Physical and Chemical Properties Division
Outputs and Interactions, FY04

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2. <u>Talks</u>

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Bruno, T.J., *"The NAS/NRC Postdoctoral Associateship Program,"* University of Denver, Denver CO, October 2, 2003. Invited

Bruno, T.J., *"Carbonyl Sulfide in LPG: The Unraveling of a Mystery,"* NIST-PCPD, Boulder CO, October 16, 2003 (contributed).

Bruno, T.J., *"Composition and Stability of RP-1,"* NASA Workshop, Boulder CO, December 11, 2003 (contributed).

Bruno, T.J., *"Improving the Copper Strip Corrosion Test,"* GTI Natural Gas Technologies Conference and Exhibition, Phoenix AZ, February 9, 2004 (contributed).

Bruno, T.J., *"Polymer Modification with Capsaicin: An Effective and Economical Approach to Rodent Control,"* S.C. Johnson, April 28, 2004.

Bruno, T.J., *"A Conceptual Introduction to Explosives,"* SURF Seminar, NIST, Boulder CO, July 23, 2004 (this talk included a demonstration of explosives).

Bruno, T.J., *"The Loss of Odor through Conjugation, Suppression and Cross-Adaptation – How One Plus One Can Sometimes Equal Zero,"* GTI Odorization Conference, Chicago IL, August 5, 2004 (Invited plenary session lecture).

Bruno, T.J., *"Introduction to Explosives,"* KUSA-9 News, Spangler Science Broadcast, September 9, 2004.

Bruno, T.J., *"Introduction to Explosives,"* Boulder Laboratories 50th Anniversary, Boulder CO, September 10, 2004 and September 11, 2004.

Bruno, T.J., *"Carbonyl Sulfide in LPG: The Unraveling of a Mystery where Chemistry Meets Engineering,"* University of Colorado, Boulder CO, September 21, 2004. Invited

Bruno, T.J., *"The Loss of Odor through Conjugation, Suppression and Cross-Adaptation – How One Plus One Can Sometimes Equal Zero,"* GTI Odorization Conference, Chicago IL, August 5, 2004 (Invited plenary session lecture).

Bruno, T.J., *"Introduction to Explosives,"* KUSA-9 News, Spangler Science Broadcast, September 9, 2004.

Bruno, T.J., *"Introduction to Explosives,"* Boulder Laboratories 50th Anniversary, Boulder CO, September 10, 2004 and September 11, 2004.

Bruno, T.J., *"Carbonyl Sulfide in LPG: The Unraveling of a Mystery where Chemistry Meets Engineering,"* University of Colorado, Boulder CO, September 21, 2004. Invited

Burgess, D.R. *"Towards a Simplest Notation and Classification Scheme for Chemical Reactions and Species,"* Constructing a Kinetics Database: An NSF-sponsored workshop NIST, Gaithersburg, Maryland, April 19, 2004.

Cafiero, M.L., *"Role of Exact Exchange and Correlation Functionals in Chemical Reactions,"* 15th Canadian Symposium on Theoretical Chemistry, Quebec, Canada, July 2, 2004.

Chaka, A.M., *"How Scientific Computing, Knowledge Management, and Databases can Enable Advances and New Insights in Chemical Technology,"* National Institute of Standards and Technology, Boulder, CO, October 27, 2003. Invited

Chaka, A.M., *"The Impact of the Environment on Chemistry at Surfaces,"* Colorado School of Mines, Golden, CO, October 24, 2003. Invited

Chaka, A.M., *"Quantum Mechanics and the Automobile,"* Howard University, Washington, DC, January 9, 2004. Invited

Chaka, A.M., *"How Scientific Computing, Knowledge Management, and Databases can Enable Advances and New Insights in Chemical Technology,"* Brock Institute for Scientific Computing, Brock University, St. Catharine, Canada February 2, 2004. Invited

Chaka, A.M., *"How Scientific Computing, Knowledge Management, and Databases can Enable Advances and New Insights in Chemical Technology,"* Chemistry Department, University of Toronto, Toronto, Canada, February 3, 2004. Invited

Chaka, A.M., *"Ab Initio Thermodynamics: Structure & Reactivity of Metal Oxide Surfaces in a Real World Environment,"* Accelrys World 2004, San Diego, CA , March 3, 2004. Invited

Chaka, A.M., *"Predicting the Impact of the Environment on the Structure and Chemistry of Metal Oxide Surfaces,"* 227th ACS National Meeting, Anaheim, CA, March 30, 2004. Invited

Chaka, A.M., *"Computational Kinetics,"* NSF Workshop on Kinetics Databases, NIST, Gaithersburg, MD, April 20, 2004. Invited

