Physical and Chemical Properties Division (838)

Outputs and Interactions

1. Publications

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Bruno, T.J. and Smith, B.L., ***"Improvements in the Measurement of Distillation Curves – Part 2: Application to Aerospace/Aviation fuels RP-1 and S-8,"*** Indust. Eng. Chem. (in press).

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Van Dresar, N.T. and Siegwarth, J.D., "***Benchmark Gauging System for a Small-Scale Liquid Hydrogen Tank,"*** Rev. Sci. Instrum. (in press).

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2. Talks

Burgess, D.R., ***"NIST Chemical Kinetics Combustion Model Database,"*** Surrogate Fuel Workshop, University of Southern California, Los Angeles, CA, February 13, 2006.

Bradley, P., **"Evaluation of total Pressure Oscillator Losses,"** 14th Int. Cryocooler Conference, Annapolis, MD June 15, 2006.

Bradley, P., ***"Low-Temperature Measurements of Regenerator and Pulse Tube Losses at High Frequencies,"*** Int. Cryogenic Engineering Conference, Prague, Czeh Republic, July 20, 2006.

Bradley, P., ***"Cryogenic Material Properties Database, Update 2006,"*** Int. Cryogenic Materials Conference, Prague, Czech Republic, July 18, 2006.

Bruno, T.J., ***"Standardizing Voodoo: Improvements in the measurement of Distillation Curves,"*** Colorado School of Mines Seminar, Golden, CO, March 10, 2006. Invited

Bruno, T.J., ***"Energetic Materials: A Practical Introduction to Explosives,"*** NIST Boulder Seminar Series, Boulder, CO, April 12, 2006. Invited

Bruno, T.J., ***"Thermophysical Properties of "Reference" JP-8,"*** Presented at the ARL/AFOSR Contractor's Meeting on Chemical Propulsion, Crystal City, VA, June 10, 2006. Invited

Bruno, T.J., ***"Improvements in the Measurement of Distillation Curves 1,"*** Rocky Mountain Conference on Analytical Chemistry, Breckenridge, CO, July 25, 2006.

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Bruno, T.J., ***"Thermal Decomposition: A Prelude to Thermophysical Property Measurements,"*** 16th Symp.on Thermophysical Properties, Boulder, CO, July 31, 2006.

Bruno, T.J., ***"Apparatus for Advanced Distillation Curve Measurement on Complex Fluids,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, August 1, 2006.

Bruno, T.J., ***"Advanced Distillation Curve Measurement: Case Studies on Complex Fluids,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, August 1, 2006.

Bruno, T.J., ***"Improvements in the Measurement of Distillation Curves,"*** Poster Session, 16th Symp. on Thermophysical Properties, Boulder, CO, August 3, 2006.

Bruno, T.J., ***"Advanced Measurement of Distillation Curves,"*** Chemical Science and Technology Laboratory Technical Achievement Awards Presentation, NIST Gaithersburg, MD, August 15, 2006.

Chaka, A., ***"Surface Structure and Reactivity of Clean and Hydrated A-Fe203,"*** AIChE 2005 Annual Meeting, Cincinnati Convention Center, Cincinnati, OH, October 31, 2005.

Chirico, R., ***"ThermoML: New IUPAC Standard for Thermodynamic Data Storage and Exchange,"*** Presented at the spring 2006 American Chemical Society meeting in Atlanta, Georgia, March 2006.

Chirico, R., ***"ThermoML: Based new Data Delivery Process and its Impact on Publication Data Quality,"*** Presented at ThermoInternational 2006, Boulder, CO, Aug 3, 2006.

Chirico, R., ***"TRC Data Entry Facility: TRC Data Collection Operations and Progress for the Data Entry Facility,"*** Presented at ThermoInternational 2006 in Boulder, CO, Aug. 4, 2006.

Frenkel, M., ***"ThermoML: A New IUPAC Standard for Thermodynamic Data Communications,"*** THERMO International 2006, Boulder, Colorado, August 1, 2006.

Frenkel, M. ***"Overview of TRC Activities,"*** 15th TRC Consortium Annual Workshop, NIST, Boulder, CO, August 3, 2006. Invited.

Friend, D.G., ***"NIST's Role in Alternative Refrigerants and the Hydrogen Economy: Metrology for Weights and Measures Development,"*** Talk for DoC Deputy Secretary and staff. Boulder, CO, October 6, 2005. Invited

Friend, D.G., ***"NIST's Role in Alternative Refrigerants and the Hydrogen Economy: Metrology and Data for Innovation and Commerce,"*** Talk for NIST Visiting Committee on Advanced Technology, Boulder, CO, December 12, 2005. Invited

Friend, D.G., ***"Background for the NIST Mercury Vapor Pressure Project,"*** Workshop on Mercury Vapor Pressure for Use in Calibrators, Orlando, FL, March 16, 2006.

Friend, D.G., ***"Overview of the Physical and Chemical Properties Division (Biosciences Emphasis),"*** CARB Follow-up Meeting, Gaithersburg, MD) 03/20/06. Invited

Friend, D.G., ***"Physical and Chemical Property Information to Support Carbon Sequestration Technologies,"*** NIST Meeting on U.S. Climate Change Technology Program, Gaithersburg, MD, March 03, 2006. Invited

Friend, D.G., ***"Brief Overview of the Physical and Chemical Properties Division"***, National Energy Technology Laboratory, Morgantown, WV, May 23, 2006. Invited

Friend, D.G., ***"Welcome to the 16th Symposium on Thermophysical Properties,"*** D.G. Friend Opening of the THERMOInternational Conference, Boulder, CO, July 31, 2006. Invited

Friend, D.G., ***"Data Activities in the Physical and Chemical Properties Division,"*** TRC Consortium Meeting, Boulder, CO, August 3, 2006.

Friend, D.G., ***"Formulation for the Viscosity of Water,"*** Annual Meeting of the International Association for the Properties of Water and Steam, Witney, England, September 5, 2006.

Friend, D.G., ***"Benchmark Data and Non-Simulation Predictive Methods,"*** Workshop of Industrial Fluid Properties Simulation, St. Paul, MN, September 18, 2006. Invited

Gonzalez, C.A., ***"Challenges to the Application of Quantum Chemical Methodologies in the Study of Physical and Chemical properties of Materials at the Nano-scale,"*** XXXI International Congress of Theoretical Chemists of Latin Expression, Margarita Island, Venezuela, October, 2005.

Harvey, A.H. ***"Thermophysical Properties of High-Temperature Gas Mixtures Containing Water,"*** National Energy Technology Laboratory, Morgantown, WV, May 2006.

Harvey, A.H.***"Humidity Standards from First Principles,"*** 16th Symposium on Thermophysical Properties, Boulder, CO, August 2006.

Huang, Y.H., ***"Equation of State and Thermophysical Properties of Helium-3,"*** Int. Cryogenic Materials Conference, Prague, Czech Republic, July 20, 2006. Invited

Huang, Y.H., ***"Debye Fluid State Equation for Helium,"*** 16th Symposium on Thermophysical Properties, Boulder, CO, August 1, 2006.

Huber, M.L., ***"Formula for the Viscosity of Water,"*** 16th Symp. on Thermophysical Properties, Boulder CO, August 2006.

Huber, M.L., ***"Correlation for the Vapor Pressure of Mercury,"*** Mercury Vapor Pressure for Use in Calibrators Meeting, Orlando FL, March 2006. Invited

Hudgens, J.W., ***"Development of a Hadamard Transform Electron Impace Ionization,"*** 17th Int. Mass Spectrometry Conf., Prague Congree, Prague, Czech Republic, August 29, 2006.

Irikura, K.K., ***"Vibrational Zero Point Energies and Their Uncertainties,"*** 19th Int. Conf. on Chemical Thermo Dynamics 2006, Boulder, CO, July 31, 2006.

Jarvis, E., ***"The Nature of Metal-Oxygen Bonding at Corundum (0001) Surfaces,"*** APS March Meeting 2006, Baltimore Convention Center, Baltimore, MD, March 14, 2006.

Jarvis, E., ***"Surface Structure & Reactivity of Cordundum Metal Oxides in the Presence of Oxygen,"*** American Chemical Society National Meeting, San Francisco, CA, September 11, 2006.

Laesecke, A., ***"100 Years Third Law of Thermodynamics: Revisiting the Consequences for Temperature,"*** 16th Symp. Thermophysical Properties, Boulder CO, July 30, 2006.

