-Phase Reaction of OH with NO_2 and NO"**
    - *L. D'Ottone, P. Campuzano-Jost, D. Bauer, and A. J. Hynes*
- **F23. "Chemical Kinetic Characterization of Combustion of Toluene"**
    - *W. J. Pitz, R. Seiser, J. W. Bozzelli, I. Da Costa, R. Fournet, F. Billaud, F. Battin-Leclerc, K. Seshadri, and C. K. Westbrook*
- **F24. "Rate Coefficients for Reaction of OH with Acetone at Low to Moderate Temperatures"**
    - *Takahiro Yamada and Philip H. Taylor*
- **F25. "Kinetic and Thermodynamic of 2-propanol Dehydration Reaction in Supercritical Water"**
    - *Vladimir Anikeev, Jeffrey Manion, and Robert Huie*
- **F26. "A Temperature-Dependent Kinetics Study of the Important Stratospheric Reaction $O(^3P) + NO_2 \rightarrow O_2 + NO$"**
    - *E. G. Estupiñán, J. M. Nicovich, and P. H.Wine*
- **F27. "Kinetics of the Reaction of OH with HCN Under Atmospheric Conditions"**
    - *R. S. Strekowski, R. E. Stickel , J. M. Nicovich , and P. H. Wine*
- **F28. "The Reaction of OH + NO_2 + M: Rate constants and branching ratios for isomer formation"**
    - *Horst Hippler, Steffen Nasterlack, Frank Striebel, and David M. Golden*
- **F29. "Kinetic and Mechanistic Studies of the OH-Initiated Oxidation of Dimethylsulfide at Low Temperature - A Reevaluation of the Rate and Branching Ratio"**
    - *M. B. Williams, P. Campuzano-Jost, D. Bauer, and A. J. Hynes*

- **F30.** "**Development of the Computational Chemistry and Reaction Engineering Workbench"**
    - *J. Thomas McKinnon, Anthony M. Dean, Jeff Grenda, Gary Mallard, Ellen Meeks, Mark N. Nimlos, George Petersson, Cheng Wang, Hai Wang*

- **F31. "Effect of Substituents on the Nature of OH Radical Reaction with Organic Sulfur Compounds"**
    - *H. Mohan and J. P. Mittal*

- **F32. "Thermochemical and Kinetic Analysis on Allyl Radical with O_2 Reaction System"**
    - *Jongwoo Lee , Joseph W. Bozzelli, and William Pitz*

- **F33. "Vibrational State Populations and Quenching of NO(X $^2\Pi$, v"=1-7) Following NO_2 Photodissociation at 193 nm Studied by Time-Resolved Fourier Transform Infrared Emission Spectroscopy"**
    - *Yuchuan Gong, Xirong Chen, and Brad R. Weiner*

- **F34. "Stereochemistry of the Thermal Retro Diels-Alder Reactions of Deuterium-Labeled Cyclohexene, Norbornene and Bicyclo[2.2.2]oct-2-ene"**
    - *David K. Lewis, David A. Glenar, Steven Hughes , Bansi L. Kalra, Jessica Schlier, Rajesh S. Shukla, and John E. Baldwin*

- **F35. "Kinetics of the Fe + NO_2 Reaction at 303 K"**
    - *K. Cappan and C. Vinckier*

- **F36. "Manganese Ions' Catalysis of Sulfite Oxidation"**
    - *A. N. Yermakov and A.P. Purmal*

- **F37. "Heterogeneous Interaction of HO2 Radicals with Organic Surfaces of Tropospheric Interest"**
    - *Andrey V. Ivanov, Allan K. Bertram, Sofia L. Trakhtenberg, Luisa T. Molina and Mario J. Molina*

- **F38. "Geminate Ion Recombination Kinetics in Liquid Hydrocarbons"**
    - *Pavel V. Poliakov, A. R. Cook, J. F. Wishart and J. R. Miller*

- **F39. "Molecular Dynamics Simulations of the Decomposition of Energetic Materials at Extreme Conditions"**
    - *M. Riad Manaa, Laurence E Fried, and Marcus Elstner*
- **F40. "Kinetics and Thermodynamics of Intramolecular Hydrogen Transfer in Alkyl Radicals and Peroxyl Radicals from Ab Initio Calculations"**
    - *Thomas C. Allison and Wing Tsang*

Session L: Poster Session 3

Thursday, 4:40 - 6:40 p.m. -- Gaithersburg Holiday Inn

- **L1. "*Ab Initio* Studies of the Kinetics of the Reactions of H Atoms with a Series of Halomethanes"**
    - *Florent Louis, Jean-Pierre Sawerysyn, and Carlos A. Gonzalez*
- **L2. "Statistical Thermodynamics of Large-Amplitude Torsions: Beyond the Conventional Separability Assumption"**
    - *Oleg A. Mazyar and William H. Green, Jr.*
- **L3. "*Ab Initio* Quantum Chemical Studies of Hydrogen Abstraction Reactions of Hydrocarbons"**
    - *Kathleen M. Jagodnik, Thomas M. Muscenti, David W. Ewing, and Michael J. Manka*
- **L4. "First-Principles Prediction of the Mechanism for the Unimolecular Decomposition of Isopropanol"**
    - *Binh Bui and M. C. Lin*
- L5. **"The Self-Reaction of Hydroperoxyl Radicals: A First-Principles Study of its Mechanism*"**
    - *Rongshun Zhu and M. C. Lin*
- **L6. "The NIST Computational Chemistry Comparison and Benchmark Database"**
    - *Russell D. Johnson III*
- **L7. "Recent Progress in Descriptive Quantum Chemistry"**
    - *Karl K. Irikura and Russell D. Johnson III*
- **L8. "Does C·H_2OBr Radical Exist? *Ab Initio* Study on CH_3OBr, C·H_2OBr, and Adduct (CH_2O~Br)**
    - *Dawoon Jung and Joseph W Bozzelli*
- **L9. "The Rate and Equilibrium Constants for the Reaction $NO_3^{\bullet} + Cl^- \rightarrow Cl^{\bullet} + NO_3^-$ in Aqueous Solutions"**
    - *G. A. Poskrebyshev, P. Neta, and R. E. Huie*

- **L10. "The Role of Nitrate Radicals in the Radiolytic Decomposition of Hydrazine in Concentrated Aqueous Nitric Acid Solutions"**
  - *G.I. Khaikin and E.L. Protasova*

- **L11. "Fluorescence Quenching Due to Diffusion-Influenced Reactions of Isolated Pairs in Solution"**
  - *Michael J. Manka, Brian Stevens, Edward C. Lim, David A. Modarelli, and Cheruvallil S. N. Rajesh*

- **L12. "Enthalpies, Entropies and Heat capacities of Formation of Oxabicyclo-heptenes"**
  - *Jin Hur and Joseph W Bozzelli*

- **L13. "Thermodynamic Properties (Enthalpies, Entropies and Heat Capacities) of Unsaturated and Polycyclic Aromatic Hydrocarbons: Molecules, Radicals and Transition States Important to Soot Formation"**
  - *Leonhard Rutz, Henning Bockhorn, and Joseph W. Bozzelli*

- **L14. "Elementary Reactions of Energy Selected Fluoroethene and 1,1-difluoroethene Ions: II. The Kinetics of HF-loss"**
  - *Felix Güthe, Helmut Baumgärtel, and Karl-Michael Weitzel*

- **L15. "A Reaction Kinetic Model of the Gas Phase, Surface Initiated Formation of PCDD/F"**
  - *Lavrent Khachatryan, Barry Dellinger, Alexander Burcat, and Ruben Asatryan*

- **L16. "Rate Constants for H + CH_4, CH_3 + H_2, and CH_4 Dissociation at High Temperature "**
  - *J. W. Sutherland, M.-C. Su, and J. V. Michael*

- **L17. "Redistribution Kinetics of Four-Atom Labeled Molecules Due to Reversible Reactions with Several Atomic Channels"**
  - *Alexander Shestov, John Hoard, Robert Burch, James Sullivan, and Vitaly Muzykantov*

- **L18. "Destruction of Isotopically Enriched Nitric Oxide, $^{15}N^{18}O$, in Corona Discharge"**
  - *Larisa G. Krishtopa and Lev N. Krasnoperov*

- **L19. "Thermodynamic Properties, Reaction Pathways, Kinetics and Chemical Activation Analysis for Addition Reactions of H atoms, O atoms and OH Radicals with Benzene"**
    - *John T. Farrell, Joseph W. Bozzelli, and Chiungju Chen*
- **L20. "Observation of the Vibrational Excitation of N_2O (100) in the Photolysis of Ozone/ N_2O Mixture"**
    - *Yongsik Lee and G.W. Flynn*
- **L21. "Kinetics of Hydroxyl Radical Reactions with Fluoroalkenes from 230 K to 480 K"**
    - *Gregory A. Poskrebyshev, Vladimir L. Orkin , Robert E. Huie, and Michael J. Kurylo*
- **L22. "Turbulent/Laminar Flow Apparatus for Thermodecomposition Kinetic Rate Measurements of Organometallic Compounds"**
    - *Edward P. Hunter and Jeffrey W. Hudgens*
- **L23. "Thermal Rate Coefficients via VTST and the Solution of Master Equation for the Unimolecular Decomposition/Isomerization of N-Pentyl Radical"**
    - *Luminita C. Jitariu, Lee D. Jones, Ian H. Hillier, Struan H. Robertson, Michael J. Pilling*
- **L24. "Mechanism for the Reaction of Phenyl Radical with Acetaldehyde"**
    - *Y. M. Choi and M. C. Lin*
- **L25. "Thermodynamic Properties (Enthalpies , Entropies and Heat Capacities) of Vinyl alcohols and ethers, corresponding radicals and values for Group Additivity"**
    - *Chol-han Kim and Joseph W. Bozzelli*
- **L26. "Thermodynamic Properties (D $H_f^o{}_{298}$, $S^o{}_{298}$, and $C_p{}^o$(T) (300□ T/K□ 1500)) of Mono-, Di-chloro dibenzo-furans and Dibenzo-*p*-dioxins"**
    - *Li Zhu, Chiung-ju Chen, and Joseph W. Bozzelli*
- **L27. "Kinetic determination of the Thermodynamic Coefficients of Partition in a Piston Flow Reactor which Presents a Double Diphasic and Monophasic Segment"**
    - *C. Duriche, M. Elkhatib, R. Metz, and H. Delalu*

- **L28. "Infrared Fluorescence Observations of E-V Transfer from $Cl^*(^2P_{½})$ to $SF_6(n_3)$ and $N_2O(n_1)$"**
    - *J. C. Batson, B. K. Berger, D. A. Dolson, and J. L. Henderson*
- **L29. "Destruction of Ethane in Corona Discharge: Experiment and Modeling"**
    - *Anatoli A. Chernov, Larisa G. Krishtopa, Oleg P. Korobeinichev and Lev N. Krasnoperov*
- **L30. "Absorption Spectrum of the Phenyl Radical in the Visible Region"**
    - *Kenichi Tonokura, Yoshihiro Norikane, and Mitsuo Koshi*
- **L31. "UV Absorption Spectrum of Formyl Radical, HCO"**
    - *Evgeni N. Chesnokov and Lev N. Krasnoperov*
- **L32. "Kinetics of the Reactions Of Fluorine and Chlorine Atoms with Ethylene Oxide"**
    - *D. Ponomarev, M. D. Hurley, and T. J. Wallington*
- **L33. "A Single Pulse Shock Tube Study of C_2Cl_6 Decomposition"**
    - *Iftikhar A. Awan, Wing Tsang, and Jeffrey A. Manion*
- **L34. "LIF study of OH from the Photodissociation of tert-Butyl Hydroperoxide"**
    - *Chan Mee Kim and Yongsik Lee*
- **L35. "Pressure Dependence of Rate Coefficients for Radical-Radical Combination Reactions: $C_2H_3+C_2H_3$, $C_2H_5+C_2H_5$ and $C_2H_3+C_2H_5$"**
    - *Dwight C. Tardy and Askar Fahr*
- **L36. "Reaction Probability of OH on Organic Surfaces of Tropospheric Interest"**
    - *Allan K. Bertram, Andrey V. Ivanov, Martin Hunter, Luisa T. Molina, and Mario J. Molina*
- **L37. "Unimolecular Dissociation Kinetics of Aromatic Halide Radical Anions Studied by Pulse Radiolysis"**
    - *Norihiko Takeda, Pavel V. Poliakov, A. R. Cook, and J. R. Miller*

- **L38. "Influence of low NOx on Maritime Halogen Activation and Uptake coefficient of HOBr on Acidified Sea-Spray Aerosol"**
    - *Wolfgang Behnke, Manfred Elend, Heinz-Ulrich Krüger and Cornelius Zetzsch*