

## Outputs and Interactions – Physical and Chemical Properties Division

### 1. Publications

#### 1a. Publications in Print

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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)

Andersen, W.C., Abdulagatov, A.I., and Bruno, T.J., "**The ASTM Copper Strip Corrosion Test: Application to Propane with Carbonyl Sulfide and Hydrogen Sulfide**," Energy and Fuels (in press).

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Polikhronidi, N.G., Abdulagatov, I.M., and Batyrova, R.G., "**Isochoric Heat Capacity Measurements for Metastable Fluids**," Int. J. Thermophys. (in press).

Poskrebyshev, G.A., Neta, P., and Huie, R.E., "**Temperature Dependence of the Acid Dissociation Constant of the Hydroxyl Radical**," J. Phys. Chem. A (in press).

Radebaugh, R., "**Cryogenics**," in Macmillan Encycl. Chem., Macmillan Pubs., New York, NY (in press).

Restrepo-Cossio, A., Gonzalez, C.A., and Mari, F., "**Comparative Ab Initio Treatment (Hartree-Fock, Density-Functional Theory, MP2 and Quadratic Configuration Interactions) of the Cycloaddition of Phosphorus Ylides with Formaldehyde**," J. Phys. Chem. A (in press).

Steele, W.V., Chirico, R.D., Nguyen, A., and Knipmeyer, S.E., "**II. The Thermodynamic Properties of 2,3-Dihydrobenzo[b]thiophene**," J. Chem. Thermodynamics (in press).

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).

Watts, L.A., "**Vapor-Liquid Equilibrium of Mixed Solvent Electrolyte Solutions: Measurements and Models**," Proc. Spectrum 2002 Conf., Reno, NV, August 4-8, 2002 (in press).

Yan, X.J., Dong, Q., Hong, X.R., and Frenkel, M., "**Reliability Analysis of Group Contribution Methods in Predicting Critical Temperatures of Organic Compounds**," Ind. Eng. Chem. Res. (in press).

Yi, X., Portnoy, J., and Pellegrino, J.J., ***“Improvement of Sample/IRE Contact Through Penetrant Fluid Pressure in ATR-FTIR Spectroscopy for Diffusion Measurements,”*** J. Polymer Sci., Part B: Polymer Physics Ed. (in press).

Yoon, Y., Amy, G., Cho, J., and Pellegrino, J., ***“Systematic Bench-scale Assessment of Perchlorate ( $\text{ClO}_4^-$ ) Rejection Mechanisms by Nanofiltration and Ultrafiltration Membranes,”*** Separation Sci. Tech. (in press).

## **2. Talks**

Allison, T.C., ***“Thermodynamics in the Experimental Kinetics and Thermodynamics Group,”*** First (Tenth) NIST/TRC Consortium, Boulder, CO, November 1, 2001.

Allison, T.C., ***“Suggestions on the Content and Structure of the Web Version of the Thermodynamics Database for Free Radicals,”*** Budapest, Hungary, September 16, 2002.

Andersen, W.C., ***“Equilibria and Kinetics of Multiphase Systems: Examples from Supercritical Fluids and Fuel Gas,”*** NIST, Boulder, CO, April 26, 2002.

Archer, D.G., ***“NIST – What It Is; What It Does,”*** Drexel University, Philadelphia, PA, May 31, 2002. Invited.

Archer, D.G., ***“Thermodynamic Properties of Water and Electrolyte Solutions at Cold and Supercooled Temperatures,”*** Drexel University, Philadelphia, PA, May 31, 2002. Invited.

Archer, D.G., ***“New NIST-Traceable Standards for Calibration and Validation of Differential Scanning Calorimetry,”*** 30<sup>th</sup> North American Thermal Analysis Society Conference, Pittsburgh, PA, September 25, 2002.

Arman, B., Larson, K., Radebaugh, R., and Bradley, P.E., ***“Pulse Tube Refrigeration for Hydrogen Densification,”*** 12<sup>th</sup> International Cryocooler Conference, MIT, Cambridge, MA, June 19, 2002.

Bruno, T.J., ***“Differential Adsorption of Odorant Compounds: A Critical Piece of the Fading Puzzle,”*** Gas Technology Institute Gas Quality and Odorization Conference, Orlando, FL, September 29, 2002.

Bruno, T.J., ***“The Copper Strip Corrosion Test: Background, Pitfalls and Improvements,”*** Gas Technology Institute Gas Quality and Odorization Conference, Orlando, FL, September 30, 2002. Invited.

Chaka, A.M., ***“Predicting Thermophysical Properties of Fluids by Molecular Simulation,”*** AIChE 2001 Annual Meeting, Reno, NV, November 5, 2001. Invited.

Chaka, A.M., ***“Effect of the Environment on Stoichiometry and Structure of Oxide Surfaces,”*** AIChE 2001 Annual Meeting, Reno, NV, November 6, 2001.

Chaka, A.M., ***“A Virtual Measurement System for Atomistic Simulations,”*** Workshop on Polarizability in Biomolecular Simulations, Snowbird, Utah, December 14, 2001. Invited.