Laesecke, A., "***Thermophysical Property Measurements in the System 2-Propanol + n-Tetradecane,"*** 16th Symp.on Thermophysical Properties, Boulder Colorado, July 30, 2006.

Laesecke, A., ***"Advanced Electromechanical Model for Torsional Crystal Viscosity Sensors,"*** 16th Symp.Thermophysical Properties, Boulder CO, July 30, 2006.

Lemmon, E.W., ***"Test of the GERG-2004 Equation of State, A Wide Range Reference for Natural Gases,"*** presented at the PRCI Measurement R&D Roadmapping Meeting, San Antonio, Texas, December 7, 2005. Invited

Lemmon, E.W., ***"Thermodynamic Properties of Air,"*** presented at U.S. Air Force T&E Days, Nashville, TN, December 8, 2005. Invited

Lewis, M., ***"Characterization of Inertance Tubes Using Resonance Effects,"*** 14th Inter. Cryocooler Conference, Annapolis, MD June 15, 2006.

Linstrom, P.J., ***"The AnIML Data Model,"*** 57th Pittsburgh Conf. on Analytical Chemistry and Applied Spectroscopy, Orlando, FL, March 16, 2006.

Linstrom, P.J., ***"The NIST Chemistry WebBook: Chemical Informatics Challenges,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, July 31, 2006.

McLinden, M., ***"Metrological Applications of Precision Gas p-ρ-T Measurements,"*** at PTB Seminar on Precision Density Measurements of Solids and Liquids, Braunschweig, Germany, October 26, 2005.

McLinden, M., ***"Adventures in Density: New (and old) Applications for p-ρ-T Measurements at NIST,"*** Ruhr Universität, Bochum, Germany, October 27, 2005. Invited

McLinden, M., ***"Adventures in Density: New (and old) Applications for p-ρ-T Measurements at NIST,"*** at Helmut Schmidt University, Hamburg, Germany, October 30, 2005.

McLinden, M., ***"Adventures in Density: New (and old) Applications for p-ρ-T Measurements,"*** at NIST, Physical and Chemical Properties Division Seminar, Boulder, CO, November 17, 2005.

McLinden, M., ***"The p-ρ-T Behavior of Propane from 265 to 500 K with Pressures to 36 MPa,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, August 1, 2006.

McLinden, M., ***"Force Transmission Errors in Magnetic Suspension Densimeters,"*** 16th Symp.on Thermophysical Properties, Boulder, CO, August 2, 2006.

Mountain, R.D., ***"Solvation Structure of Ions in Water,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, July 31, 2006.

Muzny, C., ***"Building ThermoML Based Bridges between Thermophysical Property Packages and Engineering Applications: ThermoData Engine,"*** ACS National Meeting, Atlanta, Georgia, March 28, 2006.

Muzny, C., ***"Web-ORACLE dissemination infrastructure and ThermoML Opener,"*** NIST/TRC Consortium Workshop, Boulder, Colorado, August 3, 2006,

Muzny, C., ***"Web-Oracle Dissemination System for NIST/TRC Databases,"*** 19th Int. Conference on Chemical Thermodynamics, Boulder, CO, July 31, 2006.

Orkin, V.L., ***"Atmospheric Fate of Halogenated Industrial Compounds: Accuracy of Photochemical Data for Atmospheric Lifetime,"*** ODP, and GWP Estimations, Int. Meeting Pacifichem 2005, Honolulu, HI, December 19, 2005.

Outcalt, S.L., ***"An Automated Densimeter for Rapid Screening of Industrial Fluids,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, August 2, 2006.

Perkins, R.A., ***"Specific Heat Capacity at Constant Volume of Propane at Temperatures from 85 K to 345 K with Pressures to 30 MPa,"*** 16th Symp. on Thermophysical Properties, Boulder, CO, August 3, 2006.

Perkins, R.A., ***"Status of the IAPWS-IATP Joint Project on the Viscosity of Water and Steam,"*** 6th Annual Meeting of the International Association for Transport Properties, Boulder, CO, July 29, 2006.

Radebaugh, R., ***"Cryogenic Refrigerators for DEW Systems Suitable for Military Applications,"*** 8th Directed Energy Symposium, Lihue, Hawaii, November 16, 2005. Invited

Radebaugh, R., ***"Consequences and Nature of Real Gas Effect Distinctions Between He^3 and He^4; Overview of Regenerator Test Lab,"*** ONR Superconductive Electronics Program Review, San Diego, CA, January 12, 2006. Invited

Radebaugh, R. ***"Cryogenic Applications,"*** 17th James Belfer Memorial Symposium, Cryogenic Engineering and Applications, Technion, Haifa, Israel, April 4, 2006. Invited

Radebaugh, R., ***"Microcryocoolers and High Power-Density Cryocoolers,"*** 17th James Belfer Memorial Symposium: Cryogenic Engineering and Applications, Technion, Haifa, Israel, April 4, 2006. Invited

Radebaugh, R.***,"Cryocooler Advances and Applications,"*** Workshop on Challenges of Applied Cryoelectrics, Weilburg, Germany, May 22, 2006. Invited

Radebaugh, R., ***"Foundations of Cryocoolers,"*** One-day short course, Cryogenic Society of America, 14th International Cryocooler Conference, Annapolis, MD, June 13, 2006. Invited

Radebaugh, R., ***"Application of Cryocoolers to Superconducting Systems,"*** Half-day short course, Cryogenic society of America, Applied superconductivity Conference, Seattle WA, August 27, 2006. Invited

Radebaugh, R., ***"Proposed Rapid Cooldown Technique for Pulse Tube Cryocoolers,"*** 14th International Cryocooler Conference, Annapolis, MD June 15, 2006.

Widegran, J., ***"Protein stability via speed of sound and density measurements,"*** Exploratory Research Proposal Symposium, NIST, Gaithersburg, Maryland, February 9, 2006.

Widegren, J., ***"Distillation of Room-Temperature Ionic Lliquids,"*** Physical and Chemical Properties Division Seminar, NIST, Boulder, CO, March 9, 2006.

Widegren, J. ***"Monitoring Protein Conformation with Speed of Sound and Density Measurements,"*** 2006 Boulder Laboratories Postdoctoral Poster Symposium, National Oceanic and Atmospheric Administration, Boulder, CO, June 14, 2006.

Widegren, J. ***"Electrolytic Conductivities and Viscosities of Hydrophobic Room-Temperature Ionic Liquids."*** 16th Symp. on Thermophysical Properties, Boulder, CO, August 3, 2006.

Widegren, J., ***"Exploring the volatility of room-temperature ionic liquids,"*** 232nd National American Chemical Society Meeting, San Francisco, CA, September 10, 2006.

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

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

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

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

Development of a Pulse Tube Cryocooler for Dermatalogic Cryosurgery, CIMEX BioTech (CN-1808)

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

Method and Apparatus for the Advanced Measurement of Distillation Curves, disclosure filed 4/24/06 Thomas J. Bruno

5. SRM Activities

SRM 211e Toluene Liquid Density-Expanded Range of Temperature and Pressure, under development.

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 12 NIST Thermophysical Properties of Pure Fluids Database (Version 5.0), Support
SRD 14 NIST Mixture Property 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, new and corrected structures
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 92 International Data Series (IDS) Floppy Book Database, new release
SRD 93 NIST/TRC VLE Floppy Book Database, Support
SRD 94 LLE Floppy Book Database, new release
SRD 95 SLE Floppy Book Database, new release
SRD 96 Heats of Mixing (HE) Floppy Book Database, new release
SRD 97 Flash Points Floppy Book 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.
SRD 103 ThermoData Engine, new release
SRD 133 NIST Chemical Kinetics Database (Web), Version 7.0, Release 1.3
SRD 147 IL Thermo: Ionic Liquids Database, version 1.0, 2006, new release

TRC Tables – Hydrocarbons, Major Upgrades
TRC Tables – Non-Hydrocarbons, Major Upgrades
International Data Series, Major Upgrades

7. Calibrations

Pratt and Whitney
Hoffer Flow Controls, Inc.

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 D03.08, Thermophysics 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 Subcommittee E37.09, Biological Calorimetry (Chair)
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 E37.01.221 on Reaction Calorimetry (Chair)
Calorimetry Conference (Director)

P.E. Bradley

NASA Cryogenic Technology Working Group for Space Exploration and Transportation
Office of Naval Research Government Advisory Panel for 100mW, 4Kcryocooler Program.

T.J. Bruno

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
Member of a review panel: Quality and Utilization of Agricultural Products – Critical Fluids Applications, November 2006.
16th Symposium on Thermophysical Properties (Session Organizer)

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

AIChE Design Institute for Physical Property Data (DIPPR): Project 991 Steering Team, Project 801 Steering Team, Administrative Committee, Technical Committee
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)
Industrial Fluids Simulation Challenge Organizing Committee
Joint IAPWS/IATP Task Group on Transport Properties, chair
Joint ASME-AIChE Committee on Thermophysical Properties,

Thermo International 2006 (Joint conference of the 16th STP, 19th ICCT, and 61st CalCon), Executive Board (Vice President)
16th Symposium on Thermophysical Properties, Co-Chair
Surrogate Fuels Joint Workshop Series, Subgroups on Diesel, Gasoline, and Rocket Propellants
UN Committee of Experts on the Transport of Dangerous Goods, Ad Hoc Task Force on Fill Densities, (chair)

C.A. Gonzalez

USDA Panel of the Nanoscale Science and Engineering for Agriculture and Food Systems
Scientific Board of the NanoTEK Consortium, KRAFT, Inc. (Member).
Scientific Advisor to the Interdisciplinary Network of Emerging Science and Technology, PMUSA.

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 (Vice-Chair)
IAPWS Task Group on Fundamental Constants (Chair)
IAPWS Editorial Committee (Chair)

W.M. Haynes

ASME K-7 Standing Committee on Thermophysical Properties
Touloukian Award Committee (Vice-Chair)
THERMO International 2006 (Joint conference of the 16th STP, 19th ICCT, and 61st CalCon),
Executive Board (President)
European Conference on Thermophysical Properties, International Organizing Committee
Asian Thermophysical Properties Conference (ATPC 2007), International Program Committee

M.L. Huber

Joint IAPWS-IATP Task Group on Transport Properties
ASME K-7 Standing Committee on Thermophysical Properties (Member)
16th Symposium on Thermophysical Properties (Session Organizer)

A. Laesecke

ASTM Committee D02 on Petroleum Products and Lubricants (voting member)
ASTM Committee D0207 on Flow Properties (voting member)
Air-Conditioning and Refrigeration Technology Institute (ARTI) Project Monitoring

Subcommittee on "Near and Supercritical Heat Transfer and Flow of R-410A in Small Diameter Tubes"
Colloquium Organizing Committee, CSTL, Boulder, CO (Co-Chair)
International Association of Transport Properties
Joint IAPWS-IATP Task Group on Transport Properties

E.W. Lemmon

Transmission Measurement Committee of the American Gas Association (AGA)
International Standards Organization
Technical Committee 193
Working Group 13
Natural gas-Calculation of thermodynamic properties International Standards Organization
Technical Committee 193
Working Group 18
Natural gas-Revision of ISO 6976

P.J. Linstrom

ASTM Subcommittee E13.15, Analytical Data
OASIS Units ML Technical Committee

W.G. Mallard

Steering Committee for the NIST/EPA/NIH Mass Spectra Database
Joint Committee on Atomic and Molecular Physical Data
NFPA 400 Hazardous Chemicals Code Task Group
Organization for the Prohibition of Chemical Weapons, Chairman, Validation Group for the Central Analytical Database

J.A. Manion

Multi-Agency Coordination Committee for Combustion Research (Member)
DOE/DOD Alternative Fuels Working Group (Member)
PrIMe Executive Board (Member)
IUPAC Task Force for Thermochemistry of Selected Free Radicals (Member)

J.W. Magee

Executive Board, 16th Symposium on Thermophysical Properties/19th IUPAC Conference on Chemical Thermodynamics (Co-Chair, ICCT; Co-Chair, Poster Sessions)
Board of Directors of the SURF NIST Boulder Program (Co-Chair)
IUPAC Project on Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems (Coordinator)
IUPAC Project on Ionic Liquids Database (Coordinator)
Boulder Laboratories Diversity Council
2007 Building Tomorrow's Workplace Conference (Chair, Local Arrangements)

M.O. McLinden

ASHRAE Standing Standards Project Committee 34 – Designation and Safety Classification of Refrigerants (Member)
ASHRAE Standards Project Committee 177 – Method of Test for Fractionation Measurement of Refrigerant Blends (Member)
ASHRAE Guideline Project Committee 6 – Guideline for Format of Info for Refrigerants (member)
ASHRAE Technical Committee 3.1 – Refrigerants and Secondary Coolants (Corresponding Member)
ISO TC86/SC8/WG7 – Refrigerant Properties (Member)
3rd IIR Conference on Thermophysical Properties and Transfer Processes of Refrigerants, Boulder, CO, June 23-26, 2009 (Co-chair).

C. Muzny

NIST/TRC Tables Editorial Board
Committee to update the American Institute of Physics' Physics and Astronomy Classification Scheme **(**PACS) codes for sections 64, 65 and 66 (Equations of State and Thermal Properties sections).

P. Neta

Member, IUPAC Committee on Standard Potentials of Radicals

V.L. Orkin

NASA Panel for Data Evaluation (Member)
CCSP Atmospheric Composition Interagency Working Group

Perkins, R.A.

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

9. Editorships

T.J. Bruno
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
TRC Tables – Hydrocarbons (Editorial Board)
TRC Tables – Non-Hydrocarbons (Editorial Board)

E.W. Lemmon
TRC Tables - Hydrocarbons (Editorial Board)
TRC Tables - Non-Hydrocarbons (Editorial Board)

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

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

E.W. Lemmon
TRC Tables - Hydrocarbons (Editorial Board)
TRC Tables - Non-Hydrocarbons (Editorial Board)

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

10. Seminars

October 4, 2005
Dr. Tongfan Sun, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, "Properties of Nanofluids and Bio-oils." (Division Sponsor: Arno Laesecke)

October 6, 2005
Dr. Andrei Kazakov, Dept. of Mechanical & Aerospace Engineering, Princeton University, "Detailed Modeling of an Isolated Droplet Combustion Under Microgravity Conditions." (Division Sponsor: Michael Frenkel)

November 10, 2005
Dr. Andrei Kazakov, Dept. of Mechanical & Aerospace Engineering, Princeton University, "Detailed Modeling of an Isolated Droplet Combustion Under Microgravity Conditions." (Division Sponsor: Michael Frenkel)

December 1, 2005
Professor Dr. Cor J. Peters, Delft University of Technology, The Netherlands, "Storage of Hydrogen as Clathrate Hydrates." (Division Sponsor: Arno Laesecke)

December 2, 2005
Prof. Dr. Satish Myneni, Dept. of Geosciences, Princeton University, Princeton, NJ, Predicting the Specification of Oxoanions in Aqueous Systems. (Division Sponsor: Orkid Coskuner)

January 26, 2006
Dr. Hans-Dieter Seelig, BioServe Space Technologies, University of Colorado, Boulder, "Plants Grown In Space - Life Support Systems For Manned Space Missions." (Division Sponsor: Arno Laesecke)

January 30, 2006
Prof. Anders Nilsson, Stanford Synchrotron Radiation Laboratory, Stanford University, Sand Hill Road, CA, The Structure of Liquid Water. (Division Sponsor: Orkid Coskuner)

February 13, 2006
Dr. Stuart M. Rothstein, Dept. of Chemistry and Physics, Brock University, St. Catharines, Ontario, Canada, Separating Signal from Noise in Protein Simulation Data. (Division Sponsor: Anne Chaka)

March 9, 2006
Dr. Jason Widegren, NIST, Physical and Chemical Properties Division, Boulder, Colorado, "Distillation of Room-Temperature Ionic Liquids or Distilling the Undistillable." (Division Sponsor: Arno Laesecke)

March 10, 2006
Dr. Bernard Delley, Paul Scherrer Institute, Villigen, Switzerland, "A Medley with Dmol3." (Division Sponsor: Anne Chaka)

March 31, 2006
Dr. Juan Jose Saenz, Dept. Fisica de la Materia Condensada, Universidad Autonoma de Madrid, "Optical Interactions between Particles in Confined Geometries: Resonant Scattering and Radiation Pressure." (Division Sponsor: Carlos Gonzalez)

April 18, 2006
Dr. Wesley Henderson, Dept. of Chemistry, U.S. Naval Academy, "Delving into the Physical Properties of Ionic Liquids." (Division Sponsor: Arno Laesecke)

April 20, 2006
Dr. Yonghua Huang, Institute of Refrigeration and Cryogenics, Zhejiang University, Hangzhou, P. R. China, "Equation of State and Thermodynamic Properties of Helium-3." (Division Sponsor: Ray Radebaugh)

May 26, 2006
Dr. Nancy M. Washton, Dept. of Chemistry, Penn State University, University Park, PA, "Quantifying Reactivity at Oxide Surfaces: Experimental Nuclear Magnetic Resonance Coupled to Density Functional Theory." (Division Sponsor: Anne Chaka)

June 2, 2006
Prof. Estela Blaisten-Barojas, Computational Materials Science Center, George Mason University, Fairfax, VA, "Calcium: from Bulk to Nano and Sub-Nano Clusters." (Division Sponsor: Carlos Gonzalez)

June 8, 2006
Peter S. Pedersen, Vice President Technology, Rentech, Inc., Denver, Colorado, "The Rentech Fischer-Tropsch Process and Products", June 8, 2006. (Division Sponsor: Arno Laesecke)

June 9, 2006
Dr. Edward N. Brothers, Rice University, Houston, TX, "The Polarizability of Carbon Nanotubes." (Division Sponsor: Carlos Gonzalez).

July 10, 2006
Sebastian Freund, Institute for Thermodynamics, Helmut-Schmidt-University of the Federal Armed Forces, Hamburg, Germany, "Measurement of Convection Coefficients with Temperature Oscillation IR Thermography." (Division Sponsor: Arno Laesecke)

July 20, 2006
Dr. Karsten Meier, Institute for Thermodynamics, Helmut-Schmidt-University of the Federal Armed Forces, Hamburg, Germany, "An Instrument for Highly Accurate

Measurements of the Speed of Sound in Fluids Under High Pressures." (Division Sponsor: Arno Laesecke)

August 14, 2006
C. P. Maggi and K. O. Henderson, President and Vice President Technology, Cannon Instrument Company, State College, Pennsylvania, "Viscometry in Modern Day Commercial Applications –
Cannon Instrument Company Products and Technical Capabilities." (Division Sponsor: Arno Laesecke)

August 21, 2006
Dr. Maaike Kroon, Delft University of Technology, Delft, The Netherlands, "Combining Reactions and Separations Using Ionic Liquids and Carbon Dioxide." (Division Sponsor: Carlos Gonzalez)

August 31, 2006
Malte Brian Freund, Leibniz-University, Hannover, Germany, "Measurements and Models of Thermophysical Properties of the Binary System n-Hexadecane + Butyl Benzoate." (Sponsor: Division Arno Laesecke)

September 6, 2006
Prof. Thanh N. Truong, University of Utah, Computational Science and Engineering Online (CSE:Online): "A Cyber-Environment for Computational Chemistry." (Division Sponsor: Carlos Gonzalez)

September 22, 2006
Dr. Luciano Triguero, Royal Institute of Technology, Stockholm, Sweden, "Methodology and Computational of X-ray Spectroscopies. Applications to Small Hydrocarbons, Molecules Interacting with Surfaces." (Division Sponsor: Carlos Gonzalez).

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

ThermoInternational 2006 held in Boulder, CO, **July 30 – Aug 4, 2006**. (D.G. Friend, M. Frenkel, M. Haynes, Organizers)

16th Symposium on Thermophysical Properties (D.G. Friend, Organizer)

19-th International Conference on Chemical Thermodynamics, Boulder, Colorado, **July 30-August 4, 2006**. (M. Frenkel, R. Chirico, J. McGee, Organizers)

61-st Calorimetry Conference, Boulder, Colorado, **July 30 – August 4, 2006**. (M. Frenkel, Organizer)

Session “ThermoML: Purpose, Structure, and Applications” at the American Chemical Society Spring National Meeting, Atlanta, Georgia, **March 27, 2006**. (M. Frenkel, Organizer)

6-th (15-th) TRC Research Consortium Annual Workshop, NIST, Boulder, Colorado, **August 3, 2006**. (M. Frenkel, Organizer)

12. Other

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