

THERMO International 2006

**Sixteenth Symposium on Thermophysical Properties
Nineteenth International Conference on Chemical Thermodynamics
Sixty-First Calorimetry Conference**

July 30 – August 4, 2006

at

University of Colorado
Boulder, Colorado, U.S.A.

Organized by

National Institute of Standards and Technology
American Society of Mechanical Engineers
American Institute of Chemical Engineers
International Association of Chemical Thermodynamics
International Union of Pure and Applied Chemistry

<http://www.thermointernational.org/>
<http://symp16.boulder.nist.gov/>
<http://www.icct2006.org/>
<http://www.calcon2006.org/>

Organizers

THERMO International 2006

W.M. Haynes
*National Institute of Standards and Technology
Boulder, Colorado, U.S.A.*

Sixteenth Symposium on Thermophysical Properties

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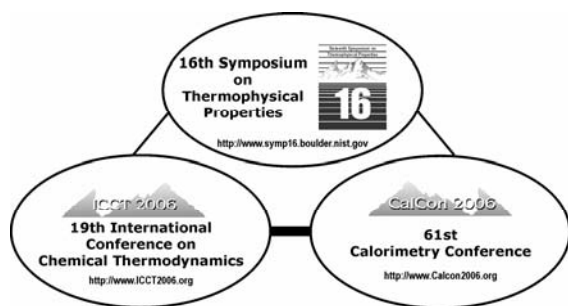
Nineteenth International Conference on Chemical Thermodynamics

M. Frenkel, R.D. Chirico and J.W. Magee
*National Institute of Standards and Technology
Boulder, Colorado, U.S.A.*

Sixty-First Calorimetry Conference

M. Gruskiewicz
*Chemical Sciences Division,
Oak Ridge National Laboratory
Oak Ridge, Tennessee, U.S.A.*

M. Frenkel
*National Institute of
Standards and Technology
Boulder, Colorado, U.S.A.*

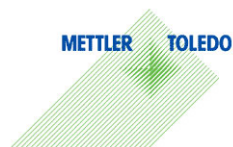


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ABOUT THERMO INTERNATIONAL 2006

THERMO International 2006 includes the 16th Symposium on Thermophysical Properties, the 19th International Conference on Chemical Thermodynamics, and the 61st Calorimetry Conference. This is the first time that these three conferences have been held jointly at the same site. This is scheduled as a one-time event. The technical program of THERMO International 2006 consists of joint sessions as well as independent sessions of the 16th Symposium on Thermophysical Properties, the 19th International Conference on Chemical Thermodynamics (ICCT 2006), and the 61st Calorimetry Conference (CalCon 2006). The program will include a keynote lecture, major award lectures, joint plenary lectures, conference-specific plenary lectures, invited lectures, oral presentations, and posters.

The Symposium on Thermophysical Properties is held in Boulder, Colorado every three years and rotates on an annual basis with the other major thermophysical properties conferences in Europe and Asia. The European conference was held in Slovakia in 2005, the Asian conference will be held in Japan in 2007, and the European Conference will be held in France in 2008. The International Conference on Chemical Thermodynamics (ICCT) is held every two years and rotates among selected sites in North America, Europe, and Asia with the last two held in Germany and China. The Calorimetry Conference is convened annually at selected sites in either the U.S. or Canada and is always held jointly with the International Conference on Chemical Thermodynamics when ICCT is convened in either the U.S. or Canada.

Because of the overlap among areas of interest of these individual conferences, members of the organizing committees for the various conferences met and decided to hold these conferences jointly. This provides a unique opportunity for researchers and practitioners worldwide to meet and discuss a broad spectrum of scientific problems in the fields of thermodynamics and thermophysical properties for a wide variety of systems as well as applications in chemistry, biology, chemical engineering, mechanical engineering, physics, and other areas of science and engineering. Perhaps more important than the distinctions among the institutional labels applied to the disciplines is the continuum of activities from fundamental science to more empirical engineering approaches to thermodynamics and thermophysical properties, and to field applications where needs may be specific and immediate. It is hoped that THERMO International 2006 will serve all these interests and will help to build bridges among communities with much to learn from each other. We look forward to interactions among members of all of these communities to make this a truly unique, worthwhile, and exciting experience!

PROCEEDINGS

Papers describing all work presented at the 16th Symposium were encouraged, but not required. A preprint volume on CD-ROM is provided to each participant. Only those papers presented by an author at the Symposium will be reviewed and considered for publication in special proceedings issues of the *International Journal of Thermophysics* and *Fluid Phase Equilibria*.

CONFERENCE INFORMATION

Award Ceremony, Lectures, and Reception (Touloukian, Rossini and Huffman): The award lectures and ceremony will be held on Tuesday, August 1, in the UMC Ballroom beginning at 1:45 p.m. A reception will follow in the UMC Courtyard.

Banquet: The conference banquet will be held on Thursday, August 3, 6:00–10:00 p.m. at the National Center for Atmospheric Research (NCAR). Buses will be available on Regent Drive near the Fiske Planetarium, and will leave starting at 5:45 p.m. Admission to the banquet is included in your registration. Tickets for guests are available at conference registration.

Breaks: All morning and afternoon breaks will be on the patio of the Mathematics Building and at the Coors Events Conference Center.

Conference Office: The main office will be located in the Engineering Center, Room 133 (303-492-7220).

Emergencies: In case of an emergency, call the Kittredge Office at 303-492-7002 or the University Police at 303-492-6666. In case of medical or other serious emergencies, dial 911.

Fax, E-Mail, and Copies: Fax and copy services are available from local vendors or Kittredge Commons (303-492-4507). There is a charge for fax and copy services. Internet and e-mail are accessible through campus computers. To logon, the conference user name is confthtr and the password is 1184a529.

Health: Boulder Community Hospital (303-440-2273) is available for serious medical attention. For urgent care and minor injuries or illnesses, the Wardenburg Student Health Center (303-492-5101), on campus, is available to conference participants. Wardenburg hours are 8 a.m. – 5 p.m. Monday – Friday, and 9 a.m. – 1 p.m. Saturday. Wardenburg is closed on Sunday.

Meal Hours: All meals will be served in the Kittredge Commons dining room during the following hours: Breakfast: 7:00–8:30 a.m.; Lunch: 11:00 a.m. - 1:30 p.m.; Dinner: 5:00-6:30 p.m. Dinner on Tuesday evening has been extended until 7:00 p.m. following the award reception.

Meal Packages: Meal packages for those not staying in campus housing can be purchased at registration for \$96.65. However, meal tickets for individual meals can be purchased at the Kittredge front desk at any time. The package includes lunch daily on Monday – Friday, and dinner daily on Sunday – Wednesday. (Thursday dinner will be a banquet – see above.)

Messages: Message boards will be located in the Kittredge Commons. You may use the Kittredge office number (303-492-7002) as your contact number for phone messages. Messages will then be placed on the message boards.

Parking: Parking permits for the week of the conference are available from the registration web site for a cost of \$19.00. They will also be sold at the Kittredge Front Desk for the duration of the conference. Permits for parking on campus are required, and tickets are issued if proper permits are not displayed.

Plenary Sessions: Plenary sessions will be held at the University Memorial Center (UMC). Buses will circulate between the Kittredge Complex and the UMC for 30 minutes before, during, and for 30 minutes after the plenary sessions. Additional stops can also be made on these circuit routes, e.g., at the Engineering Center, Math Building, etc.

(Conference Information Continues on Next Page)

CONFERENCE INFORMATION (CONTINUED)

Registration: On-site registration and pickup of Conference materials will be in the UMC Ballroom from 4:00-8:00 p.m. on Sunday, July 30th. Registration will continue on Monday morning at the UMC Ballroom. Starting with Monday afternoon, registration will be located in the Engineering Center, Room 133. Advance registration is available through the conference web site. The cost is \$475 for advance registration through June 30th, and \$525 thereafter.

Session Locations: Sessions will be held in the Engineering Classroom Building, Benson Earth Sciences Building, Coors Events Conference Center, the Mathematics Building, the Stadium Club at Folsom Field, and the University Memorial Center, as indicated in the program.

Socials: The social area will be located in the Hardrive Café in the Kittredge Commons, and will be open from 8:00-11:00 p.m. on Sunday and Tuesday. On Monday and Wednesday the social area will be open from 9:00-11:00 p.m. due to later evening sessions. Beverages and light snacks will be provided. There will be no social area on Thursday because of the banquet.

Tours: There will be four tours offered as a part of THERMO International 2006: (1) Flatiron Crossing Shopping, Monday, July 31. 10:00 a.m. – 3:00 p.m.; (2) Welcome to the Mile High City (Denver), Tuesday, August 1. 10:00 a.m. – 1:00 p.m.; (3) Discover Gold at Phoenix Gold Mine, Wednesday, August 2. 10:00 a.m. – 3:00 p.m.; (4) A Day of Wings and Things in the Springs (Colorado Springs), Friday, August 4. 1:30 p.m. – 10:30 p.m. The tours will start from the UMC building unless otherwise indicated on your ticket in the registration package.

Transportation: Boulder is 27 miles northwest of Denver via U.S. 36. The airport serving Denver is Denver International Airport (DIA). Boulder is approximately 45 miles northwest of the airport. Several forms of surface transportation are available from DIA to Boulder.

PRESENTATION INFORMATION:

Oral Sessions: In every room where talks will be held, an overhead projector will be provided for transparencies and a computer will be provided with projection capabilities for Power Point presentations. It is preferred that you bring your presentation on a CD or USB flash drive ("memory stick") and use the computer provided in the room. This computer will already be set up to work with the projection equipment. You may use your own laptop, but in this case be sure to allow ample extra setup time. It is recommended you test your presentation in advance. Equipment will be available for this purpose in Room 131, Engineering Center (Building 23 on the campus map). If you want to use slides, or have other special needs, arrangements must be made in advance during registration or by e-mail to confreg@housing.colorado.edu, or fax to 303-492-5959.

Poster Sessions: The poster sessions will take place in the CU Stadium Club at Folsom Field on Wednesday, August 2, and Thursday, August 3, from 1:45-3:30 p.m. Folsom Field is the football stadium located just north of Benson Earth Sciences Building and northwest of the Engineering Center. To reach the Stadium Club, cross the street directly north of Benson, enter the arched entry on the east side of Folsom Field, and walk 50 meters to the bank of four elevators on your right side. Enter the double doors, choose any elevator, and select the "CL" button. There will be signs and a map to identify the location of your poster; they are arranged by topic area. You will be provided with half the space on a board approximately 4 feet by 8 feet (1.22 m $\times$ 2.44 m), push pins, and velcro sticky tape. You may set up as early as 8:00 a.m. on the day of your poster presentation, and must remove all materials by 5:00 p.m. that evening. If you have special needs or questions, these must be addressed in advance during registration or by e-mail to confreg@housing.colorado.edu, or fax to 303-492-5959.

Software-Demonstration Sessions: The software-demonstration sessions will be held concurrently with the Poster Sessions on Wednesday, August 2 and Thursday, August 3 from 1:45 p.m. to 3:30 p.m. Both sessions will be held at the CU Stadium Club at Folsom Field on the campus of the University of Colorado. Folsom Field is the football stadium located just north of Benson Earth Sciences Building and northwest of the Engineering Center. To reach the Stadium Club, cross the street directly north of Benson, enter the arched entry on the east side of Folsom Field, and walk 50 meters to the bank of four elevators on your right side. Enter the double doors, choose any elevator, and select the "CL" button. Signs will identify the software demonstration area. A table 6 feet long and 30 inches wide (1.8 m $\times$ 0.76 m), 2 chairs, a poster board approximately 4 feet (1.2 m) wide, push pins, velcro sticky tape, access to electrical outlets and wireless Internet will be provided for each demonstration. You may set up as early as 8 a.m. on August 2, and we request that all materials be removed by 5:00 p.m. on August 3. If you have special needs or questions, these must be addressed in advance during registration or by e-mail to confreg@housing.colorado.edu, or fax to 303-492-5959.

Exhibits: Exhibits will be held concurrently with the Poster Sessions on Wednesday, August 2 and Thursday, August 3 from 1:45 p.m. to 3:30 p.m. Both sessions will be held at the CU Stadium Club at Folsom Field on the campus of the University of Colorado. Folsom Field is the football stadium located just north of Benson Earth Sciences Building and northwest of the Engineering Center. To reach the Stadium Club, cross the street directly north of Benson, enter the arched entry on the east side of Folsom Field, and walk 50 meters to the bank of four elevators on your right side. Enter the double doors, choose any elevator, and select the "CL" button. Signs will identify the exhibit area. A table 6 feet long and 30 inches wide (1.8 m $\times$ 0.76 m) in a booth measuring 8 feet $\times$ 8 feet (2.44 m $\times$ 2.44 m), 2 chairs, a poster board approximately 4 feet (1.2 m) wide, push pins, velcro sticky tape, access to electrical outlets and Internet will be provided for each exhibit. You may set up as early as 8 a.m. on August 2, and we request that all materials be removed by 5:00 p.m. on August 3. If you have any additional needs or questions, these must be addressed in advance during registration or by e-mail to confreg@housing.colorado.edu, or fax to 303-492-5959.

CONTACTS

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Michael Frenkel, 19th ICCT and 61st Calorimetry Conference

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Housing and Registration Information:

Virginia Schultz

CU Conference Services
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Boulder, CO 80310
Phone: 303-492-5151 Fax: 303-492-5959
E-mail: Virginia.Schultz@Colorado.edu

General Information:

Conference Secretariat

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E-mail: symp16@boulder.nist.gov

16th SYMPOSIUM SESSIONS

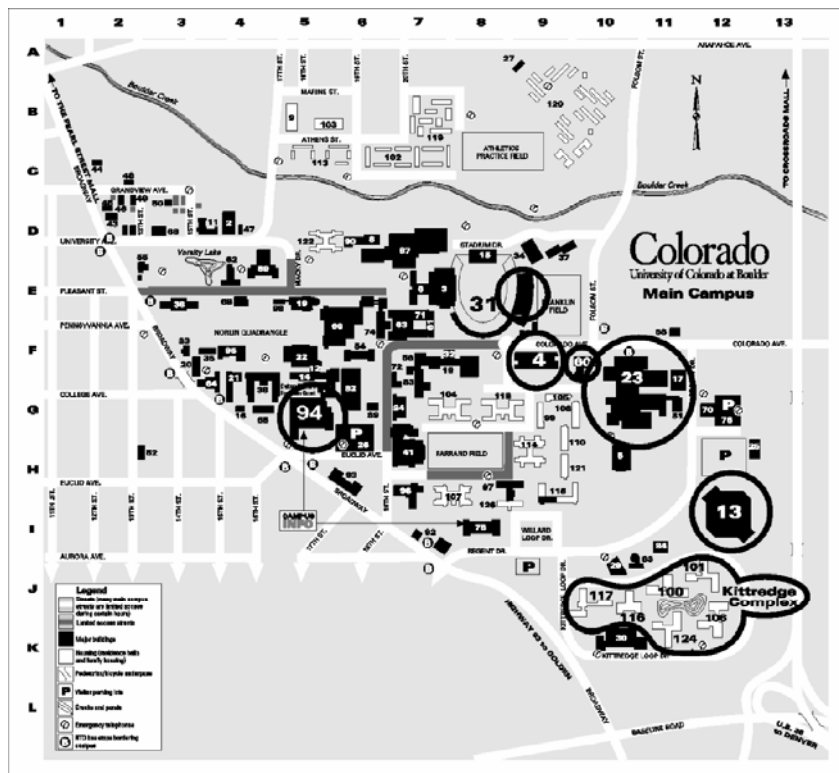
Fluid Property Measurements	Rakesh Srivastava, <i>Dow</i>
Instrumentation and Measurement Techniques	Tom Bruno, <i>NIST</i>
Inverse Problems and Non-Destructive Evaluation	Roberto Li Voti, <i>University of Rome</i>
Optical and Thermal Radiative Properties of Materials	Zhuomin Zhang, <i>Georgia Tech</i>
Photothermal and Photoacoustic Techniques	Gerald Diebold, <i>Brown University</i> Andreas Mandelis, <i>University of Toronto</i>
Properties at the Nanoscale	Pamela Norris, <i>University of Virginia</i> Robert Stevens, <i>Rochester Inst. Tech.</i>
Properties for Metallurgical Process Design	Tony Overfelt, <i>Auburn University</i> Ivan Egry, <i>German Aerospace Center</i>
Properties for Sustainable Development	Anthony Rutz, <i>INL</i> Paul Wichlacz, <i>INL</i>
Properties of Aqueous Systems	Allan Harvey, <i>NIST</i> Ilja Siepmann, <i>University of Minnesota</i>
Properties of Fuels, Including Natural Gas Systems	Jim Holste, <i>Texas A&M University</i> Ken Hall, <i>Texas A&M University</i>
Properties of Mesoscopic, Self-Assembled, and Strongly Fluctuating Systems	Mikhail Anisimov, <i>University of Maryland</i>
Properties of Polymers	Chad Snyder, <i>NIST</i> Alamgir Karim, <i>NIST</i>
Properties of Solids	Andreas Mandelis, <i>University of Toronto</i>
Properties of Working Fluids, Including Refrigerants	Mark McLinden, <i>NIST</i> Rajiv Singh, <i>Honeywell</i>
Property Needs in Biothermophotonics	Andreas Mandelis, <i>University of Toronto</i> J.J. Alvarado-Gil, <i>CINVESTAV IPN</i>
Subsecond Thermophysics	Gernot Pottlacher, <i>TU-Graz</i>
Theory of Thermophysical Properties, Including Statistical Mechanics	John Kincaid, <i>SUNY – Stony Brook</i>
Wetting, Interfaces, and Membranes	Marcus Müller, <i>Georg-August-University</i>

19th ICCT/61st CALCON SESSIONS

Colloid and Interface Science	Margarida Bastos, <i>University of Porto</i> Watson Loh, <i>State University of Campinas</i>
Electrolyte and Non-Electrolyte Solution Thermodynamics	Jean-Pierre E. Grolier, <i>Blaise Pascal University</i> Emmerich Wilhelm, <i>University of Vienna</i>
New Experimental Techniques	Tooru Atake, <i>Tokyo Inst. Technol.</i> Anthony R.H. Goodwin, <i>Schlumberger</i>
New Materials	Ramón Burriel, <i>University of Zaragoza</i> Rüdiger N. Lichtenthaler, <i>University of Heidelberg</i>
Phase Equilibrium, Supercritical Fluids, and Separation Technologies	Theodoor W. De Loos, <i>Delft University of Technol.</i> Ulrich Deiters, <i>University Cologne</i>
Thermochemistry and Molecular Energetics	Juliana Boerio-Goates, <i>Brigham Young University</i> Manuel A.V. Ribeiro da Silva, <i>University of Porto</i>
Thermodynamic Frontiers and Education	Trevor M. Letcher, <i>University of Natal</i> Ron D. Weir, <i>Royal Military College</i>

JOINT SESSIONS

Ionic Liquids	Andreas Heintz, <i>University of Rostock</i> Ken Marsh, <i>University of Canterbury</i>
Molecular Modeling, Including Simulation	Ray Mountain, <i>NIST</i> Susumu Okazaki, <i>Inst. Molecular Science</i>
Properties and Processes for a Hydrogen-based Economy	Richard Jacobsen, <i>University of Idaho</i>
Databases, Data Systems, Software Applications, and Correlations	Marcia Huber, <i>NIST</i> Andy Johns, <i>Software Products TUV NEL</i>
Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors	Mike Henzl, <i>University of Missouri</i> David Remeta, <i>Rutgers University</i> Neil Wright, <i>Michigan State University</i>
Posters	Joseph Magee, <i>NIST</i> Jason Widegren, <i>NIST</i>
Software Demonstrations	Marcia Huber, <i>NIST</i>
Exhibits	Rob Chirico, <i>NIST</i>