Chaka, A.M., *"How Scientific Computing, Knowledge Management, and Databases can Enable Advances and New Insights in Chemical Technology,"* Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD, April 21, 2004. Invited

Chaka, A.M., *"The Importance of Complexity: The Structure and Reactivity of Metal Oxide Surfaces in a Realistic Environment,"* University of Maryland, Departments of Chemistry and Biochemistry Seminar, College Park, MD, April 23, 2004. Invited

Chaka, A.M., *"How Scientific Computing and Computational Chemistry Fit into the Industrial Problem Solving Process,"* 58th Annual Quality Congress, Toronto, Canada, May 26, 2004. Invited

Chaka, A.M., *"Quantum Mechanics and the Automobile,"* Iowa State University, Ames, IA, July 14, 2004. Invited

Chaka, A.M., *"Theoretical Tools for Investigating the Chemistry of Surfaces in the Environment,"* Stanford University, Stanford, CA, July 16, 2004. Invited

Chaka, A.M., *"Predicting the Impact of the Environment on the Structure and Chemistry of Metal Oxide Surfaces,"* Department of Chemical Engineering Seminar, University of Maryland, College Park, MD, September 21, 2004. Invited

Chaka, A.M., *"How High-End Computing can Enable Advances in Chemical and Materials Technology,"* Interagency Task Force on High-End Computing, Arlington, VA, September 24, 2004. Invited

Chirico, R.D., *"New Era in Technical Data Communications: Efficient Management, Data Collection, Delivery and Standardization of Communications, and Critical Evaluation of Thermodynamic Data (a Possible Model for Kinetic Data),"* Kinetic Database Workshop, Gaithersburg MD, April 21, 2004. Invited

Chirico, R.D., *"Development of an XML-Based IUPAC Standard for Thermodynamic Data Communications: New Extensions and Applications of ThermoML,"* 2004 Calorimetry Conference, Santa Fe NM, June 28-July 1, 2004.

Chirico, R.D., *"TRC Data Entry Facility: Improving In-house and Cooperative Data Entry Operations with Guided Data Capture Software and ThermoML,"* 4th Annual NIST/TRC Consortium Workshop, Boulder CO, July 23, 2004.

Chirico, R.D., *"Themodynamic Data Processing and Delivery Within the TRC Data Infrastructure,"* International Conference on Chemical Thermodynamics – 2004, Beijing, China, August 15-19, 2004.

Chirico, R.D., *"New Era in Technical Data Communications: Efficient Management, Data Collection, Delivery and Standardization of Communications, and Critical Evaluation of Thermodynamic Data (a Possible Model for Kinetic Data),"* Kinetic Database Workshop, Gaithersburg MD, April 21, 2004. Invited

Chirico, R.D., *"Development of an XML-Based IUPAC Standard for Thermodynamic Data Communications: New Extensions and Applications of ThermoML,"* 2004 Calorimetry Conference, Santa Fe NM, June 28-July 1, 2004.

Chirico, R.D., *"TRC Data Entry Facility: Improving In-house and Cooperative Data Entry Operations with Guided Data Capture Software and ThermoML,"* 4th Annual NIST/TRC Consortium Workshop, Boulder CO, July 23, 2004.

Chirico, R.D., *"Themodynamic Data Processing and Delivery Within the TRC Data Infrastructure,"* International Conference on Chemical Thermodynamics – 2004, Beijing, China, August 15-19, 2004.

Frenkel, M., *"Communications in Thermodynamics: Establishing a 'Bridge' between Property Measurement and Chemical Process Design,"* University of Alabama at Birmingham, October 30. 2003. Invited

Frenkel, M., *"Thermodynamic Data Engine for the 21st Century,"* University of South Alabama at Mobile, October 28, 2003. Invited

Frenkel, M., *"ThermoML and IUPAC Activities in Standardizing Thermodynamic Data Communications,"* IUPAC Workshop 'XML Data Dictionaries and IUPAC Chemical Identifier', NIST, Gaithersburg MD, November 13, 2003. Invited

Frenkel, M., Diky, V.V., Chirico, R.D., Yan, X., and Wilhoit, R.C., *"Dynamic Data Evaluation: Concept and Implementation for Pure Compounds,"* AIChE Annual Meeting, San Francisco CA, November 18, 2003.

Frenkel, M. and Magee, J.W., *"A Comprehensive Data Retrieval System for Ionic Liquids,"* IUPAC Task Group meeting for the project 'Ionic Liquids Database', Delft University of Technology, Delft, Netherlands, January 26, 2004. Invited

Frenkel, M., *"New Era in Technical Data Communications: Highly Efficient Delivery and Guided Quality Control,"* Elsevier Publishers Headquarters, Amsterdam, Netherlands, January 27, 2004. Invited

Frenkel, M., *"ThermoML: Basic Principles, Scope, Description of Major Structural Elements, and New Data Delivery Process Infrastructure,"* IUPAC Task Group meeting for the project 'XML-Based IUPAC Standard for Thermodynamic Property Data Capture and Storage', ESDU Headquarters, London, United Kingdom, January 29, 2004. Invited

Frenkel, M., *"Thermodynamic Data Engine for the 21st Century: Comprehensive Data Storage Facilities, Platform-Independent Data Communications, and on-Demand Data Evaluation and Prediction Expert Systems,"* 10th International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird UT, May 18, 2004. Invited

Frenkel, M., *"Managing Thermodynamic Property Data for on-Demand Use in Chemistry and Engineering,"* DIPPR Midyear Executive Committee Meeting, Provo UT, May 22, 2004 Invited

Frenkel, M., Chirico, R.D., Diky, V.V., Yan, X., and Dong, Q., *"ThermoData Engine (TDE): A Software 'Bridge' from Experimental Measurement to Chemical Process Design,"* The 59th Calorimetry Conference, Santa Fe NM, July 1, 2004.

Frenkel, M., *"Overview of TRC Activities in 2003-2004,"* Fourth (Thirteenth) NIST/TRC Research Consortium Annual Workshop, Boulder CO, July 23, 2004.

Frenkel, M., *"Report on the IUPAC Project: 'Ionic Liquids Database',"* International Conference on Chemical Thermodynamics, Beijing, China, August 17, 2004.

Frenkel, M., *"Global Communications and Expert Systems in Thermodynamics: Connecting Property Measurement and Chemical Process Design,"* International Conference on Chemical Thermodynamics, Beijing, China, August 20, 2004 (Plenary Lecture).

Friend, D.G., *"Thermophysical Property Modeling,"* Rocket Propellant RP-1 Workshop, Boulder CO, December 11, 2003.

Friend, D.G.. *"From Cryogenics to Steam,"* Boulder Labs 50th Anniversary Lecture Series, Boulder CO, July 21, 2004.

Friend, D.G., *"Properties of Water and Aqueous Systems: Metrological Applications,"* 14th ICPWS, Kyoto, Japan, August 31, 2004. Invited

Friend, D.G., *"Thermophysical Property Modeling,"* Rocket Propellant RP-1 Workshop, Boulder CO, December 11, 2003.

Friend, D.G.. *"From Cryogenics to Steam,"* Boulder Labs 50th Anniversary Lecture Series, Boulder CO, July 21, 2004.

Friend, D.G., *"Properties of Water and Aqueous Systems: Metrological Applications,"* 14th ICPWS, Kyoto, Japan, August 31, 2004. Invited

Gonzalez, C., *"Simplified Quantum-Chemical Models to Molecular Conductance: A Comparison with Experiment,"* 3rd Int'l Conf. Computational Modeling and Simulation of Materials, Acireale, Italy, May 30, 2004.

Gonzalez, C., *"The Role of Quantum Chemistry in Molecular Electronics,"* Nanotek Consortium, KRAFT FOODS, Inc., Lanview, IL, June 2, 2004.

Gonzalez, C., *"Role of Exact Exchange and Correlation Funcationals in Chemical Reactions,"* 15th Canadian Symposium on Theoretical Chemistry, Quebec, Canada, July 2, 2004.

Harvey, A.H. and Mountain, R.D., *"Molecular Simulation of the Diffusivity of NaCl and NaOH in Steam,"* AIChE Annual Meeting, San Francisco CA, November 2003.

Harvey, A.H. and Mountain, R.D., *"Molecular Simulations of the Diffusivity of NaOH in Steam,"* 14th ICPWS, Kyoto, Japan, August 2004.

Huber, M.L., *"Viscosity correlations for minor constituent fluids in natural gas: n-octane, n-nonane, and n-decane,"* poster presentation at Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird UT, May 18, 2004.

Ihmels, E.C., Lemmon, E.W., Fischer, K., and Gmehling, J., *"Experimental Thermodynamic Properties and Fundamental Equations of State for the Four Butene Isomers,"* presented at Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird UT, May 18, 2004.

Irikura, K.K., *"Ab initio Characterization of van der Waals Excited States of C1OO,"* 227th ACS National Meeting, Anaheim, CA, March 31, 2004.

Irikura, K.K., *"Uncertainty from Bias in Virtual Measurements and the NIST Computational Chemistry Comparison and Benchmark Database (CCCBDB),"* Mathematical and Computational Science Division, NIST, April 20, 2004. Invited

Linstrom, P.J., *"Data Handling in the NIST Chemistry WebBook,"* American Chemical Society National Meeting, Philadelphia, PA, August 26, 2004.

Laesecke, A. and McLinden, M.O., *"Viscosity Measurements and Model Comparisons for the Refrigerant Blends R-410A and R-507A,"* ASHRAE Annual Meeting, Nashville TN, June 27, 2004.

Laesecke, A., *"The Tragicomical (Hi)story of Viscosity Measurements of Alternative Refrigerants,"* SURF NIST Boulder Seminar, July 2, 2004.

Lemmon, E.W., *"Thermodynamic Properties of Air,"* presented at AFOSR Test & Evaluation Program Review, Washington DC, June 22-23, 2004.

Lewis, M.A., *"Measurement of Phase Shifts and Power Flows in Inertance Tubes,"* 13th International Cryocooler Conference, New Orleans LA, March 31, 2004.

Manion, J.A., *"Gas Phase Kinetics Data And Database: What Information Is Needed And How To Use It,"* Constructing a Kinetics Database - An NSF Sponsored Workshop, NIST, Gaithersburg, MD, April 19, 2004. Invited

Manion, J.A., *"Collaborative Approaches to Database Development: Kinetic Data and the NIST Real Fuels Program,"* DuPont, Wilmington, DE, April 28, 2004. Invited

Manion, J.A., *"Combustion Kinetics Databases for Real Fuels,"* Basic Energy Science Contractors Meeting, Warrenton, VA, June 2, 2004. Invited

Manion, J.A., *"Databases For Combustion Kinetics Of Real Fuels: NIST Programs And Perspectives,"* International Workshop on CHEMKIN in Combustion, Chicago, IL, July 25, 2004. Invited

Manion, J.A., *"An Overview of the NIST Real Fuels Program,"* Johns Hopkins University, Applied Physics Laboratory, Laurel, MD, August 9, 2004. Invited

Matheu, D.M., *"Automated Construction of Gas-Phase Kinetic Models: New Pathways for Old Problems,"* Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA, November 18, 2003.

Matheu, D.M., *"New Models and Pathways for Methane and Ethane Pyrolysis from Automated, Pressure-Dependent Mechanism Generation,"* Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA, November 18, 2003.

Matheu, D.M., *"Automated Construction of Chemical Mechanisms for Challenging Pyrolysis Systems,"* 227th ACS National Meeting, Anaheim, CA, March 31, 2004.

Matheu, D.M., *"Pressure-Dependent Automated Mechanism Generation,"* 227th ACS National Meeting, Anaheim, CA, April 4, 2004.

Matheu, D.M., *"Systematic, Automated Model Construction for High-Conversion Ethane Pyrolysis,"* 18th Int'l Conf. on Chemical Kinetics, Bristol, UK, August 10, 2004.

McGivern, W.S., *"Decomposition and Isomerization of 1-Octyl Radicals,"* 30th International Symposium on Combustion, Chicago, Illinois, July 25, 2004.

Mountain, R.D., *"Introduction to Molecular Dynamics,"* 15th ACBM/NIST Computer Modeling Workshop, NIST, Gaithersburg, MD, June 21, 2004.

Mountain, R.D., *"The Industrial Fluid Properties Simulation Challenge,"* Gordon Research Conference, Plymouth, NH, July 6, 2004.

McLinden, M.O., *"Refrigerant Properties for Cycle Analysis and Simulation, Short Course: Simulation Tools for Vapor Compression System and Component Analysis,"* Purdue University, July 10, 2004. Invited

Muzny, C., *"The Future of Membrane Science at NIST,"* EUWP Desalination Kick-off Meeting & Interagency Desalination Consortium, San Antonio TX, January 6-9, 2004.

Orkin, V., *"Precise Measurements Of Hydroxyl Reaction Rate Constants And Atmospheric Lifetimes Of Industrial Pollutants,"* Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia, August 17, 2004.

Radebaugh, R., *"A Career in Cryogenic Engineering,"* Society of Women Engineers, Colorado School of Mines, Golden CO, October 22, 2003. Invited

Radebaugh, R., *"A Review of Cryocoolers and their Applications,"* Military and Commercial Applications of Low-Cost Cryocoolers (MCALC-IV), San Diego CA, November 20, 2003. Invited

Radebaugh, R., *"Foundations of Cryocoolers,"* Cryogenic Society of America, One-Day Short Course, New Orleans LA, March 28, 2004. Invited

Radebaugh, R., *"Minimum Reservoir Volumes in Large Pulse tube Refrigerators,"* 13th International Cryocooler Conference, New Orleans LA, March 31, 2004.

Radebaugh, R., *"Cryogenics: Nobel Prizes, Everyday Uses, and Technical Challenges,"* NIST Research Advisory Committee Summer Seminar, NIST/Boulder, June 22, 2004; NIST/Gaithersburg, June 25, 2004. Invited

Radebaugh, R., *"Microscale Heat Transfer at Low Temperatures,"* NATO Advanced Study Institute on Microscale Heat Transfer – Fundamentals and Applications, Cesme, Turkey, July 20, 2004. Invited

Radebaugh, R., *"Heat Transfer Issues in Cryogenic Catheters,"* NATO Advanced Study Institute on Microscale Heat Transfer – Fundamentals and Applications, Cesme, Turkey, July 28, 2004. Invited

Rosasco, G.R., *"Information and Knowledge Management at NIST,"* DoE Office of Science Data Management Workshops, Palo, CA, March 16, 2004.

Rosasco, G.R., *"New Data Activities in the NIST Physical and Chemical Properties Division,"* Dupont, Wilmington, DE, April 28, 2004.

Rosasco, G.R., *"Future Thrusts in Information and Knowledge Management,"* TRC Consortium Meeting, NIST, Boulder, CO, July 24, 2004.

Shen, V.K., *"Mechanical Properties of n-Alkane Glasses via the Energy Landscape,"* American Institute of Chemical Engineers Annual Meeting 2003, San Francisco, CA, November 21, 2003.

Shen, V.K., *"Computational and Theoretical Study of Metastability and Instability: Does Size Matter?"* Statistical Mechanics Seminar Series, University of Texas at Austin, Dept. of Chemical Engineering, February 26, 2004.

Shen, V.K., *"Phase Behavior of Binary Mixtures by Transition-Matrix Monte Carlo,"* Midwest Thermodynamics and Statistical Mechanics Conference, Buffalo, NY, June 3, 2004.

Tsang, W., *"Energy Transfer Effects During The Multichannel Decomposition Of Ethanol,"* Eastern States Meeting of the Combustion Institute, Penn State University/Nittany Lion Inn, State College, PA, October 27, 2003.

Tsang, W., *"Non-Equilibrium Effects During Disilane Decomposition,"* AIChE 2003 Annual Meeting/San Francisco Hilton, San Francisco, CA, November 17, 2003.

Tsang, W., *"Heptane Combustion Data Base,"* 42ND Aerospace Sciences Meeting & Exhibit/Reno Hilton, Reno, Nevada, January 8, 2004.

Tsang, W., *"Thermal Decomposition Of Hexyl Radicals,"* Fuel Division, American Chemical Society, Anaheim Hilton, Anaheim, CA, April 1, 2004.

Tsang, W., *"Chemical Kinetics Issues In Combustion,"* For Jason Group Panel Review on Recent Progress in Hypersonic Science & Technology, San Diego, CA, June 22, 2004. Invited

Tsang, W., *"Mechanism And Rate Constants For The Decompsition Of 1-Pentenyl Radicals,"* 30th Symposium on Combustion, University of Illinois Alumni Association, Chicago, IL, July 26, 2004.

Tsang, W., *"Fuel Cracking And Combustion Kinetics Databases,"* 228th American Chemical Society (ACS) National Meeting, Pennsylvania Convention Center, Philadelphia, PA, August 24, 2004.

Tsang, W. *"Combustion Kinetics Databases and the Uses of Chemical Inhibition"* Applied Physics Laboratory, Johns Hopkins University, August 9, 2004. Invited

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

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

Development of Pulse Tube Refrigeration Technology for a Fully Acoustic Densifier that Simultaneously Conditions Two Cryogenic Fluids, R. Radebaugh
Sierra Lobo (CN-1744) (CRADA)

Development of a Two-Stage Pulse Tube Cryocooler for Superconducting Motors, R. Radebaugh
American Superconductor Corporation (CN-1762) (CRADA)

Development of a Pulse Tube Cryocooler for Dermatalogic Cryosurgery
CIMEX BioTech (CN-1808) (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
Shell Development Company, Conoco Phillips, Chevron Texaco, Eastman Chemical Company, Virtual Materials Group, Inc.

4. Patents

5. SRM Activities

SRM 2234 Gallium for Thermal Analysis (completed)
SRM 2235 Bismuth for Thermal Analysis (completed)

6. SRD Activities

SRD   NIST Chemical Kinetics Mechanism Database CKMech
hppt://srdata.nist.gov/ckmechx/
SRD 4   NIST Thermophysical Properties of Hydrocarbon Mixtures Database, Major
        Upgrade (Version 3.01), Support
SRD 10 NIST Thermophysical Properties of Water Database, Support
SRD 17 NIST Chemical Kinetics Database on the Web, Version 7.0, Release 1.1
SRD 23 NIST Reference Fluid Thermodynamic and Transport Properties, Major
        Upgrade (Version 7), Support
SRD 23 NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures
Database, Major Upgrade (Version 7.0), Support
SRD 40 NDRL/NIST Solution Kinetics Database on the Web, New Release
SRD 69 NIST Chemistry Webbook, Contributions on Fluid Properties, New Release
TRC Tables – Hydrocarbons, Major Upgrades
TRC Tables – Non-Hydrocarbons, Major Upgrades
International Data Series, Major Upgrades
SRD 85 NIST/TRC Table Database, WinTable 1.5 (2001), New Release
SRD 87 NIST/TRC Vapor Pressure Database, Version 2001, New Release
SRD 88 NIST/TRC Ideal Gas Database, New Release
SRD 101 NIST Computational Chemistry Comparison and Benchmark Database,
        Release 10-09-2003
SRD 101 NIST Computational Chemistry Comparison and Benchmark Database, Release
        05-10-2004.

7. Calibrations

8. Committee Assignments

T.C. Allison
Collaboratory for Multi-Scale Chemical Sciences

D.G. Archer
ASTM International Committee D03 on Gaseous Fuels (Member)
ASTM International Subcommittee D03.05, Thermophysical Properties (Chair)
ASTM International Committee E37 on Thermal Measurements (Officer, Membership
Secretary)
ASTM International Subcommittee E37.02, Standard Reference Materials for Thermal

Measurements (Chair)
ASTM International Subcommittee E37.90, Executive Subcommittee (Member)
ASTM International Taskgroup E37.01.06 on Heat Capacity (Chair)
ASTM International Taskgroup E37.01.17 on Differential Scanning Calorimetry
    Calibration (Chair)
ASTM International Taskgroup E37.01.21 on Reaction Calorimetry (Chair)

P.E. Bradley
NASA Cryogenic Technology Working Group for Space Exploration and Transportation

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

A.M. Chaka
Secretary, Theoretical Subdivision, American Chemical Society
Member, Executive Committee, Physical Division, American Chemical Society
Secretary, Computational Molecular Science and Engineering Forum, American Institute
    of Chemical Engineers
National Energy Technology Laboratory Review Panel Member, DoE
NIH Chemical Diversity Roadmap Committee
Techical Advisory Committee, International Conference on Physical Properties and
    Phase Equilibria
Organizing Committee, Foundations of Molecular Modeling and Simulation Conference
AFOSR Proposal Review Panel
DOE BES Proposal Reviewer
Organizing Committee for NSF Chemistry Division Cyber-Enabled Chemistry Workshop

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)
Board of Directors of International Association of Chemical Thermodynamics
Chair, Organizing Committee of ICCT-2006
Chairman, IUPAC Task Group
Program Chair, Calorimetry Conference-2006

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
ASME Codes and Standards Institute, Air Properties Committee
IAPWS, U.S. National Representative
IAPWS Working Group on Thermophysical Properties of Water and Steam (Chair)
IAPWS Task Group on Transport Properties (Chair)
AIChE Design Institute for Physical Property Data (DIPPR): Project 991 Steering Team,
    Project 801 Steering Team, Administrative Committee, Technical Committee
Fourteenth International Conference on the Properties of Water and Steam Organizing
    Committee (Member)
Joint Conference of the 16th STP and ICCT 19, Executive Board (Vice President)
Industrial Fluids Simulation Challenge Organizing Committee (Member)
Industrial Fluids Simulation Challenge Benchmark Committee (Chair)
Joint ASME-AIChE Committee on Thermophysical Properties (Member)

A.H. Harvey
ASME Research and Technology Committee on Water and Steam in Thermal Systems
    (First Vice-Chair)
ASME Research Subcommittee on the Properties of Water and Steam (Secretary)
Colloquium Organizing Committee, CSTL, Boulder, CO (Co-Chair).
IAPWS Working Group on Thermophysical Properties of Water and Steam
IAPWS Task Group on Fundamental Constants (Chair)
IAPWS Editorial Committee (Chair)

M.L. Huber
Joint IAPWS-IATP Task Group on Transport Properties

Gonzalez, G.
USDA Panel of the Nanoscale Science and Engineering for Agriculture and Food
    Systems
Scientific Board of the NanoTEK Consortium, KRAFT, Inc. (Member)

A. Laesecke
Colloquium Organizing Committee, CSTL, Boulder, CO (Co-Chair).
Board of Directors of the SURF NIST Boulder program.
IUPAC Project on Thermochemical, Thermodynamic, and Transport Properties of
    Halogenated Organic Compounds and Mixtures (Coordinator) jointly with Prof. John
    Dymond (Glasgow, UK), Prof. Ulrich K. Deiters (Cologne, Germany), and Prof.
    Andreas Heintz (Rostock, Germany).
International Association of Transport Properties.

E.W. Lemmon
Transmission Measurement Committee of the American Gas Association (AGA)

P.J. Linstrom
ASTM Subcommittee E13.15, Analytical Data

J.W. Magee
IUPAC Project on Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the
    Development of Standardized Systems (Coordinator)
IUPAC Project on Ionic Liquids Database (Coordinator)
Executive Board, 16th Symposium on Thermophysical Properties/19th IUPAC Conference
    on Chemical Thermodynamics
Board of Directors of the SURF NIST Boulder Program (Co-Chair)

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

M.O. McLinden
ASHRAE Standards Project Committee 34 – Designation and Safety Classification of
    Refrigerants (Member)
ASHRAE Technical Committee 3.1 - Refrigerants and Secondary Coolants
    (Corresponding Member)
ISO TC86/SC8/WG7 – Refrigerant Properties (Member)

P. Neta
Member, IUPAC Committee on Standard Potentials of Radicals

V.L. Orkin
NASA Panel for Data Evaluation

R.A. Perkins
ASTM Committee D34 on Waste Management
International Association for Transport Properties
Joint IAPWS-IATP Task Group on Transport Properties

R. Radebaugh
International Cryocooler Conference, Inc., Advisory Committee
Cryogenic Society of America, Editorial Committee

S.E. Stein
ASMS Subcommittee on Measurements and Standards – Methodology
IUPAC Committee on Printed and Electronic Publishing
IUPAC, The IUPAC Chemical Identifier (Project Leader)
IUPAC, Standard XML Data Dictionaries for Chemistry (Project Leader)
Association of Biomolecular Resource Facilities Committee
Proteomics Standards Research Group

7. Editorships

T.J. Bruno
Journal of Process Analytical Chemistry (Associate Editor)
Industrial and Engineering Chemistry Research (Editorial Board)

R.D. Chirico
Journal of Chemical Thermodynamics (Editorial Board)
TRC Tables – Hydrocarbons (Editorial Board)
TRC Tables – Non-Hydrocarbons (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)
TRC Tables – Hydrocarbons (Editorial Board)
TRC Tables – Non-Hydrocarbons (Editorial Board)

A. Laesecke
Journal of Chemical and Engineering Data (Advisory Board)
TRC Tables – Hydrocarbons (Editorial Board)
TRC Tables – Non-Hydrocarbons (Editorial Board)
Guest Editor of a Special Issue of "Fluid Phase Equilibria" (Vol. 210, No. 1) with contributions to the 3rd IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons and Mixtures, July 28-August 2, 2002, Rostock, Germany. (Invited)

J.W. Magee
Journal of Chemical and Engineering Data (Associate Editor)
TRC Tables – Hydrocarbons (Editorial Board)
TRC Tables – Non-Hydrocarbons (Editorial Board)

J.A. Manion
International Journal of Chemical Kinetics (Associate Editor)

P. Neta
Radiation Physics and Chemistry (Editor)

R. Perkins
TRC Tables – Hydrocarbons (Editorial Board)
TRC Tables – Non-Hydrocarbons (Editorial Board)
Journal of Chemical and Engineering Data (Advisory Board)

R. Radebaugh
Cryogenics (International Advisory Editor)

J.C. Rainwater
International DATA Series, Selected Data on Mixtures (Editor)

W. Tsang
International Journal of Chemical Kinetics (Editor)

10. <u>Seminars</u>

October 24, 2003
J. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, "A Comparison of Computed and Observed Heats of Formation." (Division Sponsor: Carlos Gonzalez)

October 29, 2003
D.P. Landau, Center for Simulation Physics, The University of Georgia, Athens, GA, "Dynamical Scaling of Surface Growth in Simple Lattice Models." (Division Sponsor: Anne Chaka)

October 30, 2003
Dr. Vladimir Kozhevnikov, University of Utah, "Liquid-liquid transitions probed by sound."
(Division Sponsor: A. Laesecke)

November 5, 2003
J.A. Kelber, University of North Texas, Denton, TX, "Forming Laminar Cu/Substrate Interfaces: Vacuum vs Electrochemical Processing." (Division Sponsor: Anne Chaka)

November 12, 2003

M. Nic and J. Jirat, Institute of Chemical Technology, Prague, Czech Republic, "Capturing Chemical Information." (Division Sponsor: Stephen Stein)

November 14, 2003

Dr. Axel Günther, Dept. of Chem. Engineering, MIT, "Multiphase MicroChemical Systems."
(Division Sponsor: A. Laesecke)

December 17, 2003

R. Eisenberg, Rush Medical Center, Chicago, IL, "Ion Channels, Natural Nanodevices." (Division Sponsor: Raymond Mountain)

January 7, 2004

C. Lo, Massachusetts Institute of Technology, Cambridge, MA, "Car-Parrinello Molecular Dynamics Investigation of the Methanol-Methanol Coupling Reaction in the Zeolite Chabazite." (Division Sponsor: Anne Chaka)

January 15, 2004

J. de la Mora, Yale University, New Haven, CT, "Analysis of the Size and Shape of Nanoparticles by Tandem Ion Mobility and Mass Spectrometry." (Division Sponsor: Stephen Stein)

February 5, 2004

Dr. Jesus Carlos Sanchez Ochoa, University College London (UK), "The Ebulliometric Method of Vapor Pressure Measurement." (Division Sponsor: A. Laesecke)

February 19, 2004

O. Mekenyan, Bourgas "Prof. Az. Zlaataraov" University, Bulgaria, "The Virtual Mouse: Building Polycompartment Models for Predicting Biological and Physicochemical Effects. Application for Predicting Biomagnification of Chemicals in Different Organisms." (Division Sponsor: Anne Chaka)

March 11, 2004

Prof. David E. Smith, New Mexico State University, "Molecular Simulations of Swelling Thermodynamics in Hydrated Clay Minerals." (Division Sponsor: A.H. Harvey)

May 7, 2004

Dr. Vladimir Kozhevnikov, University of Utah, "Measurement of Thermodynamic Properties of Fluids at High Temperatures and Pressures." (Division Sponsor: J.W. Magee)

May 12, 2004

M. Kertesz, Georgetown University, Washington, DC, "Structural and Electronic Properties of Carbon Nanotubes and Organic Crystals." (Division Sponsor: Anne Chaka)

May 24, 2004

Dr. Christian Ihmels, Laboratory for Thermophysical Properties GmbH, University of Oldenburg, Germany, "From High Temperature and High Pressure Densities to Pascal Range Vapor Pressures: A Short Experimental Survey." (Division Sponsor: E.W. Lemmon)

June 17, 2004

Prof. Ken Marsh, University of Canterbury, "Ionic Liquids - Possible New Solvents for Green Chemistry." (Division Sponsor: J.W. Magee)

July 1, 2004

Prof. Jan V. Sengers, University of Maryland, "Fluctuations in Fluids in Thermal Nonequilibrium States." (Division Sponsor: D.G. Friend)

July 14, 2004

L. Ervin, Medical University of South Carolina, Charleston, SC, "Mass Spectrometric Analysis of Tryptic Peptides Reveals Novel Sites of Modifications in Lens Membrane Protein 20." (Division Sponsor: Stephen Stein)

August 19, 2004

S. Hewitt, California State University, Fullerton, CA, "A Physical and Analytical Chemist's Perspective of Several Atmospheric, Combustion, and Biological Systems." (Division Sponsor: Jeff Hudgens)

August 19, 2004

Dr. Ing. Piero Colonna, Associate Professor, Delft University of Technology, The Netherlands, "Nonclassical Gasdynamics: Planned Theoretical and Experimental Investigation at TU Delft." (Division Sponsor: E.W. Lemmon)

August 23, 2004

Dr. Karsten Meier, Helmut-Schmidt-University, University of the Federal Armed Forces, Hamburg, Germany, "An Apparatus for Measurements of the Speed of Sound in Liquids under High Pressures." (Division Sponsor: A. Laesecke)

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

IUPAC Project Meeting-XML Data Dictionary & Chemical Identifier, November 12-14, 2003 (S. Stein)

AIChE Annual Meeting, November 17-21, 2003, San Francisco CA (A. Laesecke – Session organizer and Chair, invited).

Constructing a Kinetics Database – NSF-Sponsored Workshop, April 19-21, 2004, Gaithersburg MD (M. Frenkel, Co-Chair).

Peptide Fragmentation and Identification Workshop (NIST/NIH/ISB), May 3-4, 2004 (S. Stein)

Publishing Workshop for the SURF NIST Boulder Program, July 13, 2004 (A. Laesecke, R. Goldfarb, J. Magee, H. McCullough).

12. Other

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

A. Laesecke
Best Paper Award Nomination for the contribution "Viscosity Measurements and Model Comparisons for the Refrigerant Blends R-410A and R-507A" at the ASHRAE Annual Meeting, June 26-30, 2004, Nashville TN.
2003 Best Paper Award by the Journal Measurement Science and Technology for the paper: R.F. Hafer and A. Laesecke, "Extension of the Torsional Crystal Viscometer to Measurements in the Time Domain," Meas. Sci. Technol., 14, 6633-673 (2003), http://www.iop.org/EJ/news/-topic=785.

J.W. Magee
Adjunct Professor, Department of Mechanical 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.

Collaborations

Prof Marco Castaldi, Columbia University – Shock tube Studies on Catalytic Processes
Prof. C. Thomas Avedesian, Cornell University, - Film Boiling as Chemical Reactor

Prof. M. R, Zachariah, University of Maryland and Mitchell Smooke, Yale University,
    Soot and Nanotube formation in NIST WSR
Dr. George Mulholland – Development of Heptane Combustion Database - SERDP