Chaka, A.M., ***“Performance Issues for Lubricant and Fuel Additives,”*** Air Force Research Laboratory, Wright-Patterson AFB, OH, January 28, 2002. Invited.

Chaka, A.M., ***“Stabilization Mechanisms for the Oxygen-Terminated Alpha-Cr<sub>2</sub>O<sub>3</sub> (0001) Surface,”*** American Physical Society Meeting, Indianapolis, IN, March 22, 2002. Invited.

Chaka, A.M., ***“Quantum Mechanics and the Automobile,”*** Kansas State University, Department of Physics, Manhattan, KS, March 28, 2002. Invited

Chaka, A.M., ***“Current and Future Needs for Improvements in Electron Correlation Methodology: The Industrial Perspective,”*** 23<sup>rd</sup> National Meeting of the American Chemical Society, Orlando, FL, April 11, 2002. Invited.

Chaka, A.M., ***“The Effect of the Environment on Aluminum, Iron, and Chromium Oxide Surfaces,”*** Department of Physics, Tulane University, New Orleans, LA, April 12, 2002. Invited.

Chaka, A.M., ***“Industrial Applications of Computational Chemistry at NIST,”*** Dow Chemical, Midland, MI, May 29, 2002. Invited.

Chaka, A.M., ***“Prediction of Surface & Interface Properties from First Principles,”*** Alcoa Technical Center, Monroe, PA, June 27, 2002. Invited.

Chaka, A.M., ***“Computational Chemistry Initiatives at NIST for Industrial Applications,”*** BP Amoco Chemicals, Naperville, IL, July 24, 2002. Invited.

Chaka, A.M., ***“How General are Hybrid Functionals?”*** Sandia National Laboratories Workshop on Quantum Mechanical Techniques: Exchange-Correlation Functionals in Density Functional Theory, Albuquerque, NM, August 14, 2002. Invited.

Chaka, A.M., ***“Surface Structure and Properties in a Complex Environment,”*** Chemistry Department, Duquesne University, Pittsburgh, PA, September 27, 2002. Invited.

Chirico, R.D., ***“TRC Data Activities, Including Guided Data Capture,”*** National Petroleum Technology Office, Department of Energy, Tulsa, OK, May 2, 2002.

Chirico, R.D., Diky, V.V., Wilhoit, R.C., Dong, Q., and Frenkel, M., ***“Data Management within the NIST/TRC Data Entry Facility: Guided Data Capture Software,”*** Calorimetry Conference, New Brunswick, NJ, August 14, 2002.

Dong, Q., ***“Data Quality Assurance Project Report: Part II. Data Analysis and Processing for Critical Constants and Normal Boiling Points,”*** Second (Eleventh) NIST/TRC Consortium Annual Workshop, Boulder, CO, June 27, 2002.

Dong, Q., Yan, X., Chirico, R.D., Wilhoit, R.C., and Frenkel, M., ***“Knowledge Management in Physicochemical Property Databases - Knowledge Recovery and Retrieval of NIST/TRC SOURCE Data System,”*** CODATA 2002 Conference, Montreal, Canada, September 30, 2002.

Dong, Q., ***“Reliability of Uncertainty Assignments: A Critical Issue in Generating Recommended Data from a Large Set of Experimental Physicochemical Data,”*** CODATA 2002 Conference, Montreal, Canada, September 30, 2002. Invited.

Fahr, A., ***“Recent Laboratory Results Relevant to the Photochemistry/Kinetics of Planetary Atmospheres,”*** Planetary Sciences Seminar Series, NASA/Goddard Space Flight Center, Greenbelt, MD, December 20, 2001.

Frenkel, M., ***“Overview of TRC Activities over 2000-2001 Period,”*** First (Tenth) NIST/TRC Consortium Annual Workshop, Boulder, CO, November 1, 2001.

Frenkel, M., ***“Striving for Data Quality: New Challenges in the New Era of the Chemical Process Design,”*** International Congress for Chemistry and Environment, Indore, India, December 16, 2001. Invited.

Frenkel, M., ***“NIST/TRC Research Activities and the Scope of the NIST/TRC Consortium,”*** Hyprotech, LTD, Calgary, Alberta, Canada, March 1, 2002.

Frenkel, M., ***“NIST/TRC Research Activities and the Scope of the NIST/TRC Consortium,”*** National Petroleum Technology Office, Department of Energy, Tulsa, OK, May 2, 2002.

Frenkel, M., ***“Thermophysical and Thermochemical Property Data Dynamic Evaluation: Concept and Reality,”*** 5<sup>th</sup> International Symposium of the ESQIE, Mexico City, Mexico, May 30, 2002. Invited.

Frenkel, M., ***“Overview of TRC Activities over 2001-2002 Period,”*** Second (Eleventh) NIST/TRC Consortium Annual Workshop, Boulder, CO, June 27, 2002.

Frenkel, M., ***“Building a New Data Pipeline: From Data Producers to Data Users,”*** 57<sup>th</sup> Calorimetry Conference, New Brunswick, NJ, August 14, 2002. Invited.

Frenkel, M., Chirico, R.D., Diky, V.V., Dong, Q., Hardin, G.R., Hong, X., Stevenson, R.A., Yan, X., and Wilhoit, R.C., ***“NIST/TRC Databases for Chemistry and Engineering,”*** 17<sup>th</sup> IUPAC Conference on Chemical Thermodynamics, Rostock, Germany, July 31, 2002.

Frenkel, M., Dong, Q., Yan, X., Hong, X., Chirico, R.D., Hardin, G.R., and Wilhoit, R.C., ***“TRC: From NBS to NIST – 60 Years in Retrospective and Many More in Perspective,”*** AIChE Annual Meeting, Reno, NV, November 6, 2001.

Friend, D.G., Lemmon, E.W., and Huber, M.L., “*Sound Speed Calculations: AGA8 and Beyond*,” American Gas Association, Operating Section Fall Committee Meetings, Phoenix, AZ, October 1, 2001.

Friend, D.G. and Huber, M.L., “*Overview of the Theory and Modeling of Fluids Group at NIST*,” First (Tenth) NIST/TRC Consortium Meeting, Boulder, CO, November 1, 2001.

Gonzalez, C.A., “*Theoretical Studies of Electrical Conductance in Molecular Wires*,” 3<sup>rd</sup> Workshop on Electronic Transport in Mesoscopic Systems,” Caracas, Venezuela, December 6, 2001. Invited.

Gonzalez, C.A., “*A Chemist’s Perspective at the Behavior of Negative Differential Resistance in Molecular Systems*,” Venezuelan Association of Physics, Caracas, Venezuela, December 14, 2001. Invited.

Gonzalez, C.A., “*Molecular Electronics at NIST*,” Special Seminar Series, Department of Chemistry, University of Akron, Akron, OH, March 8, 2002.

Gonzalez, C.A., “*On the Transferability of Hybrid Density Functional*,” 223<sup>rd</sup> ACS National Meeting, Orlando, FL, April 8, 2002.

Gonzalez, C.A., “*Practical Aspects of Computational Kinetics*,” 223<sup>rd</sup> ACS National Meeting, Orlando, FL, April 10, 2002.

Gonzalez, C.A., “*Current Challenges in Computational Kinetics*,” Department of Chemistry, University of Lille, France, July 15, 2002.

Gonzalez, C.A., “*Computational Chemistry Studies of Molecular Electronics at NIST*,” Department of Chemistry, University of Chile, Santiago, Chile, August 15, 2002.

Gonzalez, C.A., “*Performance of Hybrid Density Functionals*,” Department of Physics, University of Chile, Santiago, Chile, August 17, 2002.

Harkless, J.A., “*Quantum Monte Carlo Studies of the Electronic Structure of Ozone and Atomization of Alcohols*,” NOBCCChE 2002 Annual Conference, New Orleans, LA, March 25, 2002.

Harvey, A., “*A Century of Fluid Property Research at NBS/NIST*,” AIChE Annual Meeting, Reno, NV, November 7, 2001.

Harvey, A., “*Thermodynamic Properties of Moist Gases from Ab Initio Potentials*,” AIChE Annual Meeting, Reno, NV, November 7, 2001.

Harvey, A., ***“U.S. Implementation of New International Water Property Standards,”*** 2001 ASME International Mechanical Engineering Congress, New York, NY, November 15, 2001. Invited.

Harvey, A., ***“Thermodynamic Properties of Moist Gases from First Principles,”*** International Association for the Properties of Water and Steam Symposium on Advances in Basic and Applied Research in Hydrothermal Systems, Buenos Aires, Argentina, July 24, 2002. Invited.

Harvey, A., ***“Thermodynamic Properties of Moist Gases from First Principles,”*** Department of Chemical Engineering, University of Wyoming, Laramie, WY, September 16, 2002. Invited.

Haynes, W.M., ***“Overview of 14th Symposium on Thermophysical Properties,”*** 2001 ASME International Mechanical Engineering Congress, New York, NY, November 15, 2001. Invited.

Haynes, W.M. and Frenkel, M., ***“Proposal for 19<sup>th</sup> International Conference on Chemical Thermodynamics,”*** IUPAC Commission 1.2 on Chemical Thermodynamics Meeting, Rostock, Germany, July 28, 2002. Invited.

Huie, R.E., ***“Environmental Impact of New Chemical Agents for Fire Suppression,”*** FY2001 Next Generation Program Annual Meeting, Gaithersburg, MD, December 17, 2001. Invited.

Huie, R.E., ***“Reactivity Research at the National Institute of Standards and Technology,”*** Reactivity Research Working Group, Research Triangle Park, NC, January 16, 2002. Invited.

Huie, R.E., ***“Effect of Bromine Substitution on the Lifetimes and Ozone Depletion Potentials of Organic Compounds,”*** Halon Options Working Conference, Albuquerque, NM, April 30, 2002.

Huie, R.E., ***“Redox Potentials We Have Determined,”*** IUPAC Task Group on Standard Potentials of Radicals, Braunwald, Switzerland, May 31, 2002. Invited.

Huie, R.E., ***“Database Activities at the National Institute of Standards and Technology,”*** U.S.-Hungary Thermodynamics Working Group, Budapest, Hungary, September 1, 2002. Invited.

Irikura, K.K., ***“Bootstrapping the Databases: New Methods for Computational Thermochemistry,”*** NIST/TRC Consortium Workshop, Boulder, CO, November 1, 2001.

Irikura, K.K., ***“An Inexpert System for Discovering Chemical Reactions,”*** Meeting of the Eastern States Section of Combustion Institute, Hilton Head, SC, December 4, 2001.

Irikura, K.K., ***“Isopotential Searching for Discovering Chemical Reactions,”*** 223<sup>rd</sup> ACS National Meeting, Orlando, FL, April 8, 2002.

Irikura, K.K., ***“New Reaction Pathways in the Decomposition of RDX,”*** Reaction Mechanisms Conference, Columbus, OH, June 29, 2002.

Jacobsen, R.T and Lemmon, E.W., "**Natural Gas Property Standards**," 2001 AIChE Annual Meeting, Reno, NV, November 7, 2001.

Johnson, III, R.D., "**NIST Computational Chemistry Comparison and Benchmark Database**," NIST/TRC Consortium Workshop, Boulder, CO, November 1, 2001.

Kirklin, D.R., "**Certification of NIST SRM 217d Isooctane – Heat of Combustion**," 29<sup>th</sup> Annual Conference of the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, New Orleans, LA, March 25, 2002. Invited.

Kurylo, M.J., "**Arctic Ozone Depletion: How Do We Measure Current Research Progress and Chart a Path for the Future?**" Workshop on Arctic Ozone Loss, Alfred Wegener Institute for Polar and Marine Research, Potsdam, Germany, March 4, 2002. Invited.

Kurylo, M.J., "**The Network for the Detection of Stratospheric Change and Its Connection to WMO's Global Atmospheric Watch**," Fifth Meeting of Ozone Research Managers of the Parties to the Vienna Convention for the Protection of the Ozone Layer, Geneva, Switzerland, March 25, 2002. Invited.

Kurylo, M.J., "**The 2002 Scientific Assessment of Ozone Depletion: Scope and Status Report**," Fifth Meeting of Ozone Research Managers of the Parties to the Vienna Convention for the Protection of the Ozone Layer, Geneva, Switzerland, March 25, 2002. Invited.

Kurylo, M.J., "**The U.S. Program on Ozone and Ground-Level UV Research and Monitoring**," Fifth Meeting of Ozone Research Managers of the Parties to the Vienna Convention for the Protection of the Ozone Layer, Geneva, Switzerland, March 26, 2002. Invited.

Kurylo, M.J., "**The Network for the Detection of Stratospheric Change: Investigating the Ozone Layer and Its Links to Global Climate**," Spring Meeting of the American Geophysical Union, Washington, D.C., May 31, 2002. Invited.

Kurylo, M.J., "**Rate Constants for the Reactions of OH with Several Halogenated Hydrocarbons Over the Temperature Range 210 K – 480 K**," 17<sup>th</sup> International Symposium on Gas Kinetics, Essen, Germany, August 26, 2002.

Laesecke, A., "**Connect Virtual Design with Physical Reality – NIST Sources of Accurate Fluid Properties Information**," Department of Chemical Engineering, Iowa State University, Ames, Iowa, November 29, 2001. Invited.

Laesecke, A., "**Sub- and Supercritical Viscosity Measurements of Ten Binary and Ternary Hydrofluorocarbon Mixtures with a Torsional-Crystal Viscometer**," 3<sup>rd</sup> IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons held during the 17<sup>th</sup> International Conference on Chemical Thermodynamics, Rostock, Germany, July 29, 2002.

Laesecke, A., "***Halocarbons I: Methane Derivatives. Our Evolving View of Molecular Structure,***" 3<sup>rd</sup> IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons held during the 17<sup>th</sup> International Conference on Chemical Thermodynamics, Rostock, Germany, July 29, 2002.

Laesecke, A., "***Understanding Mixture Viscosity by Means of Molecular Modeling,***" Department of Chemical Engineering, UMIST, Manchester, UK, August 9, 2002. Invited.

Lemmon, E.W., "***Thermophysical Property Measurement and Correlation Techniques at NIST,***" Thermophysical Properties of Humid Air and Combustion Gases Workshop, Baden-Dattwil, Switzerland, October 1, 2001.

Lemmon, E.W. and Jacobsen, R.T., "***A Mixture Model for Dew Points of Natural Gases with Heavy Components,***" 81st Annual GPA Convention, Dallas, TX, March 12, 2002.

Lemmon, E.W. and McLinden, M.O., "***Method for Estimating Mixture Equation of State Parameters,***" Thermophysical Properties and Transfer Processes of New Refrigerants Conference, Paderborn, Germany, October 3, 2001. Invited.

Lewis, M.A. and Radebaugh, R., "***Measurement of Heat Conduction Through Bonded Regenerator Matrix Materials,***" 12<sup>th</sup> International Cryocooler Conference, MIT, Cambridge, MA, June 19, 2002.

Linstrom, P.J., "***The NIST Chemistry WebBook,***" NIST/TRC Consortium Workshop, Boulder, CO, November 1, 2001.

Linstrom, P.J., "***The NIST Chemistry WebBook,***" 17<sup>th</sup> IUPAC Conference on Chemical Thermodynamics, Rostock, Germany, July 30, 2002.

Linstrom, P.J., "***Combining Heterogeneous Physical Property Data Sets,***" 224<sup>th</sup> ACS National Meeting, Boston, MA, August 19, 2002.

Linstrom, P.J., "***Expressing Measurements and Chemical Systems for Physical Property Data,***" CODATA 2002 Conference, Montreal, Canada, September 30, 2002. Invited.

Magee, J.W., "***Thermodynamic Properties of Natural Gas Mixtures,***" 5<sup>th</sup> International Symposium of the ESQIE, Instituto Politecnico Nacional, Mexico City, Mexico, May 30, 2002. Invited.

Magee, J.W., "***Experimental Properties of Fluids Group Overview,***" Physical and Chemical Properties Division Seminar, Boulder, CO, June 25, 2002. Invited.

Mallard, W.G., "***Thermochemical, Thermophysical and Spectroscopic Data Activities in the Reference Data Group at Gaithersburg,***" NIST/TRC Consortium Workshop, Boulder, CO, November 2, 2001.

Mallard, W.G., ***“XML Projects at the National Institute of Standards and Technology (NIST),”*** IUPAC Meeting on XML in Chemistry, Cambridge, UK, January 24, 2002.

Miller, K.E., ***“Adsorption of Fuel Gas Odorants on Surrogate Soil Surfaces,”*** Chemistry Department, The Metropolitan State College of Denver, Denver, CO, March 8, 2002. Invited.

Miller, K.E., ***“Measurements at the Boundary: Investigation of Interfacial Properties of Industrial Systems,”*** NIST, Boulder, CO, April 5, 2002.

Miller, K.E. and Bruno, T.J., ***“Heat of Adsorption and Interaction Determinations of Fuel Gas Odorants on Surrogate Soil Surfaces by Gas Chromatography,”*** 39<sup>th</sup> Annual Meeting of the Clay Minerals Society, Boulder, CO, June 12, 2002.

Mountain, R.D., ***“Introduction to Molecular Dynamics,”*** 13<sup>th</sup> Advanced Cement Based Materials/NIST Computer Modeling Workshop, NIST, Gaithersburg, MD, June 13, 2002.

Mountain, R.D., ***“A Molecular Dynamics Sampler,”*** Physical and Chemical Properties Division Colloquium, Gaithersburg, MD, June 25, 2002.

Muzny, C.D., Hedden, R., and Bauer, B., ***“High-Throughput Membrane Transport Analysis,”*** Combinatorial Approaches for New Materials Discovery, San Diego, CA, January 23, 2002.

Muzny, C.D., Scott, P., Hedden, R., Alamgir, K., and Pellegrino, J., ***“High-Throughput-Experimentation (HTE) for Measurement of Molecular Transport through Membranes,”*** International Congress on Membranes and Membrane Processes, Toulouse, France, July 9, 2002.

Neta, P., ***“Pulse Radiolysis Measurement of One-Electron Reduction Potentials in Aqueous Solutions,”*** Symposium on “Electron Transfer in DNA,” Max-Planck Institute of Radiation Chemistry, Mulheim, Germany, June 7, 2002. Invited.

Neta, P., ***“Pulse Radiolysis Studies of Reaction Kinetics in Ionic Liquids,”*** Symposium on “Ionic Liquids as Green Solvents: Progress and Prospects,” 224<sup>th</sup> ACS National Meeting, Boston, MA, August 22, 2002. Invited.

Orkin, V.L., ***“Atmospheric Fate of Short-Lived Hydrohalocarbons - Bromofluoroalkenes, Fluoroalkenes, and a Bromofluoroether: OH Reactions and UV Spectra,”*** Partners in Environmental Technology, Technical Symposium & Workshop, Washington D.C., November 27, 2001.

Orkin, V.L., ***“Rate Constants for the Reactions between OH Radicals and Hydrocarbons over the Extended Temperature Range,”*** Mass Spectrometry Conference in Chemical Physics, Biophysics, and Environmental Sciences, Zvenigorod, Moscow, Russia, April 25, 2002. Invited.

Orkin, V.L., ***“Rate Constant Measurements for Reactions of Hydroxyl Radicals with Halogenated Alkanes, Alkenes and Ether from 210 K to 480 K,”*** XXV Informal Conference on Photochemistry, University of Miami, Coral Gables, FL, June 3, 2002.

Orkin, V.L., "**Absorption Cross Sections of Low Molecular Weight Silicon Containing Organic Compounds at Lithography Relevant Wavelengths,**" Extraction's Contamination Control and Monitoring Roadmap for Lithography Workshop, Newport, RI, June 17, 2002. Invited.

Orkin, V.L., "**Atmospheric Fate of Selected Halogenated Hydrocarbons: Reactivity towards OH from 210 K to 480 K and UV Spectra,**" 10<sup>th</sup> Scientific Conference of the International Association of Meteorology of Atmospheric Sciences Commission for Atmospheric Chemistry and Global Pollution and 7<sup>th</sup> Scientific Conference of the International Global Atmospheric Chemistry Project, Crete, Greece, September 18, 2002.

Radebaugh, R., "**Introduction to Cryocoolers,**" Military and Commercial Applications of Low-Cost Cryocoolers (MCALC-III), San Diego, CA, October 25, 2001. Invited.

Radebaugh, R., "**Cryosurgical Applications of Cryocoolers,**" Military and Commercial Applications of Low-Cost Cryocoolers (MCALC-III), San Diego, CA, October 26, 2001. Invited.

Radebaugh, R., "**Foundations of Cryocoolers,**" Cryogenic Society of America, One-Day Short Course, MIT, Cambridge, MA, June 17, 2002. Invited.

Radebaugh, R., "**Microscale Heat Transfer at Low Temperatures,**" NATO Advanced Study Institute on Low Temperature and Cryogenic Refrigeration, Cesme, Turkey, June 28, 2002. Invited.

Radebaugh, R., "**Pulse Tube Cryocoolers,**" NATO Advanced Study Institute on Low Temperature and Cryogenic Refrigeration, Cesme, Turkey, July 2, 2002. Invited.

Radebaugh, R., Bradley, P.E., Arman, B., and Bonaquist, D., "**Pulse Tube Refrigerator for Neon Liquefaction,**" 12<sup>th</sup> International Cryocooler Conference, MIT, Cambridge, MA, June 19, 2002.

Rainwater, J.C., "**Topics in SLE: Fluctuating Cell Model, Sulfur Dioxide, and Alternative to Frenkel-Ladd,**" AIChE Annual Meeting, Reno, NV, November 7, 2001.

Stein, S.E., "**Towards the Development of a Standard Chemical Identifier,**" Molecular Design Limited, San Leandro, CA, October 8, 2001. Invited.

Stein, S.E., "**The NIST Mass Spectrometry Data Program,**" NIST Mass Spectral Library Distributors Meeting, PITTCON 2002, New Orleans, LA, March 19, 2002.

Stein, S.E., "**The IUPAC Chemical Identifier,**" CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry, Columbus, OH, July 1, 2002. Invited.

Stein, S.E., "**A XML Namespace for IUPAC,**" CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry, Columbus, OH, July 2, 2002. Invited.

Stein, S.E., *“Comparing Mass Spectra: When Do They Match?”* 14<sup>th</sup> International Conference on Racing Analysts and Veterinarians, Orlando, FL, July 7, 2002. Invited.

Tsang, W., *“Chemical Kinetic Database Requirements for the Real Fuels,”* Technical Meeting of the Eastern States Section of the Combustion Institute, Hilton Head, SC, December 5, 2001. Invited.

Tsang, W., *“Important Factors in the Development of Combustion Mechanisms for Realistic Fuels,”* 40<sup>th</sup> Aerospace Sciences Meeting and Exhibit, Reno, NV, January 15, 2002.

Tsang, W., *“Fundamental Issues in the Incineration of Chlorinated and Fluorinated Organics,”* DuPont Experimental Station, Wilmington, DE, March 6, 2002. Invited.

Tsang, W., *“Progress Report – Database for Soot Formation in Heptane Combustion,”* Wright-Patterson AFB, OH, March 21, 2002.

Tsang, W., *“Important Issues in the Mechanism of JP-10 Decomposition,”* 15<sup>th</sup> ONR Propulsion Meeting, Washington, D.C., August 7, 2002.

Tsang, W., *“Some Issues on the Development of a Kinetic Model for PAH Formation from Heptane Combustion,”* 224<sup>th</sup> ACS National Meeting, Boston, MA, August 22, 2002.

Tsang, W., *“Decomposition and Isomerization of Some Alkyl Radicals,”* 17<sup>th</sup> International Symposium on Gas Kinetics, Essen, Germany, August 26, 2002.

Watts, L., *“Vapor-Liquid Equilibrium of Mixed Solvent Electrolyte Solutions: Measurements and Models,”* Spectrum 2002, American Nuclear Society, Reno, NV, August 7, 2002.

Yan, X., Dong, Q., Hong, X., Chirico, R.D., and Frenkel, M., *“Prototype of TRC Integrated Information System for Physicochemical Properties of Organic Compounds: Evaluated Data, Models, and Knowledge,”* CODATA 2002 Conference, Montreal, Canada, September 30, 2002.

### **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 (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 Dermatologic Cryosurgery  
**CIMEX BioTech (CN-1808) (CRADA)**

Praxair Pulse Tube Liquefier, R. Radebaugh  
**Praxair, Inc. (CN 1677) (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. Patents**

Bruno, T.J. and Lagalante, A.F., "Method for the Removal of Carbonyl Sulfide from Liquefied Petroleum Gas (LPG)," U.S. Patent Number 6,334,949 (1/1/02).

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**

SRM 217d 2, 2, 5 – Trimethylpentane (Iso-octane), Renewal, In Progress, Certificate in 2003

## Thermal Analysis Suite

- SRM 2233 Cyclopentane, New, Certificate Issued in FY2002
- SRM 2234 Gallium, New, Certificate Issued in FY2002
- SRM 2235 Bismuth, New, In Progress, Certificate in 2003
- SRM 2236 Silver Bromide, New, In Progress, Certificate in 2003

Fluid Density Over Wide Ranges of Temperature and Pressure, New SD Project  
Macropore Size Distribution Standard Disk (Membrane), New SD Project

### **5b. SRD Activities**

- SRD NIST Chemical Kinetics Mechanism Database CKMech  
hppt://srdata.nist.gov/ckmechx/
- SRD 1/1ANIST/EPA/NIH Mass Spectral Library (Update: July 2002)
- 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, Upgrade in Progress
- 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
- 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

### **5c. Calibrations**

Pratt and Whitney  
Hoffer Flow Controls, Inc.

## **6. Committee Assignments**

### **T.C. Allison**

Collaboratory for Multi-Scale Chemical Sciences

### **D.G. Archer**

ASTM Committee E37 on Thermal Measurements (Membership Secretary)

ASTM Subcommittee E37.02, Standard Reference Materials for Thermal Measurements (Chair)  
ASTM Subcommittee E37.90, Executive Subcommittee (Member)  
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)

**P.E. Bradley**

NASA Cryogenic Technology Team for Exploration 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

**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

**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)  
AIChE Design Institute for Physical Property Data (DIPPR): Project 991 Steering Team, Project 801 Steering Team, Administrative Committee, Technical Committee  
Fifteenth Symposium on Thermophysical Properties (Organizer and Co-Chair)

**A.H. Harvey**

ASME Research and Technology Committee on Water and Steam in Thermal Systems  
ASME Research Subcommittee on the Properties of Water and Steam (Chair)  
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)

**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  
International Advisory Committee, 17<sup>th</sup> IUPAC Conference on Chemical Thermodynamics  
International Scientific Committee, 17<sup>th</sup> IUPAC Conference on Chemical Thermodynamics  
International Organizing Committee, European Conference on Thermophysical Properties  
Scientific Programme Committee, 16<sup>th</sup> European Conference on Thermophysical Properties  
International Advisory Committee, 6<sup>th</sup> International Asian Thermophysical Properties  
Conference

**R.E. Huie**

TSCA Interagency Testing Committee  
NASA Panel for Data Evaluation  
Titular Member, IUPAC Commission on Chemical Kinetics  
IUPAC Task Group on Standard Potentials of Radicals

**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**

Colloquium Organizing Committee, CSTL, Boulder, CO (Co-Chair).  
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).  
Scientific Organizing Committee, 3<sup>rd</sup> IUPAC Workshop on Thermochemical, Thermodynamic,  
and Transport Properties of Halogenated Hydrocarbons during the 17<sup>th</sup> International  
Conference on Chemical Thermodynamics, July 28-August 2, 2002, Rostock, Germany.  
Invited.

**E.W. Lemmon**

Transmission Measurement Committee of the American Gas Association (AGA)

**B. Louie**

University of Colorado Chemical Engineering Advisory Committee

**J.W. Magee**

IUPAC Project on Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the  
Development of Standardized Systems (Coordinator)

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

**P. Neta**

Member, IUPAC Committee on Standard Potentials of Radicals

**V. Orkin**

NASA Panel for Data Evaluation

**R.A. Perkins**

ASTM Committee D34 on Waste Management  
International Association for Transport Properties

**R. Radebaugh**

International Cryocooler Conference, Inc., Advisory Committee  
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**

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)

**7. Editorships**

**T.J. Bruno**

Journal of Process Analytical Chemistry (Associate Editor)

**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)

**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 (Advisory Board)  
TRC Tables – Hydrocarbons (Editorial Board)  
TRC Tables – Non-Hydrocarbons (Editorial Board)  
Guest Editor of a Special Issue of “Fluid Phase Equilibria” with contributions to the 3<sup>rd</sup> IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons during the 17<sup>th</sup> International Conference on Chemical Thermodynamics, July 28-August 2, 2002, Rostock, Germany. Jointly with Ulrich K. Deiters (Cologne, Germany).

**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)

**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 15, 2001**

J.S. Wilkes, Department of Chemistry, U.S. Air Force Academy, USAF Academy, CO, "Ionic Liquids in Perspective." (Division Sponsor: R.E. Huie)

**November 27, 2001**

S.R. Gwaltney, Head-Gordon Group, University of California, Berkeley, CA, "Inner Sphere Electron Transfer Complexes." (Division Sponsor: A.M. Chaka)

**December 20, 2001**

V.K. Shen, Department of Chemical Engineering, Princeton University, Princeton, NJ, "Computational and Theoretical Study of Fracture in Liquids and Glasses." (Division Sponsor: A.M. Chaka)

**January 7, 2002**

D.M. Matheu, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, "Screening of Pressure-Dependent Reactions: Reliable  $k(T,P)$  for Automated Mechanism Generation." (Division Sponsor: A.M. Chaka)

**January 31, 2002**

I. Carmichael, Radiation Laboratory, University of Notre Dame, South Bend, IN, "Early Events in the Radiolysis of Amino Acids: Insights from Theory." (Division Sponsor: A.M. Chaka)

**February 25, 2002**

S. Matsika, Department of Chemistry, Johns Hopkins University, Baltimore, MD, "Conical Intersections in Non-Adiabatic Processes." (Division Sponsor: A.M. Chaka)

**March 11, 2002**

B. Delley, Paul Scherrer Institute, Villigen, Switzerland, "Molecular, Surface and Bulk Electronic Properties from Dm013 DFT Studies." (Division Sponsor: A.M. Chaka)

**April 17, 2002**

J.L. Beauchamp, Department of Chemistry, California Institute of Technology, Pasadena, CA, "Chemistry of Highly Charged Nanodroplets." (Division Sponsor: K.K. Irikura)

**April 17, 2002**

Alexei Alexandrov, Gosstandard of Russia, Russian Research Center for Standardization, Information and Certification of Materials, Moscow, Russia, "Development of a Computer

Program for a Calculation of Thermophysical Properties of Water and Steam.” (Division Sponsor: M. Frenkel)

**April 17, 2002**

Alexei Alexandrov, Gosstandard of Russia, Russian Research Center for Standardization, Information and Certification of Materials, Moscow, Russia, “Thermophysical Data Evaluation Activities in Russia.” (Division Sponsor: M. Frenkel)

**May 24, 2002**

Clare McCabe, Colorado School of Mines, Golden, CO, “Molecular Modeling of Phase Equilibria and Transport Properties,” (Division Sponsor: A. Laesecke).

**June 7, 2002**

Leslie V. Woodcock, Department of Chemistry, UMIST, Manchester, UK, “Molecular Simulations and a New Thermodynamic Approach to Nanotechnology,” (Division Sponsor: A. Laesecke).

**July 19, 2002**

David M. French, Aspen Resources Ltd., Inc., Golden, CO, “Regulatory Compliance in a Post Modern Era of Lowered Societal Expectations, and Other Drivel,” July 19, 2002 (Division Sponsor: T. Bruno).

**August 14, 2002**

P.S. Raghavan, Department of Chemistry, Madras Christian College, Tambaram, Chennai, India, “Chemistry of Surfactants.” (Division Sponsor: R.E. Huie)

**September 20, 2002**

L. Shilkrot, Division of Engineering, Brown University, Providence, RI, “Coupled Atomistic and Discrete Dislocation Plasticity.” (Division Sponsor: A.M. Chaka)

**September 20, 2002**

Maciej Radosz, Department of Chemical and Petroleum Engineering, University of Wyoming, Laramie, WY, “Solid-Fluid Phase Equilibria in Compressed Polymer Solutions,” (Division Sponsor: A. Harvey).

**September 25, 2002**

Werner Martienssen, Johann Wolfgang Goethe University Frankfurt/Main, Germany, “The Role of Scientific Data in a Complex World.” (Division Sponsor: M. Frenkel)

**September 25, 2002**

Rainer Poerschke, Landolt-Börnstein, Springer-Verlag, Berlin, Germany, “Physicochemical Data in Landolt-Börnstein Online.” (Division Sponsor: M. Frenkel)

## **September 27, 2002**

Joan F. Brennecke, Department of Chemical Engineering, University of Notre Dame, South Bend, IN, "Thermophysical Properties of Ionic Liquids: Experiments and Simulations," (Division Sponsor: A. Laesecke)

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

First Industrial Fluid Properties Simulation Challenge, COMSEF of AIChE sponsor (R.D. Mountain, A. Chaka. D. Friend, R. Johnson on organizing committee).

## **10. Other**

### **T.J. Bruno**

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

### **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.

### **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.

### **W. Tsang**

Scientific Advisory Board – Reaction Engineering on models for the incineration of chemical agents.  
Scientific Advisory Board – Collaboratory for Multi-scale Chemical Science (CMCS) – DOE,

development of an informatics based approach to the synthesis of multi-scale information.  
Consultant – Critical Infrastructure Assurance Office (CIAO): Security concerns dealing with U.S. polysilicon manufacturing facilities.