Key to Conference Specific Buildings

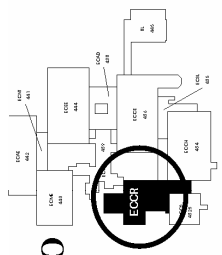
- 4 Benson Earth Sciences Building
- 13 Coors Events Conference Center
- 23 Engineering Center
- 31 Folsom Field (Stadium Club)
- 60 Mathematics Building
- 94 UMC (University Memorial Center)
- 100 Andrews Hall (Kittredge Complex)
- 101 Arnett Hall (Kittredge Complex)
- 116 Kittredge Commons
- 117 Kittredge West Hall (Kittredge Complex)
- 124 Smith Hall (Kittredge Complex)

UNIVERSITY BUILDINGS

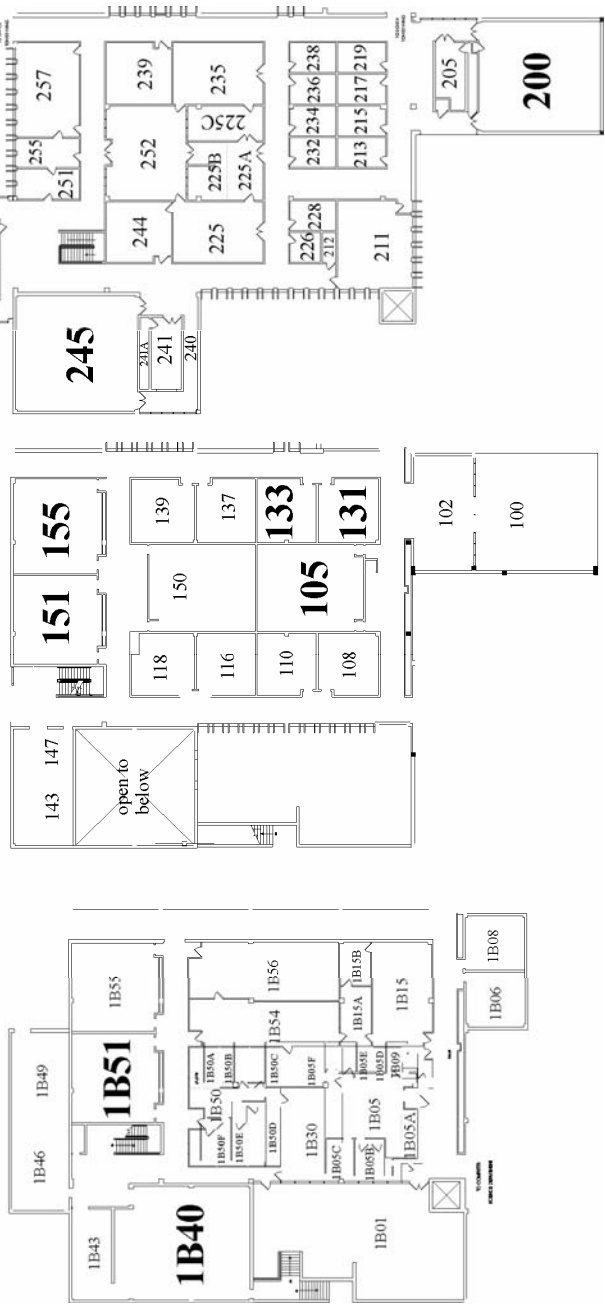
1. Administrative and Research Center
2. Armory
3. Balch Fieldhouse
4. Benson Earth Sciences Building
5. Business
6. Carlson Gymnasium
7. Ctr. For Astrophysics and Space Astronomy
8. Clare Small Arts and Sciences
9. College Inn Conference Center
10. Computing Center
11. Continuing Education
12. Coop. Inst. For Res. in Envir. Sciences
13. Coors Events/Conference Center
14. Cristol Chemistry and Biochemistry
15. Dal Ward Athletic Center
16. Denison Arts and Sciences
17. Discovery Learning Center
18. Duane Physics and Astrophysics
19. Eaton Humanities Building
20. Economics
21. Education
22. Ekeley Sciences
23. Engineering Center
24. Environmental Design
25. Envir. Health and Safety Center
26. Eudlid Avenue AutoPark
27. Family Housing Children's Center
28. Fam. Housing Children's Ctr. Colo. Court
29. Fiske Planetarium and Science
30. Fleming Law
31. Folsom Stadium
32. Gamow Tower (DUAN)
33. Gates Woodruff Women's Studies Cottage
34. Grounds and Service Center
35. Guggenheim Geography
36. Hale Science
37. Health Physics Laboratory
38. Helles Arts and Science/Rippon Theatre
39. Housing System Maintenance
40. Housing Suystem Service Center
41. Imig. Music
42. Inst. For Behavioral Genetics
43. Inst. Behavioral Science No. 2
44. IBS No. 2
45. IBS No. 3
46. IBS No. 4
47. IBS No. 5
48. IBS No. 6
49. IBS No. 7
50. IBS No. 8
51. Integrated Teaching/Learning Lab
52. International English Center
53. Joint Inst. For Laboratory Astrophysics
54. Ketchum Arts and Sciences
55. Koenig Alumni Center
56. Lab for Atmospheric and Space Physics
57. LASP Space Tech Research Ctr.
58. Lesser House
59. Macky Auditorium
60. Mathematics Building
61. MCD Biology
62. McKenna Languages
63. Muenzinger Psychology
64. Museum Collections (Bruce Curtis Bldg)
65. Museum of Natural History, Univ. of Colo
66. Norlin Library
67. Nuclear Physics Laboratory
68. Old Main
69. Page Foundation Center
70. Police and Parking Services
71. Porter Biosciences
72. Power House
73. Qwest Research Park
74. Ramaley Biology
75. Regent Administrative Center
76. Regent Drive Auto Park
77. Res. Lab, Litman RL1
78. Res Lab, WICHE (RL2)
79. Res Lab, Life Science RL4
80. Res Lab (Marine St. Science Center) RL6
81. Research Park Greenhouse
82. Sibell Wolle Fine Arts
83. Sommers-Bausch Observatory
84. Speech, Language, and Hearing Sciences
85. Stadium Offices
86. Stadium Ticket BuildingRecreation Center
87. Stadium Recreation Center
88. Sybase
89. Telecommunications Building
90. Temporary Building No. 1
91. Transportation Center
92. University Admin. Ctr and Annex
93. University Club
94. University Memorial Center
95. University Theatre
96. Wardenburg Health Center
97. Willard Administrative
98. Woodbury Arts and Sciences

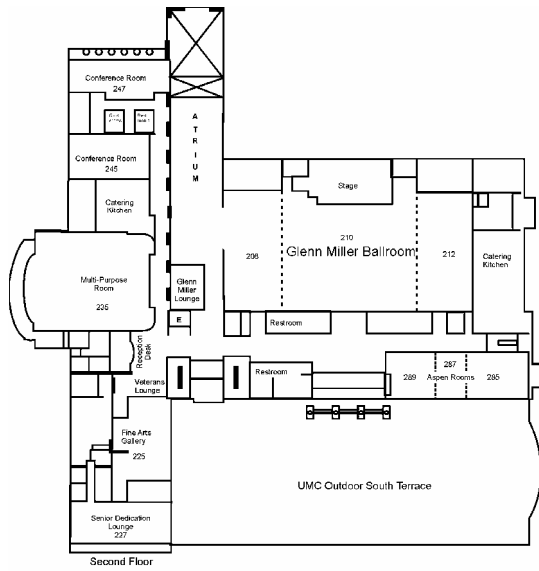
UNIVERSITY HOUSING

99. Aden Hall Quadrangle
100. Andrews Hall Kittredge Complex
101. Arnett Hall Kittredge Complex
102. Athens Court
103. Athens North Court
104. Baker Hall
105. Brackett Hall Quadrangle
106. Buckingham Hall Kittredge Complex
107. Cheyenne Arapaho Hall
108. Cockerell Hall Quadrangle
109. Colorado Court
110. Crosman Hall Quadrangle
111. Darley Commons Williams Village
112. Darley Towers Williams Village
113. Faculty-Staff Court
114. Farrand Hall
115. Hallett Hall
116. Kittredge Commons Kittredge Complex
117. Kittredge West Hall Kittredge Complex
118. Libby Hall
119. Marine Court
120. Newton Court
121. Reed Hall (REED)
122. Sewall Hall (SWLL)
123. Smiley Court (SMCT)
124. Smith Hall Kittredge Complex
125. Stearns Towers Williams Village
126. Willard Hall South Wing

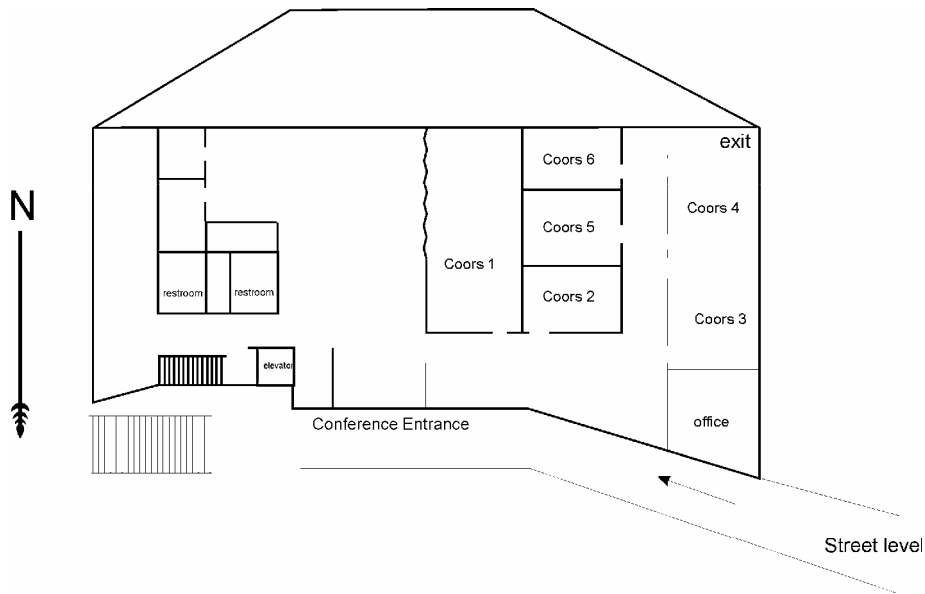


UNIVERSITY OF COLORADO ENGINEERING CENTER CLASSROOM WING FLOOR PLAN





UMC - University Memorial Center



COORS EVENTS CONFERENCE CENTER
Lower Level

Enter on North Side of the building at the street level
through doorway marked Conference Entrance

PROGRAM SUMMARY TABLE

Sunday, July 30, 2006

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UMC Ballroom

Monday, July 31, 2006

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UMC Ballroom

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- Fluid Property Measurements 1
- Ionic Liquids 1
- Molecular Modeling, Including Simulation 1
- Properties and Processes for a Hydrogen-based Economy 1
- Properties of Mesoscopic, Self-Assembled, and Strongly Fluctuating Systems 1
- Properties of Polymers 1
- Subsecond Thermophysics 1
- Theory of Thermophysical Properties, Including Statistical Mechanics 1
- Thermochemistry and Molecular Energetics 1
- Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors 1

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Coors 4
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Coors 5

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- Fluid Property Measurements 2
- Ionic Liquids 2
- Molecular Modeling, Including Simulation 2
- Molecular Modeling, Including Simulation 3
- Properties of Polymers 2
- Subsecond Thermophysics 2
- Theory of Thermophysical Properties, Including Statistical Mechanics 2
- Thermochemistry and Molecular Energetics 2

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| • Molecular Modeling, Including Simulation 5 | Benson 180 |
| • Properties for Metallurgical Process Design 1 | Eng-200 |
| • Properties of Mesoscopic, Self-Assembled,
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| • Thermodynamics and Properties in the Biological, Medical,
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- Instrumentation and Measurement Techniques 1
- Ionic Liquids 4
- Molecular Modeling, Including Simulation 6
- Properties for Metallurgical Process Design 2
- Properties of Mesoscopic, Self-Assembled, and Strongly Fluctuating Systems 3
- Properties of Polymers 3
- Theory of Thermophysical Properties, Including Statistical Mechanics 3
- Thermochemistry and Molecular Energetics 3
- Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors 3

Room

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- Properties for Metallurgical Process Design 3
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- Properties of Polymers 4
- Properties of Working Fluids, including Refrigerants 1
- Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors 4

Eng-245
Coors 5
Eng-105
Coors 4
Math 100
Coors 1
Eng-200

Eng-1B40
Eng-151
Eng-265

Coors 3

Afternoon – 1 1:45 PM

(Pages 61 - 62)

- Plenary 4,5 Awards

UMC Ballroom

Morning - 1 8:30 AM

(Page 63)

Room

- Plenary 6

UMC Ballroom

Morning – 2 10:35 AM

(Pages 64 -71)

- Fluid Property Measurements 3
- Instrumentation and Measurement Techniques 3
- Photothermal and Photoacoustic Techniques 1
- Plenary 19ICCT/61CalCon 1
- Properties for Metallurgical Process Design 4
- Properties of Solids 1
- Properties of Working Fluids, including Refrigerants 2

Eng-1B40
Eng-245
Eng-155
UMC Ballroom
Eng-200
Eng-151
Eng-265

Afternoon - 1 1:45 PM

(Pages 72 -123)

- Exhibitions 1
- Posters 1
- Software Demonstrations 1

Stadium Club
Stadium Club
Stadium Club

Afternoon – 2 3:50 PM

(Pages 124 - 136)

- Databases, Data Systems, Software Applications, and Correlations 5
- Electrolyte and Non-Electrolyte Solution Thermodynamics 6
- Fluid Property Measurements 4
- Ionic Liquids 6
- Molecular Modeling, Including Simulation 8
- Optical and Thermal Radiative Properties of Materials 1
- Phase Equilibrium, Supercritical Fluids, and Separation Technologies 2
- Photothermal and Photoacoustic Techniques 2
- Properties of Working Fluids, Including Refrigerants 3
- Theory of Thermophysical Properties, Including Statistical Mechanics 4
- Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors 5
- Wetting, Interfaces, and Membranes 1

Eng-245
Coors 5
Eng-1B40
Coors 4
Math 100
Eng-200
Coors 1
Eng-155
Eng-265
Eng-151

Coors 3
Benson 180

(Continued on Next Page)

Evening 7:30 PM**(Pages 137 – 151)****Room**

- | | |
|---|------------|
| • Colloid and Interface Science 1 | Coors 5 |
| • Databases, Data Systems, Software Applications, and Correlations 6 | Eng-245 |
| • Instrumentation and Measurement Techniques 4 | Eng-105 |
| • Ionic Liquids 7 | Coors 4 |
| • Molecular Modeling, Including Simulation 9 | Math 100 |
| • Optical and Thermal Radiative Properties of Materials 2 | Eng-200 |
| • Phase Equilibrium, Supercritical Fluids, and Separation Technologies 3 | Coors 1 |
| • Photothermal and Photoacoustic Techniques 3 | Eng-155 |
| • Properties of Aqueous Systems 1 | Eng-1B40 |
| • Properties of Working Fluids, Including Refrigerants 4 | Eng-265 |
| • Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 6 | Coors 3 |
| • Wetting, Interfaces, and Membranes 2 | Benson 180 |

Morning – 1 8:30 AM

(Pages 152 – 161)

- Instrumentation and Measurement Techniques 5
- Optical and Thermal Radiative Properties of Materials 3
- Photothermal and Photoacoustic Techniques 4
- Plenary 19ICCT/61CalCon 2
- Properties at the Nanoscale 1
- Properties of Aqueous Systems 2
- Properties of Fuels, Including Natural Gas Systems 1
- Properties of Working Fluids, Including Refrigerants 5
- Wetting, Interfaces, and Membranes 3

Room

Eng-151
Eng-200
Eng-155
UMC Ballroom
Eng-245
Eng-1B40
Eng-105
Eng-265
Benson 180

Morning – 2 10:35 AM

(Pages 162 - 176)

- Ionic Liquids 8
- Molecular Modeling, Including Simulation 10
- New Experimental Techniques 1
- New Materials 1
- Phase Equilibrium, Supercritical Fluids, and Separation Technologies 4
- Photothermal and Photoacoustic Techniques 5
- Properties for Sustainable Development 1
- Properties of Aqueous Systems 3
- Properties of Fuels, Including Natural Gas Systems 2
- Properties of Solids 2
- Thermodynamic Frontiers and Education 1
- Wetting, Interfaces, and Membranes 4

Coors 3
Math 100
Coors 2
Coors 5
Coors 1
Eng-155
Eng-265
Eng-1B40
Eng-105
Eng-200
Coors 4
Benson 180

(Continued on Next Page)

Thursday, August 03, 2006 (Continued)
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Afternoon – 1 1:45 PM
(Pages 177 – 218)

- Exhibitions 2
- Posters 2
- Software Demonstrations 2

Room

Stadium Club
Stadium Club
Stadium Club

Afternoon – 2 3:50 PM
(Pages 219 – 231)

- Colloid and Interface Science 2
- Molecular Modeling, Including Simulation 11
- New Experimental Techniques 2
- New Materials 2
- NIST/TRC Consortium Workshop 1
- Phase Equilibrium, Supercritical Fluids, and Separation Technologies 5
- Properties at the Nanoscale 2
- Properties for Sustainable Development 2
- Properties of Aqueous Systems 4
- Properties of Working Fluids, Including Refrigerants 6
- Property Needs in Biothermophotonics 1
- Thermodynamic Frontiers and Education 2
- Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural and Food Sectors 7

Coors 2
Math 100
Eng-105
Coors 5
Eng-151
Coors 1
Eng-245
Eng-200
Eng-1B40
Eng-265
Eng-155
Coors 4

Coors 3

Evening 6:00 PM
(Page 232)

- Banquet at National Center for Atmospheric Research

NCAR

Morning – 1 8:30 AM
(Pages 233 - 243)
Room

- | | |
|---|---|
| <ul style="list-style-type: none"> • Colloid and Interface Science 3 • Instrumentation and Measurement Techniques 6 • Inverse Problems and Non-Destructive Evaluation 1 • Molecular Modeling, Including Simulation 12 • New Materials 3 • Phase Equilibrium, Supercritical Fluids, and Separation Technologies 6 • Properties at the Nanoscale 3 • Properties of Aqueous Systems 5 • Properties of Fuels, Including Natural Gas Systems 3 • Properties of Working Fluids, Including Refrigerants 7 • Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural and Food Sectors 8 | <ul style="list-style-type: none"> Coors 2 Eng-105 Eng-155 Math 100 Coors 5 Coors 4 Eng-245 Eng-1B40 Eng-200 Eng-265 Coors 3 |
|---|---|

Morning – 2 10:35 AM
(Pages 244 - 248)

- | | |
|---|---|
| <ul style="list-style-type: none"> • Instrumentation and Measurement Techniques 7 • Inverse Problems and Non-Destructive Evaluation 2 • Plenary 19ICCT/61CalCon 3 • Properties of Aqueous Systems 6 • Theory of Thermophysical Properties, Including Statistical Mechanics 5 | <ul style="list-style-type: none"> Eng-105 Eng-155 UMC Ballroom Eng-1B40 Eng-265 |
|---|---|

