

Outputs and Interactions – Physical and Chemical Properties Division

1. Publications

1a. Publications in Print

- Ali, M.A., Irikura, K.K., and Kim, Y.-K., “*Electron-Impact Total Ionization Cross Sections of SF_x (x = 1-5)*,” *Int. J. Mass Spectrom.* 201, 187-195 (2000).
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- Dorofeeva, O., Novikov, V.P., and Neumann, D.B., "***NIST-JANAF Thermochemical Tables. I. Ten Organic Molecules Related to Atmospheric Chemistry,***" J. Phys. Chem. Ref. Data 30, 475-513 (2001).
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1b. Manuscripts in review

(manuscripts that have been approved by the NIST internal review process and submitted for publication, but have not yet appeared in print)

Archer, D.G., "***Response to 'Comments on the Article Entitled: Thermodynamic Properties of the KCl + H₂O System'***," J. Phys. Chem. Ref. Data (in press).

Archer, D.G. and Kirklin, D.R., "***Enthalpies of Solution of Sodium Chloride and Potassium Sulfate in Water. Thermodynamic Properties of the Potassium Sulfate + Water System***," J. Chem. Eng. Data (in press).

Babushok, V. and Tsang, W., "***Suppressant Rankings for Hydrocarbon Combustion***," Combustion and Flame (in press).

Bruno, T.J., Andersen, W.C., and Henning, K.I., "***Hydrolysis of Carbonyl Sulfide: A Potential Source of Downstream Sour Gas***," Proc. Gas Technology Inst. Conf. on Odorization and Gas Quality, Chicago, IL, July 22-24, 2001 (in press).

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Bruno, T.J. and Mayrath, J.E., "***Polychlorinated Biphenyls: Physical and Analytical Properties - A Comprehensive Literature Search***," NIST Technical Note 1362 (in press).

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Chaychian, M., Jones, C., Poster, D.L., Silverman, J., Neta, P., Huie, R.E., and Al-Sheikhly, M.I., "***Radiolytic Dechlorination of PCBs in Transformer Oil and Marine Sediment***," Rad. Phy. Chem. (in press).

Davis, R.W., Moore, E.F., Maslar, J.E., Burgess, D.R., Jr., Kremer, D.M., and Ehrman, S.H., "***A Numerical/Experimental Investigation of Microcontamination in a Rotating Disk Chemical Vapor Deposition Reactor***," Characterization and Metrology for ULSI Technology: 2001, New York, American Institute of Physics (in press).

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- Evans, D.J. and Rondoni, L., ***“Comments on the Entropy of NonEquilibrium Steady States,”*** J. Stat. Physics (in press).
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Tsang, W. and Mokrushin, V., ***“Determination of Energy Transfer Effects for Molecular Decomposition,”*** Proc. Fifteenth Int. Conf. on Chemical Vapor Deposition: CVD XV, Toronto, Canada, May 15, 2000 (in press).

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2. Talks

Allison, T.C. and Tsang, W., ***“Kinetics and Thermodynamics of Intramolecular Hydrogen Transfer in Alkyl Radicals and Peroxyl Radicals from Ab Initio Calculations,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 17, 2001

Andersen, W.C., ***“Non-Invasive Vapor-Liquid Equilibrium Measurements,”*** A Symposium in Honor of Professor Daniel E. Martire, Georgetown University, Washington D.C., May 4, 2001.

Archer, D.G. and Kirklin, D.R., ***“Enthalpies of Solution of Sodium Chloride and Potassium Sulfate in Water ,”*** 56th Calorimetry Conference, Colorado Springs, CO, August 1, 2001.

Awan, I.F., Tsang, W., and Manion, J.A., ***“A Single Pulse Shock Tube Study of C₂ Cl₆ Decomposition,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 19, 2001

Benko, K., ***“Apparatus to Measure Unsteady, Water Back-Diffusion Through RO and NF Membranes: A Potential Integrity Test,”*** North American Membrane Society 2001 Meeting, Lexington, KY, May 16, 2001.

Bradley, P.E., ***“A Low Cost Pulse Tube and a Thermoelectric Cooler for Temperatures of 180 K,”*** NIST, Boulder, CO, June 15, 2001.

Bradley, P.E., ***“A Low-Cost Pulse Tube Cryocooler for High-Speed Gas Chromatography,”*** Cryogenic Engineering Conference, Madison, WI, July 19, 2001.

Bruno, T.J., ***“Kinetics of Hydrolysis of Carbonyl Sulfide,”*** Annual Convention of the Gas Processors Association, San Antonio, TX, March 11, 2001. Invited.

Bruno, T.J., ***“Enthalpy of Adsorption of Pollutants on Clay Surfaces: A New Chromatographic Approach,”*** Symposium in Honor of Professor Daniel E. Martire, Georgetown University, Washington D.C., May 5, 2001. Invited.

Bruno, T.J., ***“NIST Chromatographic Databases for the Natural Gas Industry,”*** Symposium in Honor of Professor Daniel E. Martire, Georgetown University, Washington D.C., May 5, 2001. Invited.

Bruno, T.J., ***“Carbonyl Sulfide: A Potential Source of Downstream Sourgas,”*** Gas Technology Institute Odorization and Gas Quality Conference, Chicago, IL, July 23, 2001. Invited.

Bruno, T.J., ***“Vapor Entraining Magnetic Mixer for Extraction, Reaction, Equilibrium Applications,”*** 43rd Rocky Mountain Conference on Analytical Chemistry, Denver, CO, July 31, 2001. Invited.

Chaka, A.M., ***“Effect of the Environment on the Structure of Metal Oxide Surfaces,”*** 33rd Central/33rd Great Lakes Joint Regional Meeting, Applications of Computational Chemistry Symposium, Grand Rapids, MI, June 13, 2001.

Chaka, A.M., ***“Effect of the Environment on the Structure of Metal Oxide Surfaces,”*** Application of Molecular Simulation to Catalysis R&D and Surface Chemistry: The Case for Enlightened Experimentation - Workshop Sponsored by Accelrys, Princeton, NJ, June 14, 2001.

Chaka, A.M., ***“Getting the Environment Right: Its Effect on Metal Oxide Surface Structure and Stoichiometry,”*** Int. Symposium on Quantum Mechanics, Seattle, WA, July 23, 2001.

Chirico, R.D., ***“Validation of Enthalpy-of-Vaporization and Vapor-Pressure Values at Low-Pressures ($P < 100$ Pa): Data Validation and SRM Candidate Development,”*** 56th Calorimetry Conference, Colorado Springs, CO, August 2, 2001.

Davis, R.W., Moore, E.F., Maslar, J.E., Burgess, D.R., Kremer, D.M., and Ehrman, S.H., ***“A Numerical/Experimental Investigation of Microcontamination in a Rotating Disk CVD Reactor,”*** American Association for Aerosol Research Annual Conference, St. Louis, MO, November 7, 2000.

Fahr, A., ***“Pressure Effect on Product Channels of Hydrocarbon Radical-Radical Reactions,”*** Combustion Research Facility, Sandia National Laboratories, Livermore, CA, April 19, 2001.

Fahr, A., Hassanzadeh, P., and Tardy, D.C., ***“A Predictive Correlation Between Rate Coefficients, Electron Affinities and Energetics of Radical-Radical Combination Reactions,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 18, 2001.

Frenkel, M., ***“TRC SOURCE Database: Potential for the Standardized Thermophysical Data Files Storage,”*** CODATA Miniworkshop on Database Interoperability, Baveno, Italy, October 16, 2000. Invited.

Frenkel, M., ***“Thermophysical Data Evaluation and Use in the 21st Century: TRC Outlook,”*** 17th CODATA Conference, Baveno, Italy, October 18, 2000.

Frenkel, M., ***“New Era in the Critical Thermophysical Data Evaluation,”*** University of Rome ‘La Sapienza’, Rome, Italy, October 23, 2000. Invited.

Frenkel, M., ***“From NBS to NIST: The TRC Quest for Dynamic Compilation,”*** NIST, Boulder, CO, January 12, 2001.

Frenkel, M., ***“From NBS to NIST: The TRC Quest for Dynamic Compilation,”*** NIST, Gaithersburg, MD, February 22, 2001.

Frenkel, M., ***“TRC Data Evaluation Program: Fresh Start at NIST and Cooperation with SRD,”*** NIST Standard Reference Data Office, Gaithersburg, MD, June 6, 2001.

Frenkel, M., ***“Data Quality: Evaluation and Role in the Development of New ‘Environment-Friendly’ Chemical Technologies,”*** World Chemistry Congress, Brisbane, Australia, July 3, 2001.

Friend, D.G., ***“Activities in the Theory and Modeling of Fluids Group,”*** NIST, Boulder, CO, May 4, 2001.

Gonzalez, C.A., ***“How to do Computational Kinetics with a Reduced Budget,”*** Department of Chemistry, Universidad Nacional Autonoma de Mexico (UNAM), Mexico City, Mexico, November 14, 2000.

Gonzalez, C.A., ***“Theoretical and Experimental Efforts at NIST in Molecular Electronics,”*** Department of Chemistry, Universidad Nacional Autonoma de Mexico (UNAM), Mexico City, Mexico, November 15, 2000.

Gonzalez, C.A., ***“Improved Methodologies for the Calculation of One-Dimensional Tunnelling Corrections,”*** Department of Chemistry, Universidad Nacional Autonoma de Mexico (UNAM), Mexico City, Mexico, November 16, 2000.

Gonzalez, C.A., ***“Theoretical and Experimental Studies of Nano-Electronics at NIST,”*** Department of Chemistry, Universidad Simon Bolivar, Caracas, Venezuela, November 21, 2000.

Gonzalez, C.A., ***“Theoretical Studies of van der Waals Interactions in Aromatic Clusters,”*** Chemistry Center, Venezuelan Institute of Scientific Research, IVIC, Caracas, Venezuela, December 28, 2000.

Gonzalez, C.A., ***“Advances in Computational Kinetics,”*** Venezuelan Institute of Scientific Research, Caracas, Venezuela, January 3, 2001.

Gonzalez, C.A., ***“Mathematics in Chemistry,”*** Society for Industrial and Applied Mathematics (SIAM), Washington, D.C., January 18, 2001.

Gonzalez, C.A., ***“Implementation of Efficient Tools for Computational Kinetics,”*** Department of Chemistry, University of Lille, France, March 19, 2001.

Gonzalez, C.A., ***“Quantum Chemistry at NIST,”*** NIST, Gaithersburg, MD, May 4, 2001.

Gonzalez, C.A., ***“Theoretical Approaches for the Study of Electron Conductance in Molecules,”*** Hewlett-Packard Inc., Palo Alto, CA, May 29, 2001.

Gonzalez, C.A., ***“General Expression for the Effective Mass in the 1-D Treatment of Tunneling Corrections,”*** 222nd American Chemical Society National Meeting, Chicago, IL, August 30, 2001.

Harkless, J.A., ***“Quantum Monte Carlo for Difficult Systems,”*** National Organization of Black Chemists and Chemical Engineers (NOBCChE), Baltimore, MD, April 10, 2001.

Harkless, J.A., ***“Comparative Excited State Studies of Selected Species Using Quantum Monte Carlo,”*** 56th Int. Symposium on Molecular Spectroscopy, Columbus, OH, June 15, 2001.

Harkless, J.A., ***“Quantum Monte Carlo: Applying Monte Carlo Integration to Problems in Quantum Chemistry,”*** 7th Annual Conference for African-American Researchers in the Mathematical Sciences, Durham, NC, June 20, 2001.

Harkless, J.A., ***“Quantum Monte Carlo: Accurate and Understandable Quantum Mechanics,”*** NIST, Gaithersburg, MD, June 29, 2001.

Harkless, J.A., ***“Quantum Monte Carlo: Accurate Understandable Quantum Mechanics for the Rest of Us,”*** Hunter College, New York City, NY, July 11, 2001.

Harkless, J.A., ***“Quantum Monte Carlo Studies of Thermodynamics and Electronic States of Ozone,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 16, 2001.

Harvey, A., ***“Properties of Moist Gases from Ab Initio Potentials,”*** 17th Thermodynamics Conference, Bristol, United Kingdom, April 4, 2001.

Harvey, A., ***“Properties of Moist Gases from Ab Initio Potentials,”*** Ruhr-University, Bochum, Germany, April 9, 2001.

Harvey, A., ***“History of Water Property Research at NBS/NIST,”*** IAPWS Annual Meeting, Gaithersburg, MD, September 13, 2001.

Holcomb, C.D., ***“High Pressure Gas Separation and Conditioning,”*** 80th Annual GPA Convention, San Antonio, TX, March 11, 2001.

Hudgens, J.W., ***“Reaction Mechanisms and Kinetics of Unsaturated C₃ Radicals Studied by Cavity Ring Down Spectroscopy and ab initio Calculations,”*** Argonne National Laboratory, Argonne, IL, April 30, 2001.

Hudgens, J.W., Atkinson, D.B., and Gonzalez, C.A., ***“Addition Reaction of Chlorine and Propargyl Chloride Studied by Cavity Ring-Down Spectroscopy and by ab initio Calculations,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 19, 2001.

Huie, R.E., ***“Environmental Impact of New Chemical Agents for Fire Suppression,”*** FY2000 NGP Annual Research Meeting, Gaithersburg, MD, November 8, 2000.

Huie, R.E., ***“Research Activities of the Experimental Kinetics & Thermodynamics Group,”*** University of Lille, France, March 16, 2001.

Huie, R.E., ***“Kinetics and Equilibria for the Reactions of NO₃ with H₂O and Cl⁻,”*** University of Lille, France, March 16, 2001.

Huie, R.E., ***“The Chemistry of NO₃ in Aqueous Solutions,”*** Workshop on Nitrogen Oxides in the Lower Stratosphere and Upper Troposphere, University of Heidelberg, Germany, March 20, 2001.

Huie, R.E., ***“Reaction of the Sulfite Radical with Ferrous Ions in Bisulfite Solutions,”*** ACS Award Symposium for Creative Advances in Environmental Science and Technology: Honoring Dr. Michael R. Hoffmann, 221st ACS National Meeting, San Diego, CA, April 4, 2001.

Huie, R.E., ***“What’s Going On in Kinetics & Thermodynamics?”*** NIST, Gaithersburg, MD, August 13, 2001.

Hunter, E.P. and Hudgens, J.W., ***“Turbulent/Laminar Flow Apparatus for Thermodecomposition Kinetic Rate Measurements of Organometallic Compounds,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 19, 2001.

Irikura, K.K. and Johnson, R.D., III, ***“Discovering Chemical Reactions by Isopotential Searching,”*** NIST, Gaithersburg, MD, October 11, 2000.

Irikura, K.K., ***“Reaction Mechanisms from Qualitative Quantum Chemistry,”*** American Institute of Chemistry Engineers (AIChE) National Meeting, Los Angeles, CA, November 15, 2000.

Irikura, K.K., ***“A New Computational Method for Predicting Reactivity,”*** American Institute of Chemical Engineers (AIChE) National Meeting, Los Angeles, CA, November 17, 2000.

Irikura, K.K., ***“Organometallic Ion Chemistry,”*** Gordon Research Conference on Gaseous Ions: Structures, Energetics, and Reactions, Ventura, CA, February 26, 2001.

Irikura, K.K., ***“Recent Progress in Descriptive Quantum Chemistry,”*** Emerging Methods in Computational Chemistry and Materials, Aberdeen, MD, June 1, 2001.

Irikura, K.K. and Johnson, R.D., III, ***“Recent Progress in Descriptive Quantum Chemistry,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 19, 2001.

Johnson, R.D., III and Huie, R.E., ***“The Reaction of NH₂ with O₂ in the Presence of H₂O,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 16, 2001.

Johnson, R.D., III, ***“The NIST Computational Chemistry Comparison and Benchmark Database,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 19, 2001.

Kurylo, M.J., ***“From CFCs to PSCs: Impacts on Stratospheric Ozone Depletion,”*** Chemistry Department, Boston College, Chestnut Hill, MA, October 12, 2000.

Kurylo, M.J., ***“Recent Advances in Our Understanding of Stratospheric Ozone Chemistry: The Coupling of Laboratory and Atmospheric Measurements,”*** Earth, Atmospheric, and Planetary Sciences Department, Massachusetts Institute of Technology, Cambridge, MA, February 27, 2001.

Kurylo, M.J., ***“Kinetic Study of the Hydroxyl Radical Reaction with H₂ from 200 K to 480 K,”*** 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 16, 2001.

Kurylo, M.J., "***Kinetics of Hydroxyl Radical Reactions with Fluoroalkenes from 230 K to 480 K***," 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 17, 2001.

Kurylo, M.J., "***Ab Initio Studies of the Kinetics of the Reactions of OH Radicals with a Series of Haloalkanes***," 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 18, 2001.

Kurylo, M.J., "***Atmospheric Fate of Some Short-Lived Br-Containing Hydrohalocarbons: OH Reactions and UV Spectra***," Workshop on Laboratory Studies of Upper Troposphere / Lower Stratosphere Processes, Breckenridge, CO, July 25, 2001.

Laesecke, A., "***From Measurements to Databases – NIST: Sources of Accurate Thermophysical Properties Information***," Swiss Federal Institute of Technology (ETH), Zurich, Switzerland, January 9, 2001.

Laesecke, A., "***Error Propagation Live: The Tragicomical History of Viscosity Measurements of Alternative Refrigerants***," University of Nevada (Reno), October 20, 2000. Invited.

Laesecke, A., "***Electrical Characterization of Ten Binary and Ternary Alternative Refrigerant Mixtures***," 2nd IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons, Paris, France, April 11, 2001. Invited.

Laesecke, A., "***Halocarbons I: Methane Derivatives. Our Evolving View of Molecular Structure***," 2nd IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons, Paris, France, April 9, 2001.

Laesecke, A., "***MO Calculations; Characterization of Molecular Structure***," 2nd IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons, Paris, France, April 11, 2001. Invited.

Laesecke, A., Outcalt, S., Frenkel, M., Huber, M., Perkins, R., and Scott, J., "***Thermophysical Properties Research***," NIST, Boulder, CO, May 11-12, 2001.

Louis, F., Sawerysyn, J.-P., and Gonzalez, C.A., "***Etude théorique de la réactivité d'une série d'halogénométhanés avec des atomes d'hydrogène***," Annual Meeting of the Groupe de Cinétique et de Photochimie en Phase Gazeuse, Villeneuve d'Ascq, France, June 20, 2001.

Louis, F., Gonzalez, C.A., Kurylo, M.J. and Huie, R.E., "***Ab Initio Studies of the Kinetics of the Reactions of OH Radicals with a Series of Haloalkanes***," 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 17, 2001.

Louis, F., Sawerysyn, J.-P., and Gonzalez, C.A., "***Ab Initio Studies of the Kinetics of the Reactions of H Atoms with a Series of Halomethanes***," 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 18, 2001.

Magee, J.W., ***“A Decade of Progress in Calorimetry: Halogenated Hydrocarbons and Their Mixtures,”*** 2nd International Workshop on Thermochemical, Thermodynamic and Transport Properties of Halogenated Hydrocarbons and Mixtures, Ecole de Mines de Paris, Paris, France, April 9, 2001.

Magee, J.W., ***“Ionic Liquids: Metrology and Structure – Property Relations,”*** Belarusian State University, Minsk, Belarus, June 27, 2001.

Magee, J.W., ***“NIST Physical Property Data Program,”*** Russian Academy of Sciences, Moscow, Russia, June 30, 2001.

Mallard, W.G., ***“AMDIS as a Tool for Increased Productivity,”*** Proctor and Gamble Company, Cincinnati, OH, October 19, 2000.

Mallard, W.G., ***“Estimation of Retention Index Values for Compounds Relevant to the Chemical Weapons Convention,”*** PacificChem (Fourth International Chemical Congress of Pacific Basin Societies), Honolulu, HI, December 16, 2000.

Mallard, W.G., ***“AMDIS and the NIST MS Library,”*** Dow Chemical Company, Midland, MI, March 20, 2001.

Mallard, W.G., ***“Master Class - The NIST MS Database and AMDIS - Methods and Algorithms,”*** Interscience Corporation, Breda, The Netherlands, June 12, 2001.

Mallard, W.G., ***“The NIST MS Database and AMDIS - Detection of CW Agents,”*** The Organization for the Prohibition of Chemical Weapons - Headquarters, The Hague, The Netherlands, June 13, 2001.

Maslar, J.E., Hurst, W.S., Burgess, D.R., Kremer, D.M., and Ehrman, S.H., ***“In Situ Gas Phase Optical Measurements of Silane Decomposition in a Thermal Chemical Vapor Deposition Reactor,”*** The Electrochemical Society Annual Conference, Washington D.C., March 26, 2001.

McLinden, M.O., ***“Impact of DOE/BES-Funded Metrology Development: Thermophysical Properties of Alternative Refrigerants,”*** 19th Symposium on Energy Engineering Sciences, Argonne, IL, May 22, 2001.

McLinden, M.O., ***“History of the NIST Refrigerants Program. Thermophysical Properties Research,”*** ASHRAE Annual Meeting, Cincinnati, OH, June 26, 2001.

Meier, K., Kabelac, S., and Laesecke, A., ***“Molekular-dynamische Simulationen des Selbstdiffusionskoeffizienten und der Viskosität des Lennard-Jones Fluids,”*** VDI/GVC Thermodynamik-Kolloquium, Frankfurt/Main, Germany, October 6, 2000.

Meier, K., Laesecke, A., and Kabelac, S., ***“The ‘Critical’ Enhancement of the Bulk Viscosity of the Lennard-Jones Fluid from Equilibrium Molecular Dynamics Simulations,”***

Thermodynamics 2001, Thermodynamics and Statistical Mechanics with Industrial Applications, University of Bristol, United Kingdom, April 5, 2001.

Miller, K. E., ***“Thermodynamics and Kinetics of Fluid-Clay Interactions,”*** Symposium in Honor of Professor Daniel E. Martire, Georgetown University, Washington D.C., May 4, 2001.

Mountain, R.D., ***“A Brief Look at Supercritical Fluids Through the Molecular Dynamics Window,”*** School of Computational Sciences, George Mason University, Fairfax, VA, February 12, 2001. Invited.

Mountain, R.D., ***“Introduction to Molecular Dynamics,”*** 12th ACBM/NIST Computer Modeling Workshop, NIST, Gaithersburg, MD, June 14, 2001. Invited.

Mountain, R.D., ***“Molecular Dynamics and the Solvation of Isopropyl Alcohol from Ambient to Supercritical Conditions,”*** 5th Int. Conf. on Chemical Kinetics, NIST, Gaithersburg, MD, July 17, 2001.

Mountain, R.D., ***“Water Potential,”*** IAWPS Meeting, NIST, Gaithersburg, MD, September 12, 2001.

Muzny, C.D., ***“High-Throughput Screening of Molecular Transport Through Films, Membranes, and Nanostructures,”*** Combinatorial Methods for R&D, Gaithersburg, MD, March 23, 2001.

Muzny, C.D., ***“High-Throughput Screening of Molecular Transport through Films, Membranes, and Nanostructures,”*** ATP National Meeting, Baltimore, MD, June 4, 2001.

Neta, P., ***“Redox Reactions of Metalloporphyrins in Catalyzed Reduction of Carbon Dioxide,”*** 4th DOE Solar Photochemistry Research Conference, Tahoe City, CA, June 6, 2001.

Neta, P., ***“Reaction Kinetics in Ionic Liquids. Pulse Radiolysis Studies,”*** 5th International Conference on Chemical Kinetics, NIST, Gaithersburg, MD, July 18, 2001.

Pellegrino, J., ***“Measurements of Diffusion in Pre-made Polymer Thin Films From FTIR-ATR Spectroscopy Using a Self-Pressing Method,”*** AIChE 2000 Annual Meeting, Los Angeles, CA, November 13, 2000.

Pellegrino, J., ***“Separations in a Busy World – The Short Course,”*** AIChE 2000 Annual Meeting, Los Angeles, CA, November 13, 2000. Invited.

Pellegrino, J., ***“Measurements of Diffusion Using FTIR-ATR: Water-Acetone Diffusion In Polypropylene - A Model System For Hydrophobic Films,”*** PACIFICHEM 2000 Meeting (ACS), Honolulu, HI, December 15, 2000. Invited.

Pellegrino, J., ***“Fingerprinting’ Complex Mixtures and Correlations to Membrane Flux Decline”*** PACIFICHEM 2000 Meeting (ACS), Honolulu, HI, December 20, 2000. Invited.

Radebaugh, R., ***“Regenerator Heat Input at Intermediate Temperatures,”*** NIST, Boulder, CO, November 10, 2000.

Radebaugh, R., ***“Pulse Tube Cryocoolers: Advancement and Status,”*** American Superconductor Corporation, Westborough, MA, December 20, 2000. Invited.

Radebaugh, R. ***“Cryocooler Technology Short Course,”*** Kirtland Air Force Base, Albuquerque, NM, February 13-15, 2001. Invited.

Radebaugh, R., ***“Government and Industry Directions in Space Cryocoolers,”*** Space Cryogenics Workshop, Milwaukee, WI, July 13, 2001. Invited.

Radebaugh, R., ***“Cooling of High Tc Superconducting Systems,”*** Short Course, Cryogenic Engineering Conference, Madison, WI, July 16, 2001. Invited.

Radebaugh, R., ***“Regenerator Behavior at 4 K: Effect of Volume and Porosity,”*** Cryogenic Engineering Conference, Madison, WI, July 18, 2001.

Radebaugh, R., ***“A Review of the Cryogenic Engineering Conference (CEC),”*** NIST, Boulder, CO, August 3, 2001.

Radebaugh, R., ***“Cryogenic Technologies Group,”*** NIST, Boulder, CO, August 13, 2001.

Rainwater, J.C., ***“New Techniques for Cell Model Calculation of Solid-Liquid Equilibria,”*** AIChE 2000 Annual Meeting, Los Angeles, CA, November 14, 2000.

Rainwater, J.C., ***“A Method to Estimate Critical Loci of Binary Azeotropic Mixtures from Subcritical Isothermal Data,”*** AIChE National Spring Meeting, Houston, TX, April 23, 2001.

Ruette, F., Sanchez, M., Martorell, G., Gonzalez, C.A., Anez, R., Sierraalta, A., and Mendoza, C., ***“Quantum Chemistry for Catalysis, CATIVIC, a New Theoretical Model,”*** Fifth Venezuelan Chemistry Congress, Maracaibo, Venezuela, April 2001.

Ruette, F., Gonzalez, C.A., Sierraalta, A., Sanchez, M., and Mendoza, C., ***“Calculations of Atomic Integrals for Parametric Methods Using the Simulating Annealing Technique,”*** Fifth Venezuelan Chemistry Congress, Maracaibo, Venezuela, April 2001.

Stein, S.E., ***“The NIST Mass Spectral Data Program,”*** Annual ANACHEM Meeting, Detroit, MI, November 16, 2000.

Stein, S.E., ***“Automated Chemical Identification by GC/MS,”*** 13th Sanibel Conference on Informatics and Mass Spectrometry, Sanibel Island, FL, January 22, 2001.

Tardy, D.C. and Fahr, A., "**Pressure Dependence of Rate Coefficients for Radical-Radical Combination Reactions: $C_2H_5 + C_2H_5$, $C_2H_3 + C_2H_3$, and $C_2H_5 + C_2H_3$** ," 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 19, 2001.

Tardy, D.C. and Fahr, A., "**Complications in Gas Phase Radical-Radical Combination Reactions: Pertinent Structural and Energetic Parameters for Bimolecular Formation and Unimolecular Removal Processes**," 2001 Free Radicals Symposium, Assisi, Italy, September 2001.

Tsang, W., "**A Virtual Data Engine for Gas Phase Chemistry**," 17th International CODATA Conference, Baveno, Italy, October 17, 2000.

Tsang, W., "**Chlorination in Combustion Systems**," ASME International Mechanical Engineering Congress and Exposition, Orlando, FL, November 6, 2000.

Tsang, W., "**Formalisms for the Description of Energy Transfer Effects in Complex Unimolecular Reactions**," AIChE - 2000 Annual Meeting, Los Angeles, CA, November 13, 2000.

Tsang, W., "**Single Pulse Shock Tube Study on the Decomposition of Indane**," AIChE - 2000 Annual Meeting, Los Angeles, CA, November 15, 2000.

Tsang, W., "**A Pre-processor for the Generation of Chemical Kinetics Data for Simulations**," 39th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 10, 2001.

Tsang, W., "**Database Issues in Soot Formation Models**," SERDP Kickoff Meeting, Wright-Patterson AFB, OH, January 29, 2001.

Tsang, W., "**Database Issues in Models for Forming Aromatics**," Soot Modeling Working Group, Salt Lake City, UT, March 16, 2001. Invited.

Tsang, W., "**Multichannel Decomposition of Ethanol**," Joint Meeting of the US Combustion Institute, Oakland, CA, March 26, 2001.

Tsang, W., "**Combustion Kinetics Databases**," Workshop on Hydrocarbon Combustion Kinetics at Sandia National Laboratory, Albuquerque, NM, March 29, 2001. Invited.

Tsang, W., "**A Virtual Data Engine for Gas Phase Chemistry**," 5th International Conference on Chemical Kinetics, Gaithersburg, MD, July 16, 2001.

Tsang, W., "**Chemical Kinetic Database for PAH/Soot Formation from Heptane Combustion - Interim Report**," Wright-Patterson AFB, OH, August 20, 2001.

3. Cooperative Research and Development Agreements (CRADAs) and Consortia

Development of Pulse Tube Refrigeration Technology for a Fully Acoustic Densifier that Simultaneously Conditions Two Cryogenic Fluids, R. Radebaugh
Sierra Lobo (CRADA)

Development of Alternative Cooling for a High Speed Gas Chromatography Inlet System, R. Radebaugh
Chromatofast (CRADA)

Development of a Two-Stage Pulse Tube Cryocooler for High Temperature Superconducting Power Applications, R. Radebaugh
American Superconductor Corporation (CRADA)

Rapid GC Analysis of Samples Desorbed from Personal Monitors for Occupational Exposure Assessment, R. Radebaugh
Chromatofast (CRADA)

Praxair Pulse Tube Liquefier, R. Radebaugh
Praxair, Inc. (CRADA)

Properties and Cycle Performance of Refrigerant Blends Operating Near and Above the Refrigerant Critical Point, P. Domanski (863) and M.O. McLinden
Air-Conditioning and Refrigeration Technology Institute (CRADA)

Coblentz Society/NIST Digitized Vibrational Spectra Database, S. Stein
The Coblentz Society (CRADA)

Library Search Identification of Chemical Structure and Substructures from MS/MS Spectra, S. Stein
Finnigan Corporation (CRADA)

North American Membrane Society Consortium: Pore Size Characterization Methodology and Standards for Ultrafiltration Membranes, C. Muzny
Merck, Millipore, Osmonics, Sartorius, Bureau of Reclamation

Thermodynamics Research Center Research Consortium
Equilon Enterprises LLC, Phillips Petroleum Company, Chevron Research and Development, Celanese, Ltd., Nova Chemicals Corporation, Virtual Materials Group, Inc.

4. Patent Awards and Applications

Bruno, T.J. and Lagalante, A.F., "Method for the Removal of Carbonyl Sulfide from Liquefied Petroleum Gas (LPG)," granted, to issue December 19, 2001.

Bruno, T.J. and Rybowski, M.C., "Method and Apparatus for Entrainment Mixing of Vapor Into Liquids," pending.

Dobak, J., Radebaugh, R., Marquardt, E., and Huber, M.L., "Miniature Mixed Gas Refrigeration System," U.S. Patent Number 6, 151, 901 (11/28/00).

Dobak, J., Radebaugh, R., Marquardt, E., and Huber, M.L., "Miniature Mixed Gas Refrigeration System," NIST #95-041PCT, International Patent Application.

Dobak, J., Radebaugh, R., Marquardt, E., and Huber, M.L., "Mixed Gas Refrigeration Method," NIST #96-040CIP-EPO, International Patent Application.

5. Measurement Services

5a. SRM Activities (Certificates Issued in FY2001)

5b. SRD Activities

SRD NIST Chemical Kinetics Mechanism Database CKMech
<http://srdata.nist.gov/ckmech/>

SRD 4 NIST Thermophysical Properties of Hydrocarbon Mixtures Database, Major Upgrade (Version 3.0), Support

SRD 10 NIST Thermophysical Properties of Water Database, Support

SRD 10 NIST Thermophysical Properties of Water Database, Upgrade (Version 2.2)

SRD 12 NIST Thermophysical Properties of Pure Fluids Database, Major Upgrade (Version 5.0), Support

SRD 14 NIST Mixture Property Database, Upgrade in Progress, Support

SRD 23 NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures Database, Upgrade in Progress, Support

SRD 72 NIST Thermophysical Properties of Air and Air Component Mixtures, Released Version 1.0

SRD 69 NIST Chemistry Webbook, Contributions on Fluid Properties, New Release (July 2001)

TRC Tables – Hydrocarbons

TRC Tables – Non-Hydrocarbons

International Data Series

SRD 85 NIST/TRC Table Database, WinTable 1.5 (2001), New Release (April 2001)

SRD 87 NIST/TRC Vapor Pressure Database, Version 2001, New Release (June 2001)

5c. Calibrations

Pratt and Whitney

Hoffer Flow Controls, Inc.

6. Committee Assignments

D.G. Archer

ASTM Subcommittee E37.02, Standard Reference Materials for Thermal Measurements (Chair)

ASTM Taskgroup E37.01.06 on Heat Capacity (Chair)
ASTM Taskgroup E37.01.17 on Differential Scanning Calorimetry Calibration (Chair)
ASTM Taskgroup E37.01.21 on Reaction Calorimetry (Chair)

T.J. Bruno

International Forum on Process Analytical Chemistry, Scientific Board
ASTM Committee D03 on Gaseous Fuels
Gas Research Institute PCB Task Force
Annual SFE-SFC International Symposium, Technical Board
National Materials Advisory Board Panel on Separation Technology for Industrial Recycling and Reuse

R.D. Chirico

ASTM Committee E27 on Hazard Potential of Chemicals

M. Frenkel

Physical Data and Reaction Kinetics Committee (PDRK) of the Engineering Sciences Data Unit (ESDU™), London, UK (Corresponding Member)
Committee for Data File Format Standardization of CODATA (IUCOSPED) (Member)

D.G. Friend

ASME K-7 Standing Committee on Thermophysical Properties
ASME Research and Technology Committee on Water and Steam in Thermal Systems
ASME Subcommittee on Properties of Water and Steam
IAPWS Working Group on Thermophysical Properties of Water and Steam (Chair)
IAPWS Task Group on Transport Properties (Chair)
IAPWS Task Group on Ammonia-Water Mixtures (Chair)
AIChE Design Institute for Physical Property Data (DIPPR): Project 991 Steering Team, Project 801 Steering Team, Administrative Committee, Technical Committee
IUPAC/CODATA/ICSTI Joint Working Group on Data Exchange Standards (IUCOSPED)
Fifteenth Symposium on Thermophysical Properties (Organizer and Co-Chair)

A.H. Harvey

ASME Research and Technology Committee on Water and Steam in Thermal Systems
AIChE Area 1a (Thermodynamics and Transport Properties) Program Committee
ASME Research Subcommittee on the Properties of Water and Steam (Chair)
IAPWS Working Group on Thermophysical Properties of Water and Steam
IAPWS Task Group on Fundamental Constants (Chair)
IAPWS Editorial Committee (Chair)

W.M. Haynes

ASTM Committee D03 on Gaseous Fuels
ASTM Subcommittee D03.08 on Thermophysical Properties of Gaseous Fuels (Chair)
ASME K-7 Standing Committee on Thermophysical Properties
International Thermophysics Congress (Chair)
International Advisory Committee, 17th IUPAC Conference on Chemical Thermodynamics

International Organizing Committee, 15th European Conference on Thermophysical Properties
International Advisory Committee, 6th International Asian Thermophysical Properties
Conference

R.E. Huie

TSCA Interagency Testing Committee
NASA Panel for Data Evaluation
Titular Member, IUPAC Commission on Chemical Kinetics

M.J. Kurylo

NASA Panel for Data Evaluation
Ex-Officio Member of the Scientific Steering Group for the Stratospheric Processes and their
Role in Climate (SPARC) Project of the World Climate Research Program.
International Steering Committee of the Network for the Detection of Stratospheric Change
(NDSC) (Co-Chair).

A. Laesecke

Subcommittee on Transport Properties of IUPAC Commission I.2: Thermodynamics
Scientific Organizing Committee, 2nd IUPAC Workshop on Thermochemical, Thermodynamic,
and Transport Properties of Halogenated Hydrocarbons
Scientific Organizing Committee, 3rd IUPAC Workshop on Thermochemical, Thermodynamic,
and Transport Properties of Halogenated Hydrocarbons

J.M.H. Levelt Sengers

International Association for Properties of Water and Steam (IAPWS) (U.S. National
Representative)
American Society of Mechanical Engineers (ASME), Research Subcommittee on the Properties
of Water and Steam (Member)
Peer Committee, Chemical Engineering Section, National Academy of Engineering Liaison,
Section 31, National Academy of Sciences

P.J. Linstrom

IUPAC Task Group on Standardization of Physico-Chemical Property Electronic Data Files
(IUCOSPED)

B. Louie

University of Colorado Chemical Engineering Advisory Committee

W.G. Mallard

Steering Committee for the NIST/EPA/NIH Mass Spectra Database
Joint Committee on Atomic and Molecular Physical Data
Organization for the Prohibition of Chemical Weapons, Advisory Panel on the Central
Analytical Database

E.D. Marquardt

Federal Interagency Cryocooler Test Working Group
NASA Cryogenic Technology Team for Exploration Transportation

M.O. McLinden

ASHRAE Technical Committee 3.1 - Refrigerants and Secondary Coolants (Chair)
ISO TC86/SC8/WG7 – Refrigerant Properties (Member)

J.J. Pellegrino

Interagency Consortium on Desalination and Membrane Separation Research
North American Membrane Society (Director)
Scientific Advisory Board of the 2002 International Congress on Membranes

R.A. Perkins

ASTM Committee D34 on Waste Management
International Association for Transport Properties

R. Radebaugh

International Cryocooler Conference, Inc., Advisory Board, Registered Agent and Treasurer
Cryogenic Society of America, Editorial Committee

J.L. Scott

Measurement Technical Committee (MTC) for the GTI Metering Research Facility (MRF) at
Southwest Research Institute (SwRI)
Transmission Measurement Committee of the American Gas Association (AGA)

S.E. Stein

E49.08 ASTM Subcommittee on ANDI Protocols for Spectroscopy
ASMS Subcommittee on Measurements and Standards - Methodology
IUPAC Committee on Printed and Electronic Publishing

7. Editorships

T.J. Bruno

Journal of Process Analytical Chemistry (Associate Editor)

R.D. Chirico

Journal of Chemical Thermodynamics (Editorial Board)
Thermodynamics Research Center Thermodynamic Tables (Editorial Board)

M. Frenkel

TRC Tables – Hydrocarbons (Editor-in-Chief)
TRC Tables – Non-Hydrocarbons (Editor-in-Chief)
International Data Series (Executive Director)
Computers and Applied Chemistry (China) (Editorial Board)
Vapor-Liquid Equilibria (Poland) (Editorial Board)

D.G. Friend

International Journal of Thermophysics (Associate Editor)
Thermodynamics Research Center Thermodynamic Tables (Editorial Board)

H.J.M. Hanley

Journal of Research of the National Institute of Standards and Technology (Editorial Board)

W.M. Haynes

International Journal of Thermophysics (Editor-in-Chief)
Proceedings of the 14th Symposium on Thermophysical Properties, International Journal of Thermophysics, Fluid Phase Equilibria, and Journal of Chemical and Engineering Data (Co-Editor)

R.E. Huie

International Journal of Chemical Kinetics (Associate Editor)

A. Laesecke

Journal of Chemical and Engineering Data (Editorial Board)
Thermodynamics Research Center Thermodynamic Tables (Editorial Board)

J.W. Magee

Journal of Chemical and Engineering Data (Associate Editor)
Thermodynamics Research Center Thermodynamic Table (Editorial Board)

J.A. Manion

International Journal of Chemical Kinetics (Associate Editor)

P. Neta

Radiation Physics and Chemistry (Editor)

J.J. Pellegrino

North American Membrane Society (World Wide Web Site Editor)
Separation Science and Technology (Editorial Board)

R. Perkins

Thermodynamics Research Center Thermodynamic Tables (Editorial Board)

R. Radebaugh

Cryogenics (International Advisory Editor)
Advances in Cryogenic Engineering (Editorial Board)

J.C. Rainwater

International DATA Series, Selected Data on Mixtures (Editor)

W. Tsang

International Journal of Chemical Kinetics (Editor)

8. Seminars

October 16, 2000

R.A. Mohling, Technology Application, Inc., Boulder, CO, "Cryogenic Information Center: Literature Database, Material Properties, and the Future." (Division Sponsor: E.D. Marquardt)

March 28, 2001

M. Sola, Institut de Quimica Computacional, Universitat de Girona, Catalonia, Spain, "The Reactivity of the [5,6]-Bond in Cycloaddition Reactions to Fullerenes." (Division Sponsor: C.A. Gonzalez)

April 6, 2001

V. Kozhevnikov, Department of Physics, University of Utah, Salt Lake City, UT, "Acoustics in Phase Transition Studies of Liquids." (Division Sponsor: W.M. Haynes)

April 20, 2001

A. Redondo, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, "Large-Scale Simulations of Materials and Chemical Systems." (Division Sponsor: C.A. Gonzalez)

April 23, 2001

C. Palmer, Shering-Plough Research Institute, Kenilworth, NJ, "Current Drug Discovery Issues in Mass Spectrometry Metabolite Profiling, LIMS and Database Integration." (Division Sponsor: S.E. Stein)

May 18, 2001

W. Gully, Ball Aerospace, Boulder, CO, "What's the Real Difference Between Pulse Tube and Stirling Coolers?" (Division Sponsor: R. Radebaugh)

July 13, 2001

J.G. Eberhart, Chemistry Department, University of Colorado, Colorado Springs, CO, "The Limit of Superheat of Liquids and Their Mixtures: Measurement, Theory, and Applications." (Division Sponsor: A. Laesecke)

September 14, 2001

J. Pfothner, Department of Mechanical Engineering, University of Wisconsin, Madison, WI, "Two-Phase Heat Transfer to Liquid Nitrogen." (Division Sponsor: R. Radebaugh)

September 24, 2001

J.S. Wilkes, Department of Chemistry, U.S. Air Force Academy, Colorado Springs, CO, "Ionic Liquids in Perspective." (Division Sponsor: A. Laesecke)

9. Conferences/Workshops/Sessions Sponsored/Co-Sponsored

September 9-14, 2001

International Association for the Properties of Water and Steam Annual Meeting, Gaithersburg MD (J.M.H. Levelt Sengers and A.H. Harvey, Organizers)

March 19-21, 2001

Workshop on Nitrogen Oxides in the Lower Stratosphere and Upper Troposphere, Heidelberg, Germany (M. Kurylo, Organizing Committee Member)

May 5-7, 2001

Symposium in Honor of Prof. Daniel E. Martire, Georgetown University, Washington D.C. (T. Bruno, Organizing Committee Member)

June 18-19, 2001

Workshop on Predicting Thermophysical Properties of Fluids by Molecular Simulation, Gaithersburg, MD (R. Mountain, A. Chaka, D. Friend, and R. Johnson, III, Organizing Committee Members)

July 16-19, 2001

5th International Conference on Chemical Kinetics, Gaithersburg, MD (R.E. Huie and J.W. Hudgens, Organizers)

July 23-27, 2001

Workshop on Laboratory Studies of Upper Troposphere/Lower Stratosphere Processes, Breckenridge, CO (M. Kurylo, Organizing Committee Member)

September 7-12, 2001

Electronic Structure of Solids and Surfaces: EuroConference on Computer Simulation of Complex Interfaces: Out of the Vacuum into the Real World, Giens, France (A. Chaka, Cochair)

September 24-28, 2001

Network for the Detection of Stratospheric Change 2001 Symposium, Arcachon, France (M. Kurylo, Organizing Committee Member)

10. Other

T.J. Bruno

Adjunct Professor, Department of Chemical and Petroleum Refining Engineering, Colorado School of Mines, Golden, CO.

A. Fahr

Hosted and collaborated with Prof. Dwight Tardy of Iowa University during his sabbatical visit to NIST.

H.J.M. Hanley

Adjoint Professor, Department of Chemical Engineering, University of Colorado, Boulder, CO.

Adjunct Professor, Research School of Chemistry, Australian National University, Canberra, Australia.

M.J. Kurylo

Program Scientist for the following NASA satellite missions/instruments:

Upper Atmosphere Research Satellite (UARS).

Total Ozone Mapping Spectrometer (TOMS) satellite instrument series.

Ozone Monitoring Instrument (OMI) on the Aura satellite to be launched in 2003.

J.W. Magee

Adjunct Professor, Department of Mechanical Engineering, University of Colorado, Boulder, CO.

W. Mallard

Technical Advisor to the United States Delegation to the Organization for the Prohibition of Chemical Weapons on Sampling for Off-Site Analysis.

J. Pellegrino

Adjunct Professor, Department of Civil and Environmental Engineering, University of Colorado, Boulder, CO.

R. Radebaugh

Adjunct Professor, Department of Chemical Engineering, University of Colorado, Boulder, CO.

J.C. Rainwater

Lecturer, Department of Physics, University of Colorado, Boulder, CO.

Ph.D. Advisor (S.A. Kadlec), Department of Physics, University of Colorado, Boulder, CO.