Sunday, July 30, 2006

Joint Session

Plenary 1

Welcoming Reception

Chair:

Evening 4:00 PM - 8:00 PM

Room: UMC Ballroom

4:00 PM Opening Reception

Monday, July 31, 2006

Joint Session

Plenary 2

Opening Ceremony and Keynote Presentation

Chair: W.M. Haynes, D.G. Friend and M. Frenkel

Morning 1 8:30 AM - 10:15 AM

Room: UMC Ballroom

8:35 AM Welcome and Introductions

9:25 AM Thermophysical Property Measurements: the Journey from Accuracy to Fitness for Purpose (Invited)

W.A. Wakeham, University of Southampton, Southampton, Highfield, U.K.*

Monday, July 31, 2006

Joint Session

Plenary 3

Chair: D.G. Friend and W.M. Haynes

Morning 2 10:35 AM - 12:20 PM

Room: UMC Ballroom

Molecular Modeling, Including Simulation

10:40 AM The Fluctuation and Nonequilibrium Free Energy Theorems - Theory & Experiment (Invited)

D.J. Evans*, E. Sevick, G. Wang, D. Carberry and J. Reid,
Australian National University, Canberra, ACT, Australia
and D.J. Searles, *Griffith University, Brisbane, Queensland, Australia*

Ionic Liquids

11:30 AM The Mark of an Educated Mind (Invited)

K.R. Seddon*, *The Queen's University of Belfast, Belfast, Northern Ireland, U.K.*

Monday, July 31, 2006

19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 1

Models of Fluids (Pure and Mixed) and Simple Solutions 1

Chair: E. Wilhelm and W. Fürst

Afternoon 1 1:45 PM - 3:30 PM

Room: Coors-1

1:50 PM From Supercritical Fluids to Polymeric Glasses: A Unified Approach (Invited)

C.G. Panayiotou*, *Aristotle University, Thessaloniki, Greece*

2:30 PM The Unified Theory of Electrolytes

E. Djamali and J.W. Cobble*, *San Diego State University, San Diego, CA, U.S.A.*

2:50 PM Models of Aggregation Phenomena in Liquid Mixtures: Thermodynamic and Related Properties

V.A Durov*, *Moscow State University, Moscow, Russia*

3:10 PM The Behavior of KI Dissolved in Supercritical Ammonia

G. Sciaini, E.J. Marceca and R. Fernandez-Prini*, *University of Buenos Aires, Buenos Aires, Argentina*

Monday, July 31, 2006

16th Symposium

Fluid Property Measurements 1

Chair: R. Srivastava

Afternoon 1 1:45 PM - 3:30 PM

Room: Eng-105

1:50 PM Thermal Decomposition: A Prelude to Thermophysical Property Measurements

T.J. Bruno*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

2:10 PM Measurements of the Thermal Conductivity of Molten Lead Using a New Transient Hot Wire Sensor

J. Bilek, J.K. Atkinson and W.A. Wakeham*, *University of Southampton, Southampton, Highfield, U.K.*

2:30 PM Measurement of the Thermal Conductivity of Dimethoxymethane and Diesel Oil Mixtures by Transient Hot Wire Method

Jiangtao Wu*, Linfeng Song and Zhigang Liu, *Xi'an Jiaotong University, Xi'an, Shaanxi, China*

2:50 PM Critical Properties of Some Aromatic Compounds

E.D. Nikitin* and A.P. Popov, *Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia*

Monday, July 31, 2006

Joint Session

Ionic Liquids 1
Liquid-Liquid Equilibria

Chair: K.N. Marsh

Afternoon 1 1:45 PM - 3:30 PM

Room: Coors-4

- 1:50 PM Ionic Liquids: What Have We Learned? A Personal, Thermodynamic Scenario (Invited)**

L.P.N. Rebelo*, *Universidade Nova de Lisboa, Oeiras, Portugal*
- 2:30 PM Liquid Phase Behavior of Ionic Liquids with Alcohols: Experimental Studies and Modeling**

J.M. Crosthwaite, M.J. Muldoon, S.N.V.K. Aki, E.J. Maginn and J.F. Brennecke*, *University of Notre Dame, Notre Dame, IN, U.S.A.*
- 2:50 PM Lower Critical Solution Temperatures of Hydrofluorocarbon + Room-Temperature Ionic Liquid Solutions**

A. Yokozeki*, *DuPont Fluoroproducts Laboratory, Wilmington, DE, U.S.A.* and M.B. Shiflett, *DuPont Central Research and Development, Wilmington, DE, U.S.A.*
- 3:10 PM The Hofmeister Series and the Mutual Solubilities of Water and Ionic Liquids**

M.G. Freire and P.J. Carvalho, *Universidade de Aveiro, Aveiro, Portugal*, L.M.N.B. Santos, *Universidade do Porto, Alegre, Portugal*, I.M. Marrucho, *Universidade de Aveiro, Aveiro, Portugal*, L.P.N. Rebelo, *Universidade Nova de Lisboa, Oeiras, Portugal* and J.A.P. Coutinho*, *Universidade de Aveiro, Aveiro, Portugal*

Monday, July 31, 2006

Joint Session

Molecular Modeling, Including Simulation 1

Nanostructure

Chair: R. Mountain

Afternoon 1 1:45 PM - 3:30 PM

Room: Math-100

**1:50 PM Formation of Ice Nanotubes with Hydrophobic Guests
(Invited)**

H. Tanaka*, *Okayama University, Okayama, Japan*

**2:30 PM A Molecular Dynamics Study of Free Energy of Micelle
Formation for SDS in Water and Its Size Distribution**

N. Yoshii and S. Okazaki*, *Institute for Molecular Science,
Myodaiji, Okazaki, Japan*

**2:50 PM Multiscale Simulation of Organic-Inorganic Polyhedral
Nano-Materials**

A. Striolo*, *University of Oklahoma, Norman, OK, U.S.A.*,
E.R. Chan, *University of Michigan, Ann Arbor, MI, U.S.A.*, C.
McCabe, *Vanderbilt University, Nashville, TN, U.S.A.*, S.C.
Glotzer, *University of Michigan, Ann Arbor, MI, U.S.A.* and
P.T. Cummings, *Vanderbilt University, Nashville, TN, U.S.A.*

**3:10 PM Slip Flow on Non-Wetting Interfaces in Nanofluidics:
Navier's Slip Lengths Determined from Nonequilibrium
Molecular Dynamics**

L.L. Lee*, *California State University, Pomona, CA, U.S.A.*
and R.S. Romanov and D.V. Papavassiliou, *University of
Oklahoma, Norman, OK, U.S.A.*

Monday, July 31, 2006

Joint Session

Properties and Processes for a Hydrogen-based Economy 1

Chair: S.G. Penoncello and R.T Jacobsen

Afternoon 1 1:45 PM - 3:30 PM

Room: Coors-5

1:50 PM Storage of Hydrogen as Clathrate Hydrate (Invited)

L.J. Rovetto, J. Schoonman and C.J. Peters*, *Delft University of Technology, Delft, Netherlands*

2:30 PM Correlating the Influence of Magnetic Fields on Solute Content in Metals Using the Thermodynamic Auxiliary Work Function

J.E. Jackson*, D.L. Olson, A.N.L. Lasseigne-Jackson and B.M. Mishra, *Colorado School of Mines, Golden, CO, U.S.A.* and T.A. Siewert, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

2:50 PM Current Status of Thermodynamic Properties of Hydrogen

R.T Jacobsen*, *University of Idaho, Idaho Falls, ID, U.S.A.*, J.W. Leachman and S.G. Penoncello, *University of Idaho, Moscow, ID, U.S.A.* and E.W. Lemmon, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

3:10 PM Current Status of Transport Properties of Hydrogen

R.T Jacobsen, *University of Idaho, Idaho Falls, ID, U.S.A.*, J.W. Leachman* and S.G. Penoncello, *University of Idaho, Moscow, ID, U.S.A.* and M.L. Huber, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

3:30 PM Reliability Modeling of Microballoon Hydrogen Storage in Transportation Systems

V.P. Utgikar* and M. Manic, *University of Idaho at Idaho Falls, Idaho Falls, ID, U.S.A.* and R.T Jacobsen, *University of Idaho, Idaho Falls, ID, U.S.A.*

Monday, July 31, 2006

16th Symposium

***Properties of Mesoscopic, Self-Assembled, and Strongly
Fluctuating Systems 1***

Chair: J.V. Sengers and M.A. Anisimov

Afternoon 1 1:45 PM - 3:30 PM

Room: Eng-1B40

1:50 PM Ionic Criticality: Recent Progress, Open Questions (Invited)

Michael E. Fisher*, *University of Maryland, College Park, MD, U.S.A.*

2:30 PM Density Profiles of Fluids near Surfaces: Surface Critical Behaviour vs Surface Phase Transitions

A. Oleinikova* and I. Brovchenko, *University of Dortmund, Dortmund, Germany*

2:50 PM Scaling Fields and the Nature of Order Parameter in Asymmetric Near-Critical Liquid Mixtures

C.A. Cerdeiriña*, *Universidad de Vigo, Ourense, Spain*
and M.A. Anisimov and J.V. Sengers, *University of Maryland, College Park, MD, U.S.A.*

3:10 PM Chemical Dynamics and Critical Phenomena: Conductivity and Reactivity of Benzylbromide Near the Consolute Point of Triethylamine + Water

C.B. Specker, J.M. Ellis and J.K. Baird*, *University of Alabama in Huntsville, Huntsville, AL, U.S.A.*

Monday, July 31, 2006

16th Symposium

Properties of Polymers 1

General 1

Chair: S. Kumar and C. Snyder

Afternoon 1 1:45 PM - 3:30 PM

Room: Eng-151

1:50 PM Charge Inversion and Layer-by-Layer Assembly of Flexible Polyelectrolytes

Q. Wang*, *Colorado State University, Fort Collins, CO, U.S.A.*

2:10 PM Phase Behavior of Polyampholytes from Charged Hard-Sphere Chain Model

J.W. Jiang*, *National University of Singapore, Singapore*

2:30 PM Mixed Lamellae in Symmetric Diblock Copolymer Thin Films

D. Meng*, *U.S.A.* and Q. Wang, *Colorado State University, Fort Collins, CO, U.S.A.*

2:50 PM Model Based Design of Structured Polymers Using the Reverse Design Approach

V. Soni*, J. Abildskov, G.E. Jonsson and R. Gani, *Technical University of Denmark, Lyngby, Denmark* and N. Karayiannis and V. Mavrantzas, *University of Patras, Patras, Greece*

3:10 PM The Effect of Molecular Weight on Liquid-Liquid Immiscibility in Aqueous Solutions of Polyethylene Glycol Polymers Using the SAFT-VR Approach with Transferable Parameters

G.N.I. Clark*, A. Galindo and G. Jackson, *Imperial College, London, South Kensington, U.K.*

Monday, July 31, 2006

16th Symposium

Subsecond Thermophysics 1

Chair: G. Pottlacher and K. Boboridis

Afternoon 1 1:45 PM - 3:30 PM

Room: Eng-200

1:50 PM Surface Position-Resolved Thermophysical Properties for Metallic Alloys

Y.W. Kim*, *Lehigh University, Bethlehem, PA, U.S.A.*

2:10 PM Electrical-Optical Hybrid Pulse-Heating Method for High-Temperature Thermal Diffusivity Measurement

H. Watanabe* and T. Baba, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

2:30 PM Density and Viscosity of Liquid Ternary Ni-Cu-Fe Alloys

J. Brillo*, *German Aerospace Center, Köln, Germany*, R. Brooks, *National Physical Laboratory, Teddington, Middlesex, U.K.*, I. Egry, *German Aerospace Center, Köln, Germany*, T. Matsushita, *Royal Institute of Technology, Stockholm, Sweden* and P. Quested, *National Physical Laboratory, Teddington, Middlesex, U.K.*

2:50 PM Physical Properties and Normal Spectral Emissivity of Iridium Up to 3500 K

C. Cagran and G. Pottlacher*, *Graz University of Technology, Graz, Austria*

3:10 PM Measurement of the Surface Tension and Viscosity of Ti-Al and Ni-Al alloys by the Oscillating Drop Technique on-Board Parabolic Flights

R.K. Wunderlich*, *Ulm University, Ulm, Germany*, K. Higuchi, *Gakushuin University, Tokyo, Japan* and H.J. Fecht, *Ulm University, Ulm, Germany*

Monday, July 31, 2006

16th Symposium

***Theory of Thermophysical Properties, Including Statistical
Mechanics 1***

Chair: J. Kincaid

Afternoon 1 1:45 PM - 3:30 PM

Room: Eng-265

**1:50 PM Self-Consistent Statistical Description of Thermodynamic
Properties of Solids: Premelting Effects**

A.I. Karasevskii* and V.V. Lubashenko, G. V. Kurdyumov
Institute for Metal Physics NASU, Kiev, Ukraine

2:10 PM Isochoric Heat Capacity of Fluid in the Two-Phase Region

A.B. Kaplun and A.B. Meshalkin*, *Russian Academy of
Sciences, Novosibirsk, Russia*

**2:30 PM Effect of Surface Area Parameters on the Vapor-Liquid
Equilibrium Calculations Using a Lattice Fluid Equation of
State with Hydrogen Bonding**

A. Breitholtz*, *Sogang University, Seoul, Korea*, Chul Soo
Lee, *Korea University, Seoul, Korea*, Ki-Pung Yoo and
Jong Sung Lim, *Sogang University, Seoul, Korea* and
Jeong Won Kang, *Korea University, Seoul, Korea*

2:50 PM The Triangle of Liquid - Gas States

V.S. Vorob'ev*, G.A. Martynov and E.M. Apfelbaum, *Russian
Academy of Science, Moscow, Russia*

3:10 PM Thermodynamic Properties and Structure of Solutions

E.S. Balankina*, *Moscow State University of Instrumentation
and Computer Science, Moscow, Russia*

Monday, July 31, 2006

19th ICCT / 61st CalCon

Thermochemistry and Molecular Energetics 1

Methods for Predictions: Theoretical and Experimental

Chair: M.A.V. Ribeiro da Silva

Afternoon 1 1:45 PM - 3:30 PM

Room: Coors-2

1:50 PM Predictive Methods: Are Experimental Measurements Still Necessary (Invited)

W.E. Acree, Jr.*, *University of North Texas, Denton, TX, U.S.A.*

2:30 PM What Can "Quantum-Black-Boxes" Do for the Inorganic Thermochemist?

S. Stølen*, J.R. Martinez, C.E. Mohn and R. Søndena, *University of Oslo, Oslo, Blindern, Norway*

2:50 PM Vibrational Zero-Point Energies and Their Uncertainties

K.K. Irikura* and R.D. Johnson III, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

3:10 PM Heat Capacity Studies of Water on Nanoparticle Surfaces vs Crystalline Hydrates

J. Boerio-Goates*, B. Lang, G. Li, S. Liu, T.K. Meldrum, T. Parry, T.F. Walker and B.F. Woodfield, *Brigham Young University, Provo, UT, U.S.A.* and A.A. Lefchenko and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.*

3:30 PM Thermophysical Properties of the Vitreous and Crystalline Phases of Alkali Disilicates

D.A. Johnson*, *Spring Arbor University, Spring Arbor, MI, U.S.A.* and A.K. Labban, S.W. Barber and E.F. Westrum, Jr., *University of Michigan, Ann Arbor, MI, U.S.A.*

Monday, July 31, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 1***
Proteins

Chair: C.A.S.A. Minetti and N. Wright

Afternoon 1 1:45 PM - 3:30 PM

Room: Coors-3

**1:50 PM Thermodynamic Barriers to Protein Folding/Unfolding
(Invited)**

J.M. Sanchez-Ruiz*, *Granada University, Granada, Spain*

2:30 PM Enzymes I of Parallel Phosphotransferase Systems in E. Coli

A. Ginsburg*, *NHLBI, NIH, Bethesda, MD, U.S.A.*

**2:50 PM Transfer Free Energies of Peptide Backbone Unit from
Water to Aqueous Electrolyte Solutions at 298.15 K**

V. Pannur*, Ming-Jer Lee and Ho-mu Lin, *National Taiwan
University of Science and Technology, Taipei, Taiwan*

**3:10 PM Characterization of Partially Folded States of Proteins by
Isothermal Titration Calorimetry and Energetics of Its
Binding with Fluorescent Probe ANS**

N. Kishore*, S. Singh and T. Banerjee, *Indian Institute of
Technology Bombay, Powai, Mumbai, India*

Monday, July 31, 2006

Joint Session

**Databases, Data Systems, Software Applications, and
Correlations 1**

In Memory of Dr. R.C. Wilhoit

Chair: A.I. Johns and M.L. Huber

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-245

**3:55 PM The Contribution of Dr. Randolph Wilhoit to Databases, Data
Evaluation, and Expert Systems for Thermophysical
Property Data for Organic Compounds**

K.N. Marsh*, *University of Canterbury, Christchurch, New
Zealand*

**4:15 PM ThermoML Based New Data Delivery Process and Its
Impact on Publication Data Quality**

R.D. Chirico*, V.V. Diky, C.D. Muzny and M. Frenkel, *National
Institute of Standards and Technology, Boulder, CO, U.S.A.*

**4:35 PM Development of a Network Database for Thermophysical
Property Data**

T. Baba*, *National Institute of Advanced Industrial Science
and Technology (AIST), Tsukuba, Ibaraki, Japan*

4:55 PM ThermoData Engine: Critically Evaluated Data on Demand

V.V. Diky*, R.D. Chirico, C.D. Muzny, E.W. Lemmon, X. Yan, Q.
Dong and M. Frenkel, *National Institute of Standards and
Technology, Boulder, CO, U.S.A.*

**5:15 PM Developing and Using Kinetics Databases in Environmental
Chemistry**

J.Z. Bandstra*, J. Moore, J. Wang, P. Mitra, C.L. Giles, S.L.
Brantley and J.D. Kubicki, *Pennsylvania State University,
University Park, PA, U.S.A.*

Electrolyte and Non-Electrolyte Solution Thermodynamics 2

Models of Fluids (Pure and Mixed) and Simple Solutions 2

Chair: J-P.E. Grolier and A.I. Victorov

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-1

3:55 PM The Solubility of Propane in Water: A High-Precision Study

E. Wilhelm*, *University of Wien, Vienna, Austria*, T.R. Rettich, *Illinois Wesleyan University, Bloomington, IL, U.S.A.* and R. Battino, *Wright State University, Dayton, OH, U.S.A.*

4:15 PM Corresponding-States Correlations for Estimating Partial Molar Volumes at Infinite Dilution of Nonelectrolytes in Water over Extended Temperature and Pressure Ranges

A.V. Plyasunov* and E.L. Shock, *Arizona State University, Tempe, AZ, U.S.A.* and J.P. O'Connell, *University of Virginia, Charlottesville, VA, U.S.A.*

4:35 PM Statistical Associating Fluid Theory Coupled with Restricted Primitive Model to Represent Aqueous Multiple-Salt Solutions

X. Ji*, S.P. Tan, H. Adidharma and M.R. Radosz, *University of Wyoming, Laramie, WY, U.S.A.*

4:55 PM Improved Thermodynamic Model for Aqueous NaCl Solutions from 350 to 400 °C

B. Liu*, J.L. Oscarson, C.J. Peterson and R.M. Izatt, *Brigham Young University, Provo, UT, U.S.A.*

5:15 PM Analytical Theory for Charged Particles with Saddle-Shaped Elements in Solution of a Symmetric Electrolyte

V.A. Andreev and A.I. Victorov*, *St. Petersburg State University, St. Petersburg, Russia*

-continued on next page-

Monday, July 31, 2006

19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 2

Models of Fluids (Pure and Mixed) and Simple Solutions 2

(continued)

Chair: J-P.E. Grolier and A.I. Victorov

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-1

**5:35 PM Heat Capacities of Concentrated Sodium Hydroxide
Solutions to 300 °C**

S. Schrödle, P.M. May and G. Hefter*, *Murdoch University,
Murdoch, WA, Australia*

Fluid Property Measurements 2

Chair: R. Srivastava

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-105

**3:55 PM Thermodynamic Properties of Acetone Calculated from
Accurate Experimental Speed of Sound Measurements at
Low Temperature and High Pressures**

S. Lago* and P.A. Albo, *Istituto Elettrotecnico Nazionale
"Galileo Ferraris", Torino, Italy*

**4:15 PM Viscosity of Ar, CO, CO₂, NH₃, SF₆, SiF₄ and C₄H₈
Gases Measured with a Greenspan Acoustic Viscometer**

A.F. Estrada-Alexanders*, *Universidad Autónoma
Metropolitana, México, DF, México* and J.J. Hurly, M.R.
Moldover and J.B. Mehl, *National Institute of Standards and
Technology, Gaithersburg, MD, U.S.A.*

4:35 PM An Industrial Reference Fluid for Moderately High Viscosity

F.J.P. Caetano, *Universidade Técnica de Lisboa, Lisboa,
Portugal*, J.M.N.A. Fareleira*, *Centro de Química
Estrutural, Lisboa, Portugal*, A.P. Fröba, *Universität
Erlangen-Nürnberg, Erlangen, Germany*, K.R. Harris,
University of New South Wales, Canberra, ACT, Australia,
A. Leipertz, *Universität Erlangen-Nürnberg, Erlangen,
Germany*, C.M.B.P. Oliveira, *Universidade Técnica de
Lisboa, Lisboa, Portugal* and W.A. Wakeham, *University of
Southampton, Southampton, Highfield, U.K.*

**4:55 PM Viscosity of Di-Isodecylphthalate by Surface Light
Scattering (SLS)**

A.P. Fröba*, C. Botero and A. Leipertz, *Universität Erlangen-
Nürnberg, Erlangen, Germany*

-continued on next page-

Monday, July 31, 2006

16th Symposium

Fluid Property Measurements 2

(continued)

Chair: R. Srivastava

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-105

**5:15 PM Density and Viscosity of Reference Fluids
Diisodecylphthalate and S20 Over a Wide Range of
Temperature and Pressure**

K.N. Marsh and M. Kandil, *University of Canterbury,
Christchurch, New Zealand* and A.R.H. Goodwin*,
*Schlumberger Technology Corporation, Sugar Land, TX,
U.S.A.*

Ionic Liquids 2

General

Chair: K.R. Seddon

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-4

3:55 PM Physical Properties of Pyridinium Fluorohydrogenate, Pyr(HF)₃

R.J.H. Hulse* and R.R.S. Singh, *Honeywell, Buffalo, NY, U.S.A.*

4:15 PM Some Physico-Chemical Properties of Imidazolium and Pyridinium Based Ionic Liquids

N. Papaiconomou*, J. Salminen and J.M. Prausnitz, *University of California, Berkeley, CA, U.S.A.*

4:35 PM Compressed Liquid Densities of EMIM Chloride + 1-Propanol mixtures at Temperatures from (313 to 363) K and Pressures up to 25 MPa

A. Zúñiga-Moreno and L.A. Galicia-Luna*, *Instituto Politécnico Nacional, México, DF, México*

4:55 PM Report on IACT/IUPAC Project: Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems

K.N. Marsh*, *University of Canterbury, Christchurch, New Zealand*

5:15 PM IUPAC Ionic Liquids Database - ILThermo

Q. Dong, C.D. Muzny, R.D. Chirico, V.V. Diky, A. Kazakov*, J.W. Magee, J.A. Widegren and M. Frenkel, *National Institute of Standards and Technology, Boulder, CO, U.S.A.* and K.N. Marsh, *University of Canterbury, Christchurch, New Zealand*

-continued on next page-

Monday, July 31, 2006

Joint Session

Ionic Liquids 2

General

(continued)

Chair: K.R. Seddon

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-4

5:35 PM Excess Molar Volumes for Binary (Ionic Liquid + Methanol or Acetone) and Ternary (Ionic Liquid + Methanol + Acetone) Systems at T = 298.15 K, 303.15 K and 313.15 K and at Atmospheric Pressure

P. Bhujrajh and N. Deenadayalu*, *Durban Institute of Technology, Durban, KwaZulu-Natal, South Africa*

Monday, July 31, 2006

Joint Session

***Molecular Modeling, Including Simulation 2
Separations***

Chair: J. Vrabec

Afternoon 2 3:50 PM - 5:35 PM

Room: Bens-180

- 3:55 PM A Monte Carlo Study of Structure and Retention in Reversed-Phase Liquid Chromatography Systems**
J.I. Siepmann*, L. Zhang and J.L. Rafferty, *University of Minnesota, Minneapolis, MN, U.S.A.* and M.R. Schure, *Rohm and Haas Company, Spring House, PA, U.S.A.*
- 4:15 PM Separation of Gas Mixtures Using a Range of Zeolite Membranes: a Molecular Dynamics Study**
W. Jia and S. Murad*, *University of Illinois at Chicago, Chicago, IL, U.S.A.*
- 4:35 PM Molecular Dynamics Simulation of Oxygen Diffusion Through Self-Assembled Monolayers**
P. Srivastava* and W.G. Chapman, *Rice University, Houston, TX, U.S.A.* and P.E. Laibinis, *Vanderbilt University, Nashville, TN, U.S.A.*
- 4:55 PM Pore Size or Geometry: Which Determines the Shape and Inverse-Shape Selective Adsorption of Alkane Isomers?**
J.W. Jiang*, *National University of Singapore, Singapore, Singapore*
- 5:15 PM Adsorption of Benzene from Dilute Aqueous Solution**
R. Tscheliessnig, C. Horejs, W. Billes, M. Wendland* and J. Fischer, *University of Natural Resources and Applied Life Sciences, Vienna, Austria* and J. Kolafa, *Prague Institute of Chemical Technology, Prague, Czech Republic*

Monday, July 31, 2006

Joint Session

Molecular Modeling, Including Simulation 3

Phase Transitions

Chair: N. Matubayasi

Afternoon 2 3:50 PM - 5:35 PM

Room: Math-100

3:55 PM Using Molecular Simulation to Understand the Surface Phase Behavior of Fluids (Invited)

J.R. Errington*, *The State University of New York at Buffalo, Buffalo, NY, U.S.A.*

4:35 PM Determination of Wetting Transitions in Binary Mixtures at Three-Phase Coexistence Using Transition-Matrix Monte Carlo and Finite-Size Scaling

V.K. Shen*, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.* and J.R. Errington, *SUNY Buffalo, Buffalo, NY, U.S.A.*

4:55 PM Molecular Dynamics Simulation of the Structure, Dynamics, and Energetics of Water at Mineral Surfaces

A.G. Kalinichev*, *University of Illinois, Urbana, IL, U.S.A.*, J. Wang, *University of California at Davis, Davis, CA, U.S.A.* and R.J. Kirkpatrick, *University of Illinois, Urbana, IL, U.S.A.*

5:15 PM Modeling of the Carbon Dioxide Solubility in Imidazolium-Based Ionic Liquids with the tPC-PSAFT Equation of State

M.C. Kroon*, *Delft University of Technology, Delft, Netherlands*, E.K. Karakatsani and I.G. Economou, *National Center for Scientific Research "Demokritos", Attikis, Greece* and G.J. Witkamp and C.J. Peters, *Delft University of Technology, Delft, Netherlands*

Monday, July 31, 2006

16th Symposium

Properties of Polymers 2

Semicrystalline and Nanofilled Polymers

Chair: A. Karim and C. Snyder

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-151

**3:55 PM Dynamics and Thermodynamics of Nanofilled Polymers
(Invited)**

S. Kumar*, *Rensselaer Polytechnic Institute (RPI), Troy, NY, U.S.A.*

4:35 PM The Calorimetry of Nanophases of Macromolecules

B. Wunderlich*, *The University of Tennessee (and Oak Ridge National Laboratory, Oak Ridge, TN), Knoxville, TN, U.S.A.*

**4:55 PM Rigid Amorphous Fraction of Semicrystalline Polymers and
Polymer Nanocomposites**

A. Wurm*, A. Sargsyan and C. Schick, *University of Rostock, Rostock, Germany*

**5:15 PM Time-Domain Spectroscopy Analysis of the Amorphous
Phase in Semicrystalline Polycarbonate**

C.R. Snyder* and B.R. Conrad, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.* and H. Marand, A. Alizadeh and S. Sohn, *Virginia Tech, Blacksburg, VA, U.S.A.*

Monday, July 31, 2006

16th Symposium

Subsecond Thermophysics 2

Chair: G. Pottlacher and C. Cagran

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-200

3:55 PM Melting and Reorganization of Polymer Crystals Studied by Fast Scanning Calorimetry (10,000 K/s)

C. Schick* and A. Minakov, *University of Rostock, Rostock, Germany*

4:15 PM Radiance Temperature and Normal Spectral Emittance (In the Wavelength Range of 1.5 to 5 Micron) of Nickel at Its Melting Point by a Pulse-Heating Technique

K. Boboridis*, *University of Cyprus, Nicosia, Cyprus*, A. Seifter and A.W. Obst, *Los Alamos National Laboratory, Los Alamos, NM, U.S.A.* and D. Basak, *Orbital Sciences Corp., Dulles, VA, U.S.A.*

4:35 PM Cobalt in the Solid and the Molten States

C. Cagran*, *Graz University of Technology, Graz, Austria*

4:55 PM Modeling of Surface Tension and Viscosity Measurements by the Oscillating Drop Method Applied to Measurements with an Electromagnetic Levitation Device on Board Parabolic Flights

K. Higuchi*, *Gakushuin University, Tokyo, Japan* and R.K. Wunderlich and H.J. Fecht, *Ulm University, Ulm, Germany*

5:15 PM Relaxation of Extremely Superheated States of Liquids and Polymeric Compounds

A.V. Shishkin, P.V. Skripov, A.A. Smotriskiy* and A.A. Starostin, *Institute of Thermal Physics, Ekaterinburg, Russia*

Monday, July 31, 2006

16th Symposium

***Theory of Thermophysical Properties, Including Statistical
Mechanics 2***

Chair: J. Kincaid

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-265

3:55 PM The Nature of Liquid-Gas Asymmetry in Fluids (Invited)

M.A. Anisimov* and J.T. Wang, *University of Maryland,
College Park, MD, U.S.A.*

**4:35 PM Multiple Critical Points for Square-Wells with Repulsive
Shoulders: Renormalization Calculations Compared with
Simulations**

J.A. White*, *American University, Washington, DC, U.S.A.*

**4:55 PM Monte Carlo Simulations of Criticality and Tricriticality:
Finite-Size Scaling**

C.J. O'Keeffe*, R. Ren and G. Orkoulas, *University of
California, Los Angeles, Los Angeles, CA, U.S.A.*

5:15 PM Nonparametric Equation of State for Critical Fluids

P.P. Bezverkhy, V.G. Martynets* and E.V. Matizen, *Institute of
Inorganic Chemistry of Russian Academy of Science,
Novosibirsk, Russia*

Monday, July 31, 2006

19th ICCT / 61st CalCon

Thermochemistry and Molecular Energetics 2

Organic and Organometallic Systems

Chair: J. Boerio-Goates

Afternoon 2 3:50 PM - 5:35 PM

Room: Coors-5

- 3:55 PM Application of Correlation-Gas Chromatography to Problems in Thermochemistry (Invited)**
J.S. Chickos*, *University of Missouri-St. Louis, St. Louis, MO, U.S.A.*
- 4:35 PM Experimental and Computational Study on the Thermochemistry of Some Isomers of Bromoaniline**
M.A.V. Ribeiro da Silva*, A.I.M.C. Ferreira and J.R.B. Gomes, *Universidade do Porto, Porto, Portugal*
- 4:55 PM Combined Experiments to Measure Low Sublimation Pressures and Diffusion Coefficients of Organometallic Compounds**
M.A. Siddiqi* and B. Atakan, *University of Duisburg Essen, Duisburg, Germany*
- 5:15 PM The Enthalpies of Formation of Asparagine and Glutamine**
I. Contineanu and A. Neacsu, *Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania* and St. Perisanu*, *Polytechnic University of Bucharest, Bucharest, Romania*

Monday, July 31, 2006

Joint Session

**Databases, Data Systems, Software Applications, and
Correlations 2**

Session 2

Chair: D L. Morgan and A.I. Johns

Evening 7:30 PM - 9:35 PM

Room: Eng-245

**7:35 PM Database Tools for Evaluating Thermophysical Property
Data (Invited)**

R.L. Rowley*, *Brigham Young University, Provo, UT, U.S.A.*

**8:15 PM The NIST Chemistry WebBook: Chemical Informatics
Challenges**

P.J. Linstrom* and D.V. Tchekhovskoi, *National Institute of
Standards and Technology, Gaithersburg, MD, U.S.A.*

**8:35 PM Rapid Evaluation of Prediction Methods with DIPPR's
Automated Property Prediction Package**

W.V. Wilding*, J.R. Rowley, J.L. Oscarson and R.L. Rowley,
Brigham Young University, Provo, UT, U.S.A.

8:55 PM Web-Oracle Dissemination System for NIST/TRC Databases

C.D. Muzny*, V.V. Diky, R.D. Chirico and M. Frenkel, *National
Institute of Standards and Technology, Boulder, CO, U.S.A.*

**9:15 PM Windows-Based Version of the Software and Database
System for Reference Table Calculations**

V.S. Iorish*, *IVTAN Association of RAS, Moscow, Russia*
and G.V. Belov, *Moscow State University, Moscow, Russia*

Monday, July 31, 2006

19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 3

Properties of Electrolyte Systems, Including High Temperature

Chair: C. Panayiotou and T. Kimura

Evening 7:30 PM - 9:15 PM

Room: Coors-1

7:35 PM Organic Solutes in Hydrothermal Systems: Ionization Constants and Standard Partial Molar Volumes of Aqueous Hydroxy Carboxylic Acids, Amines and Amino Acids at Temperatures up to 335 °C and Functional Group Additivity Effects (Invited)

P.R. Tremaine* and E. Bulemela, *University of Guelph, Guelph, ON, Canada*

8:15 PM Solubility in Hydrometallurgical Processes

J. Salminen*, *University of California, Berkeley, CA, U.S.A.*
and T. Kaskiala and P. Kobylin, *Helsinki University of Technology, HUT, Helsinki, Finland*

8:35 PM Influence of Methanol Addition to the Speciation in the Water - CO₂ - Diethanolamine System

A. Archane, L. Gicquel, E. Provost and W. Fürst*, *Ecole Nationale Supérieure de Techniques Avancées, Paris, France*

8:55 PM Hydrothermal Synthesis, Heat Capacity Functions and Enthalpy of Formation for Sodium Titanium Hydroxyphosphate, Na₄Ti(OH)₂(PO₄)₂

M. Madekufamba*, L.N. Trevani and P.R. Tremaine, *University of Guelph, Guelph, ON, Canada*

Monday, July 31, 2006

Joint Session

Ionic Liquids 3

Gas Solubility

Chair: C.J. Peters

Evening 7:30 PM - 9:15 PM

Room: Coors-4

7:35 PM Thermodynamics of Solvation of Small Solutes on Ionic Liquids

M.F. Costa Gomes*, J. Jacquemin, P. Husson and A.A.H. Padua, *CNRS/Université Blaise Pascal, Aubière, France* and V. Majer, *Université Blaise Pascal/CNRS, Aubière, France*

7:55 PM Ionic Liquids As CO₂ Capture Media

J.K. Dixon*, M.J. Muldoon, J.L. Anderson, S.N.V.K. Aki, J.F. Brennecke and E.J. Maginn, *University of Notre Dame, Notre Dame, IN, U.S.A.*

8:15 PM Solubility of Some Single Gases in the Ionic Liquid [HMIM][Tf₂N]

G. Maurer*, *University of Kaiserslautern, Kaiserslautern, Germany*

8:35 PM Solvent Strength Effects on the Antisolvent Ability of CO₂ with Organic/IL Mixtures

B.R. Mellein*, R.L. Ladewski, S.N.V.K. Aki and J.F. Brennecke, *University of Notre Dame, Notre Dame, IN, U.S.A.*

8:55 PM Pure and Mixed Gas Solubilities in Tunable Ionic Liquids

J.L. Anderson*, D.J. Couling, D.G. Hert, S.N.V.K. Aki, J.K. Dixon, M.J. Muldoon and J.F. Brennecke, *University of Notre Dame, Notre Dame, IN, U.S.A.*

Monday, July 31, 2006

Joint Session

***Molecular Modeling, Including Simulation 4
Solvation***

Chair: S. Murad

Evening 7:30 PM - 9:15 PM

Room: Math-100

- 7:35 PM Free Energy of Solvation in the Method of Energy Representation**
N. Matubayasi*, *Kyoto University, Kyoto, Japan*
- 7:55 PM Solvation Structure of Ions in Water**
R.D. Mountain*, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*
- 8:15 PM Accurate Prediction of Key Electrolyte Properties Using a Chemical Physics Approach Based on Ion Solvation**
K.L. Gering*, *Idaho National Laboratory, Idaho Falls, ID, U.S.A.*
- 8:35 PM Calorimetry and Molecular Dynamics Simulations for Surfactant-Cyclodextrin Inclusion Complexes**
X. Banquy, N. Diaz-Vergara, Á. Piñeiro and M. Costas*, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*
- 8:55 PM Determining Stoichiometries and Equilibrium Constants of Supramolecular Complexes from Surface Tension, Isothermal Titration Calorimetry and Molecular Dynamics Simulations**
É. Tovar and A. García, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*, A. Villa and A.E. Mark, *Univ. of Groningen, Groningen, Netherlands*, X. Banquy, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*, A. Amigo, *Universidad de Santiago de Compostela, Santiago de Compostela, Spain* and S. Pérez-Casas and Á. Piñeiro*, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*

Monday, July 31, 2006

Joint Session

Molecular Modeling, Including Simulation 5

Crystallization-Melting

Chair: H. Torri

Evening 7:30 PM - 9:00 PM

Room: Bens-180

7:35 PM Homogenous Melting Mechanism in Superheated Crystals

G. Grimvall*, *Royal Institute of Technology, Stockholm, Sweden*

7:55 PM Microscopic Modeling of Current Spikes due to Phase Transitions at Electrode-Electrolyte Interfaces

I. Medved*, *Constantine the Philosopher University, Nitra, Slovakia* and D.A. Huckaby, *Texas Christian University, Fort Worth, TX, U.S.A.*

8:15 PM Simulation of Methane Hydrate Formation Employing a Model That Relates the Stochastic Nature of Crystallization and the Phase Equilibria

J.R. Avendano-Gomez*, R. Limas Ballesteros and M. Corea-Tellez, *Instituto Politecnico Nacional, México, DF, México*

8:35 PM Cluster Mechanism of Homogeneous Crystallization (Computer Study)

D.K. Belashchenko*, *Moscow Institute of Steel and Alloys, Moscow, Russia*

Monday, July 31, 2006

16th Symposium

Properties for Metallurgical Process Design 1

Chair: R. Overfelt and I. Egry

Evening 7:30 PM - 9:15 PM

Room: Eng-200

- 7:35 PM Measurement of the Thermophysical Properties of an NPL Thermal Conductivity Standard Stainless Steel 310**
- J. Blumm* and A. Lindemann, *NETZSCH-Geraetebau GmbH, Selb, Bavaria, Germany* and R. Campbell, *NETZSCH Instruments, Burlington, MA, U.S.A.*
- 7:55 PM Thermal Diffusivity Prediction of Liquid Metals with an Applied Magnetic Field**
- R.M. Banish* and Y.Y. Khine, *University of Alabama in Huntsville, Huntsville, AL, U.S.A.*
- 8:15 PM Thermal Diffusivity of the Aluminum Alloy Al-17Si-4Cu (A390) in the Solid and Liquid State**
- E. Kaschnitz*, *Oesterreichisches Giesserei-Institut, Leoben, Austria* and R. Ebner, *Materials Center Leoben, Leoben, Austria*
- 8:35 PM Thermal Diffusivity Measurements of Some Industrially Important Alloys by a Laser Flash Method**
- R.A. Abas*, *Royal Institute of Technology, Stockholm, Sweden*, M. Hayashi, *Tokyo Institute of Technology, Tokyo, Japan* and S. Seetharaman, *Royal Institute of Technology, Stockholm, Sweden*
- 8:55 PM Thermal Diffusivity/Conductivity of MgAlON-BN Composites**
- T. Matsushita* and Z.T. Zhang, *Royal Institute of Technology, Sweden, Stockholm, Sweden* and S. Seetharaman, *Royal Institute of Technology, Stockholm, Sweden*

Monday, July 31, 2006

16th Symposium

***Properties of Mesoscopic, Self-Assembled, and Strongly
Fluctuating Systems 2***

Chair: W. Köhler and M.A. Anisimov

Evening 7:30 PM - 9:15 PM

Room: Eng-1B40

**7:35 PM Apparent Mean-Field Criticality of Liquid-Liquid Phase
Transitions in Ionic Solutions (Invited)**

W. Schröer*, M. Wagner, O. Stanga and D. Saracsan,
University Bremen, Bremen, Germany

**8:15 PM Universal Behavior in Star Polystyrene + Methylcyclohexane
Systems Near the Critical Point**

D.T. Jacobs*, M.T. Wellons, S.J. Suddendorf, A.L. Triplett, M.
Lightfoot and N.L. Venkataraman, *The College of Wooster,
Wooster, OH, U.S.A.*

**8:35 PM Measurement of Diffusion in Ternary Liquid Mixtures by
Light Scattering Technique and Comparison with Data
Obtained by Taylor Dispersion**

D.A. Ivanov* and J. Winkelmann, *University Halle, Halle,
Germany*

**8:55 PM Light-Scattering Study of a Ternary Fluid Mixture Near the
Liquid-Vapor Critical Point**

V.N. Kouryakov*, *Russian Academy of Sciences, Moscow,
Russia*, E.E. Gorodetskii, *Oil and Gas Research Institute
of the Russian Academy of Sciences, Moscow, Russia* and
V.A. Deshabo, V.I. Kosov, D.I. Yudin and I.K. Yudin, *Russian
Academy of Sciences, Moscow, Russia*

Monday, July 31, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 2***

Biomacromolecules

Chair: D.P. Remeta

Evening 7:30 PM - 9:35 PM

Room: Coors-3

7:35 PM Progress in Designing Nucleic Acid Structures and Fine-Tuning Their Interactions (Invited)

H.H. Klump*, M. Chauhan, M. Mills and E. Lin, *University of Cape Town, Rondebosch, South Africa*

8:15 PM Specific DNA Binding by the Homeodomain Nkx2.5(C56S): Detection of Impaired DNA or Unfolded Protein by Isothermal Titration Calorimetry

E. Fodor* and A. Ginsburg, *NHLBI, NIH, Bethesda, MD, U.S.A.*

8:35 PM Alcohol-Salt Induced Partially Folded State of α -Lactalbumin and Energetics of ANS-Binding: Isothermal Titration Calorimetric and Spectroscopic Studies

R. Sharma* and N. Kishore, *Indian Institute of Technology Bombay, Powai, Mumbai, India*

8:55 PM Interactions of Magnesium and Calcium Chloride with Lysozyme: Thermodynamic and Spectrophotometric Approach

P. Patyar*, B.S. Lark and T.S. Banipal, *Guru Nanak Dev University, Amritsar, India*

Tuesday, August 01, 2006

Joint Session

**Databases, Data Systems, Software Applications, and
Correlations 3**

Session 3

Chair: C.D. Muzny and A.I. Johns

Morning 1 8:30 AM - 10:15 AM

Room: Eng-245

**8:35 AM Thermophysical Property Databases in Chemical
Engineering - A Survey of Existing Data Bases with the
Focus on Electrolyte Solutions (Invited)**

R. Sass*, *DECHEMA e.V., Frankfurt am Main, Germany*

**9:15 AM Infotherm: Thermophysical Data of Mixtures and Pure
Compounds**

J. Homann* and M. Schmidt, *FIZ CHEMIE Berlin, Berlin,
Germany*

**9:35 AM ThermoML: a New IUPAC Standard for Thermodynamic Data
Communication**

M. Frenkel*, R.D. Chirico, V.V. Diky and Q. Dong, *National
Institute of Standards and Technology, Boulder, CO, U.S.A.*,
K.N. Marsh, *University of Canterbury, Christchurch, New
Zealand*, J.H. Dymond, *University of Glasgow, Glasgow,
East Kilbride, U.K.*, W.A. Wakeham, *University of
Southampton, Southampton, Highfield, U.K.*, S.E. Stein,
*National Institute of Standards and Technology,
Gaithersburg, MD, U.S.A.*, E. Königsberger, *Murdoch
University, Murdoch, WA, Australia* and A.R.H. Goodwin,
*Schlumberger Technology Corporation, Sugar Land, TX,
U.S.A.*

**9:55 AM Website: a New Tool for Experts in the Development of the
International Thermodynamic Databases**

I.L. Khodakovsky*, *Dubna International University for Nature,
Society and Man, Dubna, Moscow Region, Russia*

Tuesday, August 01, 2006 19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 4

Properties of Electrolyte Systems, Including High Temperature

Chair: P.R. Tremaine and V.A. Durov

Morning 1 8:30 AM - 10:35 AM

Room: Coors-1

8:35 AM Osmotic Coefficients, Solubilities, and Deliquescence Relations in Mixed Aqueous Salt Solutions at Elevated Temperature

M.S. Gruszkiewicz* and D.A. Palmer, *Oak Ridge National Laboratory, Oak Ridge, TN, U.S.A.*

8:55 AM Modification of the RIII Model to Describe Interactions of Carbon Dioxide with Aqueous NaCl Solutions at Temperatures from 350 to 400 °C and Pressures from 18 to 40 MPa

C.J. Peterson*, J.L. Oscarson, B. Liu and R.M. Izatt, *Brigham Young University, Provo, UT, U.S.A.*

9:15 AM Standard Partial Molar Volumes of Aqueous Alkanolamines at Temperatures up to 325°C: Functional Groups Contributions

E. Bulemela* and P.R. Tremaine, *University of Guelph, Guelph, ON, Canada*

9:35 AM Physicochemical Properties of Bayer Liquors: Experimental Aspects

L.C. Königsberger*, E. Königsberger, G. Hefter and P.M. May, *Murdoch University, Murdoch, WA, Australia*

9:55 AM Physicochemical Properties of Bayer Liquors: A Comprehensive Model

E. Königsberger*, P.M. May and G. Hefter, *Murdoch University, Murdoch, WA, Australia*

-continued on next page-

Tuesday, August 01, 2006 19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 4

Properties of Electrolyte Systems, Including High Temperature

(continued)

Chair: P.R. Tremaine and V.A. Durov

Morning 1 8:30 AM - 10:35 AM

Room: Coors-1

**10:15 AM Application of Neural Network in Prediction of Activity
Coefficient in Single and Mixed Electrolyte Solution**

M.R. Dehghani*, *Research Institute of Petroleum Industry,
Iran*, H. Modarress, *Amir Kabir University of Technology,
Iran*, A. Bakhshi, *National Petrochemical Company, Iran*
and H. Manafi, *Research Institute of Petroleum Industry,
Iran*

Tuesday, August 01, 2006

16th Symposium

Instrumentation and Measurement Techniques 1

Chair: T.J. Bruno

Morning 1 8:30 AM - 9:55 AM

Room: Eng-105

8:35 AM Progress Towards a Determination of the Molar Gas Constant at INRIM

R.M. Gavioso* and G. Benedetto, *Istituto Nazionale di Ricerca Metrologica, Torino, Italy*

8:55 AM Johnson Noise Thermometry in the Range 505 K to 933 K Using Resistance-Based Scaling

W.L. Tew and J.R. Labenski*, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.* and S.W. Nam, S. P. Benz, P. Dresselhaus and C.J. Burroughs, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

9:15 AM Progress Towards a Primary Pressure Standard Based on the Dielectric Permittivity of Helium

R.M. Gavioso, *Istituto Nazionale di Ricerca Metrologica, Torino, Italy*, E.F. May, *University of Western Australia, Crawley, WA, Australia* and J.W. Schmidt* and M.R. Moldover, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

9:35 AM Will Acoustic Gas Thermometry Lead to a New Temperature Scale?

L. Pitre*, *Institut National de Métrologie, Saint Denis, France* and M.R. Moldover and W.L. Tew, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Tuesday, August 01, 2006

Joint Session

Ionic Liquids 4

Vapor-Liquid and Liquid-Liquid Equilibria

Chair: G. Maurer

Morning 1 8:30 AM - 10:15 AM

Room: Coors-4

- 8:35 AM High-Pressure Phase Equilibria of Binary and Ternary Systems with Ionic Liquids (Invited)**
A. Shariati, K.E. Gutkowski, L.J. Florusse and C.J. Peters*,
Delft University of Technology, Delft, Netherlands
- 9:15 AM Vapor-Liquid-Liquid Equilibria of Hydrofluorocarbons and 1-Butyl-3-Methylimidazolium Hexafluorophosphate**
M.B. Shiflett*, *DuPont Central Research and Development, Wilmington, DE, U.S.A.* and A. Yokozeki, *DuPont Fluoroproducts Laboratory, Wilmington, DE, U.S.A.*
- 9:35 AM Supercritical Fluid Chromatography As a Source of Solute Partition Coefficients in Room-Temperature Ionic Liquid-sc CO₂ Systems**
J. Planeta, P. Karasek and M. Roth*, *Academy of Sciences of the Czech Republic, Brno, Czech Republic*
- 9:55 AM Corresponding States Analysis and Criticality of the Liquid-Liquid Phase Transition of Ionic Liquids in Solution**
W. Schröer* and D. Saracsan, *University Bremen, Bremen, Germany*

Tuesday, August 01, 2006

Joint Session

Molecular Modeling, Including Simulation 6

Simulation Methods

Chair: A. Kalinichev

Morning 1 8:30 AM - 9:55 AM

Room: Math-100

8:35 AM Sequential Metropolis Algorithms for Fluid Simulations

R. Ren*, C.J. O'Keeffe and G. Orkoulas, *University of California, Los Angeles, Los Angeles, CA, U.S.A.*

8:55 AM Transient Molecular Dynamics Simulations of Viscosity and Thermal Diffusivity for Simple Fluids

J.C. Thomas* and R.L. Rowley, *Brigham Young University, Provo, UT, U.S.A.*

9:15 AM Replica-Exchange Molecular Dynamics Simulations on the Phosphorylation of Phospholamban at Ser16

Y. Sugita*, *University of Tokyo, Tokyo, Japan*

9:35 AM Thermodynamics of Roses-Toward Predictive Thermodynamic Models and Simulations

M. Stan*, J.C. Ramirez, P. Cristea, M.I. Baskes, S.M. Valone and Z. Hu, *Los Alamos National Laboratory, Los Alamos, NM, U.S.A.*

Tuesday, August 01, 2006

16th Symposium

Properties for Metallurgical Process Design 2

Chair: I. Egry and R. Overfelt

Morning 1 8:30 AM - 10:15 AM

Room: Eng-200

- 8:35 AM Establishment of Noncontact AC Calorimetry of High-Temperature Melts Using Solid Platinum Spheres as a Reference**
- H. Fukuyama*, H. Kobatake, I. Minato and T. Nakamura, *Tohoku University, Aoba-ku, Sendai, Japan*, T. Tsukada, *Osaka Prefecture University, Sakai, Osaka, Japan* and S. Awaji, *Tohoku University, Aoba-ku, Sendai, Japan*
- 8:55 AM Noncontact AC Calorimetry of Liquid Silicon with Suppressing Convections in a Static Magnetic Field**
- H. Kobatake*, H. Fukuyama, I. Minato and T. Nakamura, *Tohoku University, Aoba-ku, Sendai, Japan*, T. Tsukada, *Osaka Prefecture University, Osaka, Sakai, Japan* and S. Awaji, *Tohoku University, Aoba-ku, Sendai, Japan*
- 9:15 AM High Temperature Emissivity of High Purity Titanium and Zirconium**
- G. Teodorescu*, P.D. Jones, R.A. Overfelt and B. Guo, *Auburn University, Auburn, AL, U.S.A.*
- 9:35 AM Measurements of Heat Capacity of Titanium and Zirconium by Electromagnetic Levitation**
- B. Guo*, G. Teodorescu, R.A. Overfelt and P.D. Jones, *Auburn University, Auburn, AL, U.S.A.*
- 9:55 AM Benard-Marangoni Instability as Possible Modifier of Surface Alloy Composition**
- Y.W. Kim*, *Lehigh University, Bethlehem, PA, U.S.A.*

Tuesday, August 01, 2006

16th Symposium

***Properties of Mesoscopic, Self-Assembled, and Strongly
Fluctuating Systems 3***

Chair: M.E. Fisher and M.A. Anisimov

Morning 1 8:30 AM - 10:15 AM

Room: Eng-1B40

8:35 AM Mesoscopic Theory for Highly Charged Colloids in Pure Water (Invited)

A. Ciach* and W.T. Gozdz, *Polish Academy of Sciences, Warsaw, Poland* and G. Stell, *State University of New York, Stony Brook, NY, U.S.A.*

9:15 AM Critical Phenomena and Crossovers in Colloidal Dispersions

D. Pini*, *Università di Milano, Milano, Italy*, F. Lo Verso, *Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany*, A. Parola, *Università dell'Insubria, Como, Italy* and L. Reatto, *Università di Milano, Milano, Italy*

9:35 AM Thermal Patterning of a Critical Polymer Blend

W. Köhler*, A. Voit, A. Krekhov, W. Enge and L. Kramer (deceased), *University of Bayreuth, Bayreuth, Germany*

9:55 AM Viscous Properties of Ferrofluids from Dynamic Light Scattering

B. Rathke*, J. Patzke and S. Will, *Universität Bremen, Bremen, Germany*

Tuesday, August 01, 2006

16th Symposium

Properties of Polymers 3

General 2

Chair: C. Snyder and A. Karim

Morning 1 8:30 AM - 10:15 AM

Room: Eng-151

8:35 AM Conformational Heat Capacity of Liquid Poly(Vinyl Methyl Ether) in the Absence and Presence of Water

M. Pyda* and E. Nowak-Pyda, *The University of Tennessee (and Oak Ridge National Laboratory, Oak Ridge, TN), Knoxville, TN, U.S.A.*, B. Wunderlich, *The University of Tennessee (and Oak Ridge National Laboratory), Knoxville, TN, U.S.A.* and K. Van Durme and B. Van Mele, *Vrije Universiteit, Brussels, Belgium*

8:55 AM Thermodynamic Characteristics and Physico-Chemical Properties of Polymethacrylic Acid and Its Blends with Water

V.F. Uryash*, S.V. Chuprova, N.Yu. Kokurina, V.N. Larina and V.A. Izvozchikova, *Nizhny Novgorod State University, Nizhny Novgorod, Russia*

9:15 AM Measurements of the PMMA by Pulse Transient Method: Methodology for the Determination of the Thermophysical Parameters Including the Heat Transfer Coefficient

L. Kubicar*, P. Dieska, V. Bohac, V. Vretenar and S. Barta, *Institute of Physics SAS, Bratislava, Slovakia*

9:35 AM Biocompatible Polymers Characterization by IGC

I. Kikic*, P. Alessi and F. Vecchione, *University of Trieste, Trieste, Italy*

9:55 AM Solubilities, Thermostabilities and Flame Retardance Behaviour of Phosphorus Containing Flame Retardants and Copolymers

L. Wang*, Jihua Kong, R. Wang and Yong Liu, *Beijing Institute of Technology, Beijing, China*

Tuesday, August 01, 2006

16th Symposium

Theory of Thermophysical Properties, Including Statistical Mechanics 3

Chair: J. Kincaid

Morning 1 8:30 AM - 10:15 AM

Room: Eng-265

- 8:35 AM A New *Ab Initio* Interaction Potential for CO-CO and Calculation of Some Selected Thermophysical Properties**
R. Hellmann*, E. Bich and E. Vogel, *University of Rostock, Rostock, Germany*
- 8:55 AM Enthalpies of Formation of Organophosphorous Compounds Determined by Current Methods of Computational Quantum Chemistry**
O.V. Dorofeeva*, Y.V. Vishnevskiy and N.F. Moiseeva, *Moscow State University, Moscow, Russia*
- 9:15 AM Transferable Potentials for Mixed Alcohol-Amine Interactions**
J.R. Elliott, Jr.* and N.H. Gray, *The University of Akron, Akron, OH, U.S.A.*
- 9:35 AM A Weighting Matrix Approach As a Substituent for Binary Interaction Parameters**
A. Al-matar*, *University of Jordan, Amman, Jordan*
- 9:55 AM Prediction of Missing UNIFAC Group-Interaction Parameters through Connectivity Indices**
H.E. González-Villalba*, *Technical University of Denmark, Lyngby, Denmark*, B. Le Bert, *Université Claude Bernard Lyon 1, Villeurbanne, France* and J. Abildskov and R. Gani, *Technical University of Denmark, Lyngby, Denmark*

Tuesday, August 01, 2006 19th ICCT / 61st CalCon

Thermochemistry and Molecular Energetics 3

Inorganic Materials

Chair: A. Navrotsky

Morning 1 8:30 AM - 10:15 AM

Room: Coors-5

8:35 AM Model-Free Kinetic Analysis: Getting the Most from Your DSC Data -James J. Christensen Award Lecture- (Invited)

S. Vyazovkin*, *University of Alabama at Birmingham, Birmingham, AL, U.S.A.*

9:15 AM The Energetics of Hematite Dissolution in Iron Ore Melts for Assimilation in Commercial Sintering Processes: *In Situ* High Temperature Calorimetric Studies

R. Morcos* and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.* and B. Ellis, *BHP Research, Shortland, NSW, Australia*

9:35 AM Synthesis, Characterization and Thermodynamic Properties of the Phosphates $\text{NaM}_2(\text{PO}_4)_3$ and $\text{Na}_5\text{M}(\text{PO}_4)_3$ (M = Ti, Zr, Hf) - IACT Doctorate Award Presentation -

V.I. Pet'kov, E.A. Asabina*, A.V. Markin and N.N. Smirnova, *Nizhni Novgorod State University, Nizhni Novgorod, Russia*

9:55 AM Comparative Studies of the Thermophysical Properties of Crystalline and Vitreous Alkali Tri-And Tetrasilicates

D.A. Johnson, *Spring Arbor University, Spring Arbor, MI, U.S.A.* and S.W. Barber, A.K. Labban, R. Berg, M. Zhou and E.F. Westrum, Jr.*, *University of Michigan, Ann Arbor, MI, U.S.A.*

Tuesday, August 01, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 3
Calorimetry of Biological Systems***

Chair: N. Wright

Morning 1 8:30 AM - 10:15 AM

Room: Coors-3

**8:35 AM A Calorimetric Investigation of the B to Z Transition in a
Model DNA Oligonucleotide**

R.D. Sheardy* and J. Ferreira, *Seton Hall University, South
Orange, NJ, U.S.A.*

8:55 AM DNA and RNA Duplex Stability by ITC and DSC

B.E. Lang*, *National Institute for Standards and Technology,
Rockville, MD, U.S.A.* and F.P. Schwarz, *Center for
Advanced Research in Biotechnology/National Institute for
Standards and Technology, Rockville, MD, U.S.A.*

9:15 AM Which Calorimeter Is the Best?

L.D. Hansen*, *Brigham Young University, Provo, UT,
U.S.A.* and D.J. Russell, *Calorimetry Sciences
Corporation, Lindon, UT, U.S.A.*

**9:35 AM Solution Calorimetry As a Tool to Assess Swelling of
Polymer Blends and Hydrogels**

S. Conti, *Pavia University, Pavia, Italy*, S. Gaisford* and G.
Buckton, *University of London, London, U.K.* and U. Conte,
Pavia University, Pavia, Italy

**9:55 AM Thermodynamic Study of 8-Hydroxyquinoline by Adiabatic
Calorimetry and Thermal Analysis**

Yan-Sheng Li and S.-X. Wang, *Dalian Jiaotong University,
Dalian, China* and Z.-C. Tan* and Li-Xian Sun, *Chinese
Academy of Sciences, Dalian, China*

Tuesday, August 01, 2006

Joint Session

**Databases, Data Systems, Software Applications, and
Correlations 4**

Session 4

Chair: J.C. Sanchez Ochoa and M.L. Huber

Morning 2 10:35 AM - 12:20 PM

Room: Eng-245

10:40 AM Generalization of the Friction Theory for Viscosity Modeling

S.E. Quiñones-Cisneros* and U.K. Deiters, *University of
Cologne, Köln, Germany*

**11:00 AM Inclusion of Physical Terms in a Simultaneously Optimized
Equation of State for the Description of Associating Fluids**

L. Piazza*, G. Herres and R. Span, *University of Paderborn,
Paderborn, Germany*

**11:20 AM Improvement of the Two Parameter Cubic Equation of State
to Represent Vapor Pressure of Pure Compound**

L.A. Galicia-Luna*, *Instituto Politécnico Nacional, México,
DF, México*

**11:40 AM Quantification of Uncertainties in Experimental Data for
Thermodynamic and Transport Properties**

K. Zou, N. Kumar and A.S. Lawal*, *Texas Tech University,
Lubbock, TX, U.S.A.*

**12:00 PM A Comparison of Scaling Models of Thermodynamic
Properties Along the Coexistence Curve Including the
Critical Point**

E.E. Ustjuzhanin*, *Moscow Power Engineering Institute,
Moscow, Russia*, I.M. Abdulagatov, *Russian Academy of
Sciences, Makhachkala, Dagestan, Russia*, P.V. Popov and
V.A. Rykov, *Moscow Power Engineering Institute, Moscow,
Russia* and J. Jata, *Kyoto Institute of Technology, Kyoto,
Japan*

Tuesday, August 01, 2006 19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 5

Properties of Electrolyte Systems, Including High Temperature

Chair: T. Tominaga and J. Salminen

Morning 2 10:35 AM - 12:40 PM

Room: Coors-5

10:40 AM Glyme-Lithium Salt Thermal Phase Behavior

W.A. Henderson*, *U.S. Naval Academy, Annapolis, MD, U.S.A.*

11:00 AM The Effect of Temperature on the Activity Coefficients of Two Macrocyclic Amines in Aqueous Solution

L.H. Blanco*, *Universidad Nacional de Colombia, Bogotá, D.C, Colombia* and M.T. Davila, *Universidad Nacional de Colombia, Sede Manizales, Manizales, Colombia*

11:20 AM Effect of Temperature on the Activity Coefficient of Amino Acids in Aqueous Solutions

C.M. Romero* and M.E. González, *Universidad Nacional de Colombia, Bogotá, D.C, Colombia*

11:40 AM Solvent Effects on Complexation of Nitrilotriacetic Acid with Molybdenum(V) in Different Aqueous Solutions of Methanol

K. Zare*, *Islamic Azad University, Tehran, Iran* and F. Gharib, *Shahid Beheshti University, Tehran, Evin, Iran*

12:00 PM Relationship Between Ionic Strength Dependence Patterns, Stability and Structure of Some Dioxovanadium(V), Molybdenum(VI) and Tungsten(VI) Complexes with Aminoacids and Aminopolycarboxylic Acids in Different Sodium Perchlorate Aqueous Solutions

K. Majlesi*, *Islamic Azad University, Tehran, Iran* and K. Zare, *Shahid Beheshti University, Tehran, Iran*

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Tuesday, August 01, 2006 19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 5

Properties of Electrolyte Systems, Including High Temperature

(continued)

Chair: T. Tominaga and J. Salminen

Morning 2 10:35 AM - 12:40 PM

Room: Coors-5

12:20 PM Cooperative Hydrogen Bonding in Solution

B.N. Solomonov* and M.A. Varfolomeev, *Kazan State University, Kazan, Russia*

Tuesday, August 01, 2006

16th Symposium

Instrumentation and Measurement Techniques 2

Chair: K. E. Miller and T.J. Bruno

Morning 2 10:35 AM - 12:00 PM

Room: Eng-105

10:40 AM Apparatus for Advanced Distillation Curve Measurement of Complex Fluids

T.J. Bruno*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

11:00 AM Advanced Distillation Curve Measurement: Case Studies on Complex Fluids

T.J. Bruno and B.L. Smith*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

11:20 AM Design of a Single Cell Ebulliometer for Vapor Pressure Measurement up to 3 MPa

V.B. Miller* and S.G. Penoncello, *University of Idaho, Moscow, ID, U.S.A.*

11:40 AM A Novel Method to Measure Saturated Vapor Pressures of Subliming Solids

P.A. Russell*, *University of Teesside, Tees Valley, Middlesbrough, U.K.* and G. Mason, I.W. Cumming and K. Hellgardt, *Loughborough University, Loughborough, Leicestershire, U.K.*

Tuesday, August 01, 2006

Joint Session

Ionic Liquids 5

Calorimetry

Chair: J.W. Magee

Morning 2 10:35 AM - 12:40 PM

Room: Coors-4

**10:40 AM Thermodynamic Properties and Polymorphism of
Bis(Trifluoromethanesulfonyl)Imide Ionic Liquids
- IACT Doctorate Award Presentation -**

Y.U. Paulechka*, A.V. Blokhin, G.J. Kabo and A.G. Kabo,
Belarusian State University, Minsk, Belarus

**11:00 AM Low Temperature Heat Capacity of 1-Hexyl-3-
Methylimidazolium Bis(Trifluoromethylsulfonyl)Imide**

Y. Shimizu*, *National Institute of Advanced Industrial
Science and Technology (AIST), Tsukuba, Ibaraki, Japan*, Y.
Ohte, *National Metrology Institute of Japan, Tsukuba,
Ibaraki, Japan*, Y. Yamamura and K. Saito, *University of
Tsukuba, Tsukuba, Ibaraki, Japan* and T. Atake, *Tokyo
Institute of Technology, Midori-ku, Yokohama, Japan*

**11:20 AM Thermal, Transport, and Electrochemical Studies of Ionic
Liquids for Lithium Ion Battery Systems**

J. Salminen* and J.M. Prausnitz, *University of California,
Berkeley, CA, U.S.A.* and J. Newman, *University of
California, Berkeley, Berkeley, CA, U.S.A.*

**11:40 AM Thermodynamic Investigation of a Room Temperature Ionic
Liquid: Heat Capacity, Standard Enthalpy of Formation and
Heat of Reaction for Synthesis of EMIES**

Z.-H. Zhang*, Z.-C. Tan, Li-Xian Sun, Q. Shi and B. Tong,
Chinese Academy of Sciences, Dalian, China

**12:00 PM Thermodynamics of Ionic Liquids Based on Transitional
Metal - Giaque Travel Award Presentation -**

Q.-G. Zhang*, *Chinese Academy of Science, Xining, China*

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Tuesday, August 01, 2006

Joint Session

Ionic Liquids 5

Calorimetry

(continued)

Chair: J.W. Magee

Morning 2 10:35 AM - 12:40 PM

Room: Coors-4

12:20 PM Studies on Thermo-Chemical Properties of a New Ionic Liquid Prepared by Mixing 1-Methyl-3-Pentylimidazolium Chloride with InCl_3

Wei Guan*, *Liaoning University, Shenyang, China*, J. Tong, *Chinese Academy of Science, Xining, China* and H. Wang and Lei Li, *Liaoning University, Shenyang, China*

Tuesday, August 01, 2006

Joint Session

***Molecular Modeling, Including Simulation 7
Transport***

Chair: S. Okazaki

Morning 2 10:35 AM - 12:00 PM

Room: Math-100

10:40 AM Molecular Simulation of the Shear Viscosity and Phase Behavior of Dendrimers

R.J. Sadus*, *Swinburne University of Technology, Hawthorn, Victoria, Australia*

11:00 AM Non-equilibrium Simulation of Polymer Shear Flow via Dynamic Monte Carlo

J.R. Dorgan*, *Colorado School of Mines, Golden, CO, U.S.A.*

11:20 AM Transport Properties of Anisotropic Polar Fluids by Molecular Dynamics: Systematic Study and Predictive Application to Real Fluids

J. Vrabec*, G.A. Fernandez and H. Hasse, *University of Stuttgart, Stuttgart, Germany*

11:40 AM Time-Domain Calculations of the Polarized Raman Spectra and the Transient IR Absorption Anisotropy of the OH Stretching Mode of Liquid Water

H. Torii*, *Shizuoka University, Shizuoka, Japan*

Tuesday, August 01, 2006 19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 1***

Theory I

Chair: U.K. Deiters and T.W. de Loos

Morning 2 10:35 AM - 12:20 PM

Room: Coors-1

**10:40 AM The Development of Soft-SAFT As a Versatile Molecular-
Based Equation of State: Phase, Interface, and Derivative
Properties Extensions (Invited)**

L.F. Vega, Consejo Superior de Investigaciones
Cientificas, Barcelona, Bellaterra, Spain*

**11:20 AM Application of the PC-SAFT Equation of State Model to Solid-
Liquid Equilibrium at High Pressures**

P.K. Jog, The Dow Chemical Company, Midland, MI,
U.S.A. and T. Laursen, VLXE, Copenhagen, Denmark*

**11:40 AM A Molecular Formulation of the Activity Coefficients and
Their Reference Fugacities for Supercritical Fluid States**

L.L. Lee, California State University, Pomona, CA, U.S.A.*

**12:00 PM Effects of Three-Body and Bonding Interactions on Phase
Separation in an Exactly Solvable Ternary or Binary Solution
on the Honeycomb and Bethe Lattices**

*R.P. Lungu, University of Bucharest, Bucharest-Magurele,
Romania, D.A. Huckaby*, Texas Christian University, Fort
Worth, TX, U.S.A. and F.D. Buzatu, National Institute for
Physics and Nuclear Engineering, Bucharest-Magurele,
Romania*

Tuesday, August 01, 2006

16th Symposium

Properties for Metallurgical Process Design 3

Chair: I. Egry and R. Overfelt

Morning 2 10:35 AM - 12:20 PM

Room: Eng-200

10:40 AM The Metastable Miscibility Gap in the Cu-Co-Fe System

S. Curiotto*, *Risø National Laboratory, Roskilde, Denmark*, R. Greco and M. Palumbo, *Università di Torino, Torino, Italy*, N.H. Pryds, *Risø National Laboratory, Roskilde, Denmark*, E. Johnson, *University of Copenhagen, Copenhagen, Denmark* and L. Battezzati, *Università di Torino, Torino,*

11:00 AM Wetting Transitions in Binary Subregular Liquid Alloys

C. Antion and D. Chatain*, *CNRS, Campus de Luminy, Marseille, France*

11:20 AM Density and Surface Tension of Liquid Ternary Cu-Co-Fe Alloys

J. Brillo*, *German Aerospace Center, Köln, Germany* and I. Egry, *German Aerospace Center, Köln, Germany*

11:40 AM Phase Transitions and Instabilities at Fluid Metal/Vapor Interfaces

W. Freyland*, *University of Karlsruhe, Karlsruhe, Germany*

12:00 PM Liquid-Liquid Interfacial Tension in Ternary Monotectic Alloys Al-Bi-Cu and Al-Bi-Si

I. Kaban, W. Hoyer and M. Kehr*, *Chemnitz University of Technology, Chemnitz, Germany*

Tuesday, August 01, 2006

16th Symposium

***Properties of Mesoscopic, Self-Assembled, and Strongly
Fluctuating Systems 4***

Chair: D.T. Jacobs and M.A. Anisimov

Morning 2 10:35 AM - 12:20 PM

Room: Eng-1B40

10:40 AM Line of Critical Points and the Giant Electromechanical Response in a Ferroelectric Relaxor System (Invited)

Z. Kutnjak*, *J. Stefan Institute, Ljubljana, Slovenia*, J. Petzelt, *Academy of Sciences of the Czech Republic, Prague, Czech Republic* and R. Blinc, *J. Stefan Institute, Ljubljana, Slovenia*

11:20 AM Multinuclear NMR Study of Supramolecular Restructuring in Organic Solute/H₂O/Ions Systems

V. Balevicius*, *Vilnius University, Vilnius, Lithuania* and H. Fuess, *University of Technology Darmstadt, Darmstadt, Germany*

11:40 AM Rheology and Microrheology in Worm-Like Micelles

J. Galvan-Miyoshi, J. Delgado and R. Castillo*, *UNAM, México, DF, México*

12:00 PM On Some Peculiarities of Pre-Transitional Behavior of the Relaxation Time of Order Parameter Fluctuations in Isotropic Phase of Nematic Liquid Crystals

D.I. Semenov*, *Samarkand State University, Samarkand, Uzbekistan*

Tuesday, August 01, 2006

16th Symposium

Properties of Polymers 4

Diffusion, Sorption, and Permeation in Polymers

Chair: A. Karim and C. Snyder

Morning 2 10:35 AM - 12:20 PM

Room: Eng-151

10:40 AM Temperature Dependent Permeation of Water Vapor Through Barrier Foils

M. Koehl*, D. Philipp, O. Angeles and H.R. Wilson,
Fraunhofer Institute for Solar Energy Systems, Freiburg, Germany

11:00 AM Polymer Microstructures: Modification and Characterisation by Fluid Sorption

S.A.E. Boyer*, *Tokyo Metropolitan University, Tokyo, Japan*
and M. Baba, J.M. Nedelec and J.P.E. Grolier, *Blaise Pascal University, Aubière, France*

11:20 AM Measurement of the Concentration Dependence of the Mutual Diffusion Coefficient in Polymer Solutions Using the Soret Forced Rayleigh Scattering Method

Y. Yamamoto*, M. Niwa and Y. Nagasaka, *Keio University, Yokohama, Kanagawa, Japan*

11:40 AM Thermal Expansion of Polymers Submitted to Supercritical Carbon Dioxide As a Function of Pressure

S.A.E. Boyer, *Blaise Pascal University, Aubière, France*,
S.L. Randzio, *Polish Academy of Sciences, Warsaw, Poland* and J.P.E. Grolier*, *Blaise Pascal University, Aubière, France*

12:00 PM CO₂ Separation from Nitrogen Using Membranes Made of Poly(2,4-dimethyl-1,6-phenylene oxide) and Its Bromine Derivatives

X.H. Hu*, H.C. Cong, A.B. Blasig, Y.S. Shen and M.R. Radosz,
University of Wyoming, Laramie, WY, U.S.A.

Tuesday, August 01, 2006

16th Symposium

Properties of Working Fluids, Including Refrigerants 1
Equations of State

Chair: M. O. McLinden and R. R. Singh

Morning 2 10:35 AM - 12:20 PM

Room: Eng-265

10:40 AM Thermophysical Properties of R410A Correlated by the Patel-Teja Equation of State

R. Akasaka*, *Kyushu Lutheran College, Kumamoto City, Kurokami, Japan*, Y. Kayukawa, *National Institute of Advanced Industrial Science and Technology (AIST), National Metrology Institute of Japan (NMIJ), Tsukuba, Japan* and N. Kagawa, *National Defense Academy, Hashirimizu, Yokosuka, Japan*

11:00 AM Debye Fluid State Equations for Helium

V. Arp, *Cryodata Inc., Boulder, CO, U.S.A.* and G.B. Chen and Y.H. Huang*, *Zhejiang University, Zhejiang, China*

11:20 AM Study on the Interaction Coefficients in PR Equation with vdW Mixing Rules for HFC and HC Binary Mixtures

J.X. Chen and P. Hu*, *University of Science and Technology of China, China* and Z.S. Chen, *University of Science and Technology of China, Hefei, Anhui, China*

11:40 AM A New Reference Quality Equation of State for Sulfur Hexafluoride

C. Guder* and W. Wagner, *Ruhr-Universität Bochum, Bochum, Germany*

12:00 PM A Reference Equation of State for the Thermodynamic Properties of Propane for Temperatures from the Melting Line to 650 K and Pressures Up to 1000 MPa

E.W. Lemmon* and M.O. McLinden, *National Institute of Standards and Technology, Boulder, CO, U.S.A.* and W. Wagner, *Ruhr-Universität Bochum, Bochum, Germany*

Tuesday, August 01, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 4
Biomedicine and Pharmaceuticals***

Chair: L.D. Hansen and D.P. Remeta

Morning 2 10:35 AM - 11:40 AM

Room: Coors-3

**10:40 AM Prediction of Sepsis in Neonate Blood: An Isothermal
Calorimetric Study**

C. Ling, C. Tuleu, A.E. Beezer, M. O'Neill*, S. Gaisford, P. Long
and I. Wong, *University of London, London, U.K.*

11:00 AM Temperature Scanning Structural Study on Stratum Corneum

I. Hatta*, *Fukui University of Technology, Fukui, Japan* and
N. Ohta, K. Inoue and N. Yagi, *Japan Synchrotron Radiation
Research Institute/Spring-8, Hyogo, Japan*

**11:20 AM The Potential of 2-Nitrobenzaldehyde As a Chemical Test
and Reference Reaction for Photocalorimetry - Giaque
Travel Award Presentation -**

M. Dhuna*, S. Gaisford, M.A.A. O'Neill and A.E. Beezer,
University of London, London, U.K., J.A. Connor,
*University of Greenwich, Medway Campus, Chatham
Maritime, Kent, U.K.* and D. Clapham, *GlaxoSmithKline,
Harlow, Essex, U.K.*

Tuesday, August 01, 2006

Joint Session

Plenary 4

Awards

Chair: M. Frenkel and D.G. Friend

Afternoon 1 1:45 PM - 3:30 PM

Room: UMC Ballroom

**1:50 PM Calorimetry of Nanoparticles, Surfaces, Interfaces, Thin
Films, and Multilayers - The Rossini Award Lecture - (Invited)**

A. Navrotsky*, *University of California at Davis, Davis, CA,
U.S.A.*

**2:40 PM A New Tool for an Old Job: Using Fixed Cell Scanning
Calorimetry to Investigate Dilute Aqueous Solutions
-The Hugh M. Huffman Memorial Award Lecture - (Invited)**

E.M. Woolley*, *Brigham Young University, Provo, UT,
U.S.A.*

Tuesday, August 01, 2006

Joint Session

Plenary 5

Awards

Chair: D.G. Friend and M. Frenkel

Afternoon 2 3:50 PM - 5:35 PM

Room: UMC Ballroom

**3:55 PM A Scientific Approach to Teaching Science - Fourth
Touloukian Memorial Lecture- (Invited)**
Carl Wieman*, *University of Colorado, Boulder, CO, U.S.A.*

4:55 PM Award Presentations and Reception

Wednesday, August 02, 2006

Joint Session

Plenary 6

Chair: W.M. Haynes and M. Frenkel

Morning 1 8:30 AM - 10:15 AM

Room: UMC Ballroom

***Thermodynamics and Properties in the Biological,
Medical, Pharmaceutical, Agricultural and Food Sectors***

**8:35 AM Thermodynamic Problems in Structural Molecular Biology
(Invited)**

P.L. Privalov*, *Johns Hopkins University, Baltimore, MD,
U.S.A.*

***Databases, Data Systems, Software Applications, and
Correlations***

9:25 AM Life, Data and Everything (Invited)

M.A. Satyro*, *Virtual Materials Group, Inc., Calgary, AB,
Canada*

Fluid Property Measurements 3

Chair: R. Srivastava

Morning 2 10:35 AM - 12:20 PM

Room: Eng-1B40

10:40 AM Liquid - Liquid - Vapor Phase Equilibria of Binary Carbon Dioxide + Formic Acid Mixture System

Jihoon Im*, G. Lee and Hwayong Kim, *Seoul National University, Seoul, Korea*

11:00 AM Association and Viscosity of Methanol-Triethylamine Vapor Mixtures

E. Vogel* and V. Teske, *University of Rostock, Rostock, Germany*

11:20 AM Measurement and Calculation of Multicomponent Diffusion Coefficients in Liquids

S. Rehfeldt* and J. Stichlmair, *Technical University Munich, Garching, Germany*

11:40 AM Turbidity and Related Properties Very Near the Critical Point of SF₆, from Measurements Under Weightlessness

C. Lecoutre-Chabot*, Y. Garrabos, D. Beysens and F. Palencia, *CNRS, Pessac Cedex, France*

12:00 PM High-Accuracy Measurements of the Electric and Magnetic Susceptibilities of O₂ and H₂ using a Quasi-Spherical Resonator and a Cross Capacitor

E.F. May*, *University of Western Australia, Crawley, WA, Australia* and M.R. Moldover and J.W. Schmidt, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Instrumentation and Measurement Techniques 3

Chair: L. Ott and T.J. Bruno

Morning 2 10:35 AM - 12:20 PM

Room: Eng-245

10:40 AM An Automated Densimeter for Rapid Screening of Industrial Fluids

S.L. Outcalt* and M.O. McLinden, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

11:00 AM Force Transmission Errors in Magnetic Suspension Densimeters

M.O. McLinden*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.* and R. Kleinrahm and W. Wagner, *Ruhr-Universität Bochum, Bochum, Germany*

11:20 AM Magnetic Effects on Fluid-Density Measurement in a Magnetic-Levitation Densimeter

Y. Kano*, *Keio University, Yokohama, Kohoku-ku, Japan*, Y. Kayukawa and K. Fujii, *National Institute of Advanced Industrial Science and Technology (AIST), National Metrology Institute of Japan (NMIJ), Tsukuba, Japan* and H. Sato, *Keio University, Yokohama, Kohoku-ku, Japan*

11:40 AM Precision Containerless Density Measurements of $\text{Zr}_6\text{Ni}_8\text{Cu}_2\text{Al}_{10}$

R.C. Bradshaw* and M.E. Warren, *University of Massachusetts, Amherst, MA, U.S.A.*, J.R. Rogers, *NASA-MSFC, Huntsville, AL, U.S.A.*, T.J. Rathz, *University of Alabama in Huntsville, Huntsville, AL, U.S.A.*, A.K. Gangopadhyay and K.F. Kelton, *Washington University, St. Louis, MO, U.S.A.* and R.W. Hyers, *University of Massachusetts, Amherst, MA, U.S.A.*

-continued on next page-

Wednesday, August 02, 2006

16th Symposium

Instrumentation and Measurement Techniques 3

(continued)

Chair: L. Ott and T.J. Bruno

Morning 2 10:35 AM - 12:20 PM

Room: Eng-245

12:00 PM Development of a Cryogenic Adiabatic Calorimeter Using a Pulse-Tube Cryocooler

H. Kato*, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*, A. Tateno, S. Goto and I. Aoki, *Jecc Torisha Co., Ltd., Kawagoe, Saitama, Japan*, H. Kawaji, *Tokyo Institute of Technology, Yokohama, Kanagawa, Japan* and T. Atake, *Tokyo Institute of Technology, Midori-ku, Yokohama, Japan*

Wednesday, August 02, 2006

16th Symposium

Photothermal and Photoacoustic Techniques 1

Chair: G.J. Diebold

Morning 2 10:35 AM - 12:40 PM

Room: Eng-155

10:40 AM Investigations of Thermal Physical Properties and Utilizations of Room Temperature Ionic Liquids by Transient Grating and Thermal Lens Techniques (Invited)

C. Frez and G.J. Diebold, *Brown University, Providence, RI, U.S.A.* and C.D. Tran*, S. Yu, S. Challa and M. Franko, *Marquette University, Milwaukee, WI, U.S.A.*

11:20 AM Pulsed Laser Opto-Acoustic Measurements in Solids from Macro- to Nano-Scale (Invited)

S.N. Jerebtsov, A.A. Kolomenskii and H.A. Schuessler*, *Texas A&M University, College Station, TX, U.S.A.*

12:00 PM Transient Grating Signals from Particulate Suspensions

C. Frez and G.J. Diebold*, *Brown University, Providence, RI, U.S.A.*

12:20 PM Optoacoustic Processes in Highly Diluted Suspensions of Gold Nanoparticles

S.V. Egerev*, *Andreyev Acoustics Institute, Moscow, Russia* and A.A. Oraevsky, *Fairway Medical Technologies, Houston, TX, U.S.A.*

Wednesday, August 02, 2006 19th ICCT / 61st CalCon

Plenary 19ICCT/61CalCon 1

Chair: E. Wilhelm and T.W. de Loos

Morning 2 10:35 AM - 12:20 PM

Room: UMC Ballroom

Electrolyte and Non-Electrolyte Solution Thermodynamics

10:40 AM Applications of Thermodynamics for Protein Solutions (Invited)

J.M. Prausnitz* and L. Hagar, *University of California
Berkeley, Berkeley, CA, U.S.A.*

Phase Equilibrium, Supercritical Fluids, and Separation Technologies

11:30 AM Computational Quantum Mechanics: An Underutilized Tool in Thermodynamics (Invited)

S.I. Sandler*, *University of Delaware, Newark, DE, U.S.A.*

Properties for Metallurgical Process Design 4

Chair: R. Overfelt and I. Egry

Morning 2 10:35 AM - 12:20 PM

Room: Eng-200

10:40 AM Application of Thermodynamics in Pb-Free Soldering Materials

Z. Moser*, *Institute of Metallurgy and Materials Science, Kraków, Poland*, K. Rzyman, *Silesian University of Technology, Katowice, Poland* and W. Gąsior and A. Dębski, *Institute of Metallurgy and Materials Science, Kraków, Poland*

11:00 AM A New High-Temperature Oscillating Cup Viscometer

M. Kehr* and W. Hoyer, *Chemnitz University of Technology, Chemnitz, Germany* and I. Egry, *German Aerospace Center, Köln, Germany*

11:20 AM Viscosity of Molten Fe-Cr-Ni Ternary Alloy

Y. Sato*, K. Sugisawa, D. Aoki, Y. Ambo, K. Yanagase and T. Yamamura, *Tohoku University, Sendai, Japan*

11:40 AM Thermophysical Properties of Titanium Aluminides - the European IMPRESS Project

I. Egry*, *German Aerospace Center, Köln, Germany*, R. Brooks, *National Physical Laboratory, Teddington, Middlesex, U.K.*, E. Ricci, *National Research Council (CNR), Genoa, Italy*, R.K. Wunderlich, *Ulm University, Ulm, Germany* and S. Seetharaman, *KTH, Stockholm, Sweden*

12:00 PM Precise Density Measurement for Electromagnetically Levitated Liquid Combined with the Surface Oscillation Analysis

M. Adachi*, A. Mizuno and M. Watanabe, *Gakushuin University, Tokyo, Japan*, H. Kobatake, *Tohoku University, Aoba-ku, Sendai, Japan* and H. Fukuyama, *Gakushuin University, Tokyo, Japan*

Wednesday, August 02, 2006

16th Symposium

Properties of Solids 1

Heat Transfer and Thermal Physics

Chair: J.J. Alvarado-Gil and A. Mandelis

Morning 2 10:35 AM - 12:00 PM

Room: Eng-151

10:40 AM Adsorption Enthalpy of Explosives and Taggants on a Polymeric Surface

T.J. Bruno, K.E. Miller* and E. Nakagawara, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

11:00 AM Predictions of the Dissociation of Hydrate in Sediment Samples with Numerical Heat Transfer Models Based on Fourier's Law

S.R. Davies* and E.D. Sloan, *Colorado School of Mines, Golden, CO, U.S.A.*

11:20 AM A Thermal Diffusivity Measurement Technique for Materials with Internal Heat Generation such as Cement Paste

R.M. Banish* and A. Hernandez-Barros, *University of Alabama in Huntsville, Huntsville, AL, U.S.A.*

11:40 AM Thermal Decomposition of Calcium Dioxodiaquaperoxyoxalatouranate(VI) Dihydrate

M.S. Prasada Rao* and B.B.V. Sailaja, *Andhra University, Visakhapatnam, India*

***Properties of Working Fluids, Including Refrigerants 2
Lubricants***

Chair: R.R. Singh and M.O. McLinden

Morning 2 10:35 AM - 12:00 PM

Room: Eng-265

10:40 AM Solubility Correlation of Carbon Dioxide + Lubricant Oil Mixtures

A. Yokozeki*, *DuPont Fluoroproducts Laboratory, Wilmington, DE, U.S.A.*

11:00 AM Density and Dynamic Viscosity of Carbon Dioxide + Polyolester Mixtures up to 353.15 K and 60 MPa at Low Lubricant Concentrations

A.S. Pensado*, *Universidad de Santiago de Compostela and Université Blaise Pascal Clermont-Ferrand, Santiago de Compostela, Spain*, A.A.H. Padua, *CNRS/Université Blaise Pascal, Aubière, France* and M.J.P. Comuñas and J. Fernández, *Universidad de Santiago de Compostela, Santiago de Compostela, Spain*

11:20 AM Solubility of Carbon Dioxide in 2-Methylpropionic, 2-Methylbutyric, 2-Methylhexanoic and 2-Methylvaleric Ester Oils

S.B. Bobbo*, R.C. Camporese, L.F. Fedele and M.S. Scattolini, *National Research Council (CNR), Padova, Italy* and R. Stryjek, *Polish Academy of Sciences (PAN), Warsaw, Poland*

11:40 AM An Experimental Investigation and Modeling of the Thermodynamic Properties of R245fa/Compressor Oil Solutions

S.N. Ancherbak* and Y.V. Semenyuk, *Odessa State Academy of Refrigeration, Odessa, Ukraine*, A.J. Grebenkov and O.V. Beliayeva, *Joint Institute of Power Engineering and Nuclear Research-Sosny, Minsk, Belarus* and V.P. Zhelezny, *Odessa State Academy of Refrigeration, Odessa, Ukraine*

Wednesday, August 02, 2006

Joint Session

Exhibitions 1

Chair: R.D. Chirico

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

1:50 PM ACS Publications

Anter Corp.

Calorimetry Sciences Corp.

Elsevier

JECC Torisha Co.

Mettler-Toledo

Netzsch Instruments Inc.

PerkinElmer

Rubotherm

Springer

TA Instruments

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Colloid and Interface Science

Dynamics of an Antimicrobial Oligopeptide: Low-Temperature Adiabatic Calorimetry and Neutron Scattering

Y. Miyazaki* and A. Inaba, *Osaka University, Toyonaka, Osaka, Japan*, N. Alves and P. Gomes, *University of Porto, Porto, Portugal*, J-M. Zanotti, *LLB (CEA-CNRS), Gif/Yvette, France*, H.D. Middendorf, *University of Oxford, Oxford, U.K.* and M. Bastos, *University of Porto, Porto, Portugal*

Effect of the Molecular Geometry on the Transient Foam Behavior of Binary Non-Aqueous Liquid Mixtures: Alkane + Alcohol, Alcoxyalcohol, Diol or Polyether Systems

L.M. Trejo*, J. Cristiani and B. Salas, *Universidad Nacional Autónoma de México (UNAM), México, DF, México* and B. Kronberg, *Institute for Surface Chemistry, Stockholm, Sweden*

Phase Behavior of Diheptadecanoyl-Phosphatidylcholine Bilayers in the Presence of KCl

H. Nakazawa*, M. Kinoshita and S. Kato, *Kwansei Gakuin University, Sanda, Hyogo, Japan*

Prediction of Transient Foam Behavior from Equilibrium Surface Tension Data for Amphiphile's Aqueous Systems

L.M. Trejo*, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*, J. Gracia-Fadrique and M.G. Lemus, *Ciudad Universitaria, México, DF, México* and Á. Piñeiro, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Colloid and Interface Science

Preparation and Characterization of Zinc Ferrite Nanospheres in Microemulsion

M. Zhang and X.-Q. An*, *Nanjing Normal University, Nanjing, China*

Study of Emulsions Stability Using a Biosurfactant from *Y. Lipolytica* (IMUFRJ 50682)

J.R. Trindade and M.G. Freire*, *Universidade de Aveiro, Aveiro, Portugal*, P.F.F. Amaral and M.A.Z. Coelho, *EQ / UFRJ, Centro de Tecnologia, Rio de Janeiro, Brazil* and J.A.P. Coutinho and I.M. Marrucho, *Universidade de Aveiro, Aveiro, Portugal*

Surface Tension of Chain Molecules - a Combination of the Gradient Theory with the CPA EOS

M.B. Oliveira, I.M. Marrucho and J.A.P. Coutinho, *Universidade de Aveiro, Aveiro, Portugal*, G.M. Kontogeorgis, *Technical University of Denmark, Lyngby, Denmark*, C. Miqueu, *Université de Pau et des Pays de L'Adour, Pau, France* and A.J. Queimada*, *Universidade de Aveiro, Aveiro, Portugal*

The Coexistence Curves for Nonaqueous Microemulsion of {Dimethylacetamide + Sodium Di(2-Ethyl-1-Hexyl)Sulphosuccinate + Octane} in the Critical Region

H.-L. Cai, *Lanzhou University, Lanzhou, Gansu, China*, X.-Q. An*, *Nanjing Normal University, Nanjing, China* and W.-G. Shen, *East China University of Science and Technology, Shanghai, China*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Colloid and Interface Science

Ultrasonic Studies and Thermal Conductivity of Sodium Silicate Glasses

S.Ç. Çolak, G. Savaroğlu*, G. Kılıç, E. Aral and S. Birdogan,
Eskisehir Osmangazi University, Eskisehir, Turkey

Electrolyte and Non-Electrolyte Solution Thermodynamics

A New Method to Estimate the Hydrophobic Effect Enthalpy

B.N. Solomonov* and I.A. Sedov, *Kazan State University, Kazan, Russia*

Activity Coefficients of Binary Mixtures Through the Whole Concentration Range from Surface Tension Measurements

Á. Piñeiro*, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*, A. Amigo, *Universidad de Santiago de Compostela, Santiago de Compostela, Spain* and J. Gracia-Fadrique, *Univ. Nacional Autonoma de Mexico, México, DF, México*

Apparent Molar Volumes and Apparent Molar Heat Capacities of Aqueous 1,2-Dimethoxyethane, Diethyl Ether, 1,4-Dioxane, Dimethyl Sulfoxide, and Tetrahydrofuran T/K = (278.15 to 393.15) and P = 0.35 MPa

M.B. Blodgett, S.P. Ziemer and E.M. Woolley*, *Brigham Young University, Provo, UT, U.S.A.*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Electrolyte and Non-Electrolyte Solution Thermodynamics

**Calorimetric Determination of the Standard State
Thermodynamic Properties for Aqueous Gadolinium
Perrhenate and Gadolinium Chloride up to 623 K**

E. Djamali* and J.W. Cobble, *San Diego State University,
San Diego, CA, U.S.A.*

**Calorimetric Determination of the Standard State
Thermodynamic Properties for Completely Dissociated
Aqueous Hydrochloric Acid and Sodium Hydroxide up to 623
K**

E. Djamali* and J.W. Cobble, *San Diego State University,
San Diego, CA, U.S.A.*

Consistency Test for Density and Refractive Index Data

P. Brocos* and A. Amigo, *Universidad de Santiago de
Compostela, Santiago de Compostela, Spain*

**Deriving Solute Activity Coefficients via Calorimetric
Measurement of Solubility**

T.I. Elwell* and R. Srivastava, *The Dow Chemical Company,
Midland, MI, U.S.A.*

Evaluating the Quality of Excess Properties Predictions

P. Brocos*, *Universidad de Santiago de Compostela,
Santiago de Compostela, Spain*, Á. Piñeiro, *Universidad
Nacional Autónoma de México (UNAM), México, DF, México*
and A. Amigo, *Universidad de Santiago de Compostela,
Santiago de Compostela, Spain*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Electrolyte and Non-Electrolyte Solution Thermodynamics

Excess and Solvation Enthalpies of Perfluoroalkane + Alkane Mixtures

L. Lepori* and E. Matteoli, *Istituto Processi Chimico-Fisici, CNR, Pisa, Italy* and C. Duce and M.R. Tine, *Università di Pisa, Pisa, Italy*

Excess Properties of Binary Mixtures of N-Methyl-2-piperidinone with Water or Water-d₂

S. Pihlasalo, *University of Turku, Turku, Finland*, K. Steinby, *Abo Akademi University, Abo, Finland* and P. Scharlin*, *University of Turku, Turku, Finland*

High Pressure Speed of Sound Measurements and the Calculation of Densities for Selected Aqueous Sugar Systems

A.W. Hakin*, *The University of Lethbridge, Lethbridge, AB, Canada* and H. Høiland, *University of Bergen, Bergen, Norway*

Liquid Renewable Fuels: Excess Thermodynamic Properties of Binary and Ternary Mixtures Containing ETBE, Cyclohexane and Toluene

J.J. Segovia, C.R. Chamorro, M.A. Villamañán*, M.C. Martín and R.M. Villamañán, *Universidad de Valladolid, Valladolid, Spain*

Measurement and Correlation of Solubility of Naphthalene in Mixed Solvents

A. Belabbaci, A. Negadi and L. Negadi*, *University Aboubakr Belkaid of Tlemcen, Tlemcen, Algeria*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Electrolyte and Non-Electrolyte Solution Thermodynamics

Mixtures of 1,1,2,2-Tetrachloroethane + Aromatic Hydrocarbons: Excess and Solvation Thermodynamic Function

L. Lepori and E. Matteoli*, *Istituto Processi Chimico-Fisici, CNR, Pisa, Italy*, A. Spanedda and G.C. Bussolino, *Istituto Processi Chimico-Fisici, CNR, Pisa, Italy* and B. Marongiu and S. Porcedda, *Università di Cagliari, Cagliari, Italy*

Modeling of Excess Molar Volume of Binary Mixtures of Water-Alkanol: a New Application of the ERAS Model

R.B. Tôrres*, M.Y. Nagamachi, A.Z. Francesconi and P.L.O. Volpe, *Instituto de Química UNICAMP, Campinas, São Paulo, Brazil*

New Mean Spherical Approximation Method for Prediction of Solid Liquid Equilibria in Mixed Aqueous Electrolyte Solution

M.R. Dehghani*, *Research Institute of Petroleum Industry, Iran*, H. Modarress, *Amir Kabir University of Technology, Iran* and A. Bakhshi, *National Petrochemical Company, Iran*

Orientational Effects in Binary Liquid Organic Mixtures: Study in Terms of the Flory Theory

N. Riesco*, *Loughborough University, Loughborough, Leicestershire, U.K.* and J.A. Gonzalez, I. Mozo, I.G. de la Fuente and J.C. Cobos, *Universidad de Valladolid, Valladolid, Spain*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Electrolyte and Non-Electrolyte Solution Thermodynamics

Partial Molar Properties of Aqueous Solution of Alcohols at 298.15 K

T. Kimura*, Shinya Inui and T. Kamiyama, *Kinki University, Kowakae, Higashi-osaka, Japan*

Quasichemical Models of Structure and Physicochemical Properties of 1,4-Dioxane-Methanol and 1,4-Dioxane-Ethanol Mixtures

V.A Durov* and O.G. Tereshin, *Moscow State University, Moscow, Russia*

Solubility and High Pressure Density of HFE-7500 in n-Alkanes

J. Cendón, B. Orge, L.M. Casás, J. Vijande, M.M. Piñeiro* and J.L. Legido, *Universidade de Vigo, Vigo, Spain*

Species Identification, Volatility and Thermodynamic Properties of Gaseous and Aqueous Arsenous Acid in High-Temperature Solutions

J.W. Cobble, D.R. Fyke, K.D. Chen and P.J. Turner*, *San Diego State University, San Diego, CA, U.S.A.*

Temperature Dependence of the Excess Heat Capacity for Associated Mixtures: Experimental Results and Modeling

C. Paz-Ramos, C.A. Cerdeiriña* and L. Romaní, *Universidad de Vigo, Ourense, Spain* and M. Costas, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Electrolyte and Non-Electrolyte Solution Thermodynamics

**Thermophysical Properties of the Quaternary Mixture
Benzene + Cyclohexane + 1-Pentanol + Anisole at 298.15 K**

L.M. Casás, M.M. Piñeiro* and B. Orge, *Universidade de
Vigo, Vigo, Spain*

**Volumetric Behavior of a Liquid Mixture of Pentaerythritol
Tetrapentanoate and Pentaerythritol Tetra(2-
Ethylhexanoate) for Broad Ranges of Temperatures and
Pressures**

O. Fandiño, M.J.P. Comuñas, L. Lugo, E.R. López and J.
Fernández*, *Universidad de Santiago de Compostela,
Santiago de Compostela, Spain*

**Volumetric Properties of Binary and Ternary Mixtures of
Diisopropyl Ether, α,α,α -Trifluorotoluene and Ethanol at
298.15 K and 101 kPa**

Z. Atik* and K. Lourdani, *University of Sciences and
Technology Houari Boumediene, Bab-Ezzouar, Algeria*

**Volumetric Properties of Binary Mixtures of Acetonitrile-
Ethers at Different Temperatures and Atmospheric Pressure**

R.B. Tôrres*, M.I. Ortolan and P.L.O. Volpe, *Instituto de
Química UNICAMP, Campinas, São Paulo, Brazil*

Instrumentation and Measurement Techniques

A Multifunctional Device for Thermophysical Measurements

S.S. Proshkin* and I.V. Baranov, *Saint-Petersburg, Russia*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Instrumentation and Measurement Techniques

A New Experimental Device for Spectral Directional Emissivity Measurements

R.B. Perez-Saez, L. del Campo* and M.J. Tello, *Universidad del Pais Vasco, Leioa, Bizkaia, Spain*

A New Small-Scale Reaction Calorimeter with Combined Temperature Control for the Determination of Kinetics Parameters

G.R. Richner*, *ETH Zürich, Zürich, Switzerland*, F.V. Visentin, *Mettler-Toledo GmbH AutoChem, Inc., Schwerzenbach, Switzerland* and G.P. Puxty and K.H. Hungerbühler, *ETH Zürich, Zürich, Switzerland*

Absorption of Sound Near Critical Point of Stratification in Binary Solutions

R.K. Turniyazov*, *Samarkand State University, Samarkand, Uzbekistan*

Advanced Distillation Curve Measurement: Applications to Gasolines, Rocket Propellant and Jet Fuels

T.J. Bruno and B.L. Smith*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Design, Development, and Testing of a Resistive Adiabatic Calorimeter

G. Barreiro-Rodríguez* and A. Herrera-Gómez, *CINVESTAV-Unidad Querétaro, Querétaro, QT, México*, E. Méndez-Lango, *Centro Nacional de Metrología, QT, México* and J.M. Yáñez-Limón, *CINVESTAV-Unidad Querétaro, Querétaro, QT, México*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Instrumentation and Measurement Techniques

Development of an Apparatus for Measurements of Thermal Expansion Coefficients of Solid Materials Around Room Temperature

N. Yamada*, *National Metrology Institute of Japan, Tsukuba, Ibaraki, Japan* and H. Kato and T. Baba, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

Development of Ripplon Scanning Technique for Surface Viscoelasticity of Polymer Solutions

T. Ueno* and Y. Nagasaka, *Keio University, Yokohama, Kanagawa, Japan*

Experimental Study of Gas-Liquid Two-Phase Flow in Glass Micromodels

B.J. Gutiérrez*, *Universidad Simón Bolívar GFT-USB, Caracas, Venezuela*, F. Juárez and L. Ornelas, *Universidad Simón Bolívar, Caracas, Venezuela* and S. Zeppieri and A.L. López, *Universidad Simón Bolívar GFT-USB, Caracas, Venezuela*

Instrumental Improvement for Calorimetric Research

V.P. Nesterenko*, *Belarusian National Technical University, Minsk, Belarus*

Measurement of Gas Mixing Volumes by Flux Response Technology

N. Riesco*, P.A. Russell, I.W. Cumming, K. Hellgardt and G. Mason, *Loughborough University, Loughborough, Leicestershire, U.K.*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Instrumentation and Measurement Techniques

New Metrology for Characterization of Nanomagnetic MRI Contrast Agents

B. Cage* and S. Russek, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

New Reference Installation for Measurement of Thermal Conductivity of Thermal Insulating Materials

N.A. Sokolov*, *D.I.Mendeleyev Institute for Metrology, St. Petersburg, Russia*

New Technology for Investigations of Photoelastic Properties of Nontransparent Crystals

F.R. Akhmedzhanov*, *Samarkand State University, Samarkand, Uzbekistan*

Oscillation Method of Phase Analysis

A.B. Kaplun and A.B. Meshalkin*, *Russian Academy of Sciences, Novosibirsk, Russia*

Photoacoustic Heat Transmission Method for Measuring the Specific Heat Capacity of Solids

O. Delgado-Vasallo, *Universidad de la Habana, Habana, Cuba*, E. Marín, A. Calderón* and J.A.I. Díaz-Góngora, *Instituto Politécnico Nacional, México, DF, México* and G. Peña-Rodríguez, *Universidad Francisco de Paula Santander, Cúcuta, Colombia*

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Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Instrumentation and Measurement Techniques

Reference Values of the Viscosity of Hydrogen, Methane, Argon, and Xenon Determined with Capillary Viscometers

R.F. Berg*, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*, E.F. May, *University of Western Australia, Crawley, WA, Australia* and M.R. Moldover, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Simultaneous Multiobjective Chemical Model Fitting of Online Measurements: Calorimetry, Spectroscopy and Gas Uptake

S.I. Gianoli, G. Puxty and K. Hungerbuehler, *ETH Hönggerberg, Zürich, Switzerland* and G.R. Richner*, *ETH Zürich, Zürich, Switzerland*

Study on Thermal Insulation Based on Polyimide Foam for Future Spacecrafts

T. Ohta*, *Tokai University, Hiratsuka, Kanagawa, Japan*, H. Nagano, *Keio University, Hiyoshi, Yokohama, Japan* and A. Ohnishi, *Japan Aerospace and Exploration Agency, Sagami-hara, Kanagawa, Japan*

Thermal Diffusivity Measurements of a Composite Material with Orthogonal Anisotropy

J. Benacka, L. Vozar* and I. Stubna, *Constantine the Philosopher University, Nitra, Slovakia*

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Chair: J.W. Magee and J.A. Widegren

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Instrumentation and Measurement Techniques

Thermal Properties of Soils and Their Relationship with Moisture Content

G. Vera, A.G. Juárez, A. Calderón*, J.A.I. Díaz-Gongora and E. Marín, *Instituto Politécnico Nacional, México, DF, México*

Ultrahigh Vacuum Quartz Crystal Microbalance Studies of Pure Compound Vapor Pressures

A. Freedman, *Aerodyne Research, Inc, Billerica, MA, U.S.A.*, Z. Li, *Aerodyne Research, Inc., Billerica, MA, U.S.A.* and J. Wormhoudt*, *Aerodyne Research, Inc, Billerica, MA, U.S.A.*

Uncertainty Evaluation of Viscosity Measurement Standards

Hae Man Choi*, Yong Bong Lee, Yong Moon Choi and S.H. Lee, *Korea Research Institute of Standards and Science, Daejeon, Yuseong-Gu, Korea*

Viscosity, Thermal Conductivity, and Surface Tension at High Pressures

E.C. Ihmels*, *DDBST GmbH, Oldenburg, Germany*, A. Grybat and S. Horstmann, *Institute at the University of Oldenburg, Oldenburg, Germany* and K. Fischer, *DDBST GmbH, Oldenburg, Germany*

New Experimental Techniques

A New Method of Measuring Second Virial Coefficients of Gases

L.L. Cortés* and E. Mendez-Lango, *Centro Nacional de Metrología (CENAM), el Marqués, QT, México*

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New Experimental Techniques

An Automated Flow Calorimeter for the Determination of Liquid Isobaric Heat Capacities

J.J. Segovia, C.R. Chamorro, R.M. Villamañán, M.C. Martín and M.A. Villamañán*, *Universidad de Valladolid, Valladolid, Spain*

Determination of Density of Argon with a Mechanical Oscillator Densimeter

L.L. Cortés* and E. Mendez-Lango, *Centro Nacional de Metrología (CENAM), el Marqués, QT, México*

Development of a Calorimetric Sensor for Medical Application

F. Socorro*, A. Mariano and M. Rodríguez de Rivera, *Universidad de Las Palmas, Las Palmas de Gran Canaria, Spain*

Multiparallel Power Compensated Calorimetry for Ultrasmall Samples

J. Higuera-Guisset, A.F. Lopeandía*, J. Valenzuela, E. León-Gutierrez and J. Rodríguez-Viejo, *Universidad Autónoma de Barcelona, Bellaterra, Spain*

Thermokinetic Study on Liquid Mixtures Through Flow Microcalorimetry

M. Rodríguez de Rivera* and F. Socorro, *Universidad de Las Palmas, Las Palmas de Gran Canaria, Spain*

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New Materials

Calorimetric Study on Cu-Al-Ni Shape Memory Alloys

A. López-Echarri*, I. Ruiz-Larrea and J.M. San Juan, *Universidad del País Vasco, Bilbao, Spain* and A. Fraile-Rodríguez, *Paul Scherrer Institut, Switzerland*

Fullerene Clusters in the Systems C60 - Polar Solvents

N.V. Avramenko*, M.V. Korobov, N.I. Ivanova, A.M. Parfenova and O.I. Kiseleva, *Moscow State University, Moscow, Russia* and M.V. Avdeev, *Frank Laboratory of Neutron Physics, Moscow, Russia*

Heat Capacity of Tricyclohexylmethanol

Y. Yamamura* and K. Amano, *University of Tsukuba, Tsukuba, Ibaraki, Japan*, H. Saitoh, *Saitama University, Saitama, Japan* and K. Saito, *University of Tsukuba, Tsukuba, Ibaraki, Japan*

Hexagonal and Versus SrMnO₃: Band Structure, Heat Capacity and Lattice Dynamics

R. Søndena, P. Ravindran and S. Stølen*, *University of Oslo, Oslo, Blindern, Norway*

Influence of Plasticizer on Glass Transition of Systems Showing a Rigid Amorphous Fraction (Semicrystalline Polymers, Polymer Nano-Composites)

A. Sargsyan*, *University of Rostock, Rostock, Germany*, S. Thomas and S. Thomas, *Mahatma Gandhi University, Kottayam, Kerala, India*, A. Wurm, *University of Rostock, Rostock, Germany*, A. Tonoyan, *State Engineering University of Armenia, Yerevan, Armenia* and C. Schick, *University of Rostock, Rostock, Germany*

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New Materials

Low-Energy Direct Synthesis of Potassium Tantalate by Hydrothermal Synthesis with Ethanol on a Substrate

T. Hashizume*, A. Saiki and K. Terayama, *University of Toyama, Toyama, Japan*

The Time-Dependent Specific Heat of $\text{Na}_{0.35}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O}$ Maintained at Ambient Temperature

R.A. Fisher*, N. Oeschler and N.E. Phillips, *University of California, Berkeley, CA, U.S.A.*, J.E. Gordon, *Amherst College, Amherst, MA, U.S.A.* and M.L. Foo and R.J. Cava, *Princeton University, Princeton, NJ, U.S.A.*

Thermodynamic Investigation of Crystalline Thorium Selenite Monohydrate

V.P. Nesterenko*, *Belarusian National Technical University, Minsk, Belarus*

Optical and Thermal Radiative Properties of Materials

Dielectric Spectroscopy of Supercooled Water in Porous Glass and Compressed Hydrophilic Aerosils

G. Sinha, J. Leys, C. Glorieux and J. Thoen*, *Katholieke Universiteit, Leuven, Belgium*

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Optical and Thermal Radiative Properties of Materials

**Spectroscopic Study of Heterogeneous Associates
Formation in Rhodamines B and S Solution with Gossipol**

S. Astanov, *Bukhara Technological Institute of Food and
Light Industry, Bukhara, Uzbekistan*, E.N. Kurtaliev,
Samarkand State University, Samarkand, Uzbekistan and
N. Nizomov*, *Bukhara Technological Institute of Food and
Light Industry, Bukhara, Uzbekistan*

**Study of Orientational Molecular Mobility of Some Mono
Substituted Benzene in Solutions**

Sh.A. Abdurakhmanova* and Sh.Sh. Isanova, *Samarkand
State University, Samarkand, Uzbekistan*

**Study of Thermodynamical Parameters of Viscous
Processes in Some Mono Substituted Benzenes**

Sh.A. Abdurakhmanova and Sh.Sh. Isanova*, *Samarkand
State University, Samarkand, Uzbekistan*

Photothermal and Photoacoustic Techniques

**A New Development of Photoacoustic Detection for
Microchip-Capillary Electrophoresis Using a Simple Pick-Up
Device**

J.-W. Kim, A.K. Lee, M.S. Jeoung, J.Y. Lee and J-G. Choi*,
Yonsei University, Seoul, Korea

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Photothermal and Photoacoustic Techniques

Algorithm for the Metrological Comparison of Two Photothermal Methods for Measurement of the Properties of Materials

R. Ivanov, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México*, E. Marín, *Instituto Politécnico Nacional, México, DF, México*, G. Gutiérrez-Juárez, *Universidad de Guanajuato, León, GT, México*, J.P. Pichardo-Molina*, *Centro de Investigaciones en Optica A.C., León, GT, México*, A. Calderón, *Instituto Politécnico Nacional, México, DF, México* and I. Moreno, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México*

Finite Element Simulation for Thermal Effusivity Measurement in Local Area by Thermal Microscope

S. Ikeuchi*, T. Yagi, N. Taketoshi, H. Kato and T. Baba, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

Generalized Parameter for Election of Suitable Technique and Optimization of Differential Photothermal Experiments

R. Ivanov, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México*, E. Marín, *Instituto Politécnico Nacional, México, DF, México*, G. Gutiérrez-Juárez, *Universidad de Guanajuato, León, GT, México*, J.P. Pichardo-Molina*, *Centro de Investigaciones en Optica A.C., León, GT, México* and I. Moreno, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México*

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Photothermal and Photoacoustic Techniques

Investigation of Thermophysical Properties of Magnetoactive Media Using Method of Resonant Photoacoustic Spectroscopy

G.S. Mityurich*, *Belarusian Trade and Economic University, Gomel, Belarus*, A.N. Emelyanovich, *Gomel State University, Gomel, Belarus* and R.M. Burbelo, *Kiev National University, Kiev, Ukraine*

Measurements of the High Pressure Ultrasonic Wave and the Cavitation Bubble by Optodynamic Method

R. Petkovsek*, G. Mocnik and J. Mozina, *University of Ljubljana, Ljubljana, Slovenia*

On the Influence of the Coupling Fluid in Auto-Normalized Front Photopyroelectric Method to Measure Thermal Effusivity in Solids

G. Gutiérrez-Juárez*, *Universidad de Guanajuato, León, GT, México*, J.P. Pichardo-Molina, *Centro de Investigaciones en Optica A.C., León, GT, México*, R. Ivanov, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México* and M.R. Huerta-Franco, *Instituto de Investigaciones Sobre el Trabajo, León, GT, México*

Optodynamic Analysis of Laser Induced Thermal Effects at Air-Water Interface

D. Horvat, R. Petkovsek* and J. Mozina, *University of Ljubljana, Ljubljana, Slovenia*

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Photothermal and Photoacoustic Techniques

Photoacoustic Method for Characterization of Natural Galena (PbS)

P.M. Nikolić and D.T. Luković, *Institute of Technical Sciences SASA, Belgrade, Serbia*, M.V. Nikolić, *University of Belgrade, Belgrade, Serbia*, S.M. Savić, *Institute of Technical Sciences SASA, Belgrade, Serbia*, S.R. Djukić, *IRITEL, Belgrade, Serbia*, S. Djurić, *Institute of Technical Sciences SASA, Belgrade, Serbia* and L.S. Lukić*, *IRITEL, Belgrade, Serbia*

Photoacoustic Thermal Characterisation of Porous Rare-Earth Phosphate Ceramics

S.D. George*, *Life Science Centre, Manipal, India*, R. Komban and K.G.K. Warriar, *Regional Research Laboratory, CSIR, Thiruvananthapuram, India* and P. Radhakrishnan, V.P.N. Nampoori and C.P.G. Vallabhan, *Cochin University of Science and Technology, Cochin, India*

Photoacoustic Thermoelastic Imaging of Vickers Indented Solids Without and Under External Loading

K.L. Muratkov* and A.L. Glazov, *A.F. Ioffe Physical-Technical Institute of RAS, St. Petersburg, Russia*

Photopyroelectric Microscopy of Biological Material

B.R. Briseño-Tepepa*, *Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada - I.P.N., México, DF, México*, R. Saavedra, *Universidad de Concepción, Concepción, Chile*, R. González-Ballesteros, *Cinvestav-IPN, México, DF, México* and J.L. Jiménez-Peréz and A. Cruz-Orea, *Centro de Investigación y de Estudios Avanzados del I.P.N., México, DF, México*

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Photothermal and Photoacoustic Techniques

Similarity Theory in Photothermal Experiments: A Condition for Neglecting Convection Effects

O. Delgado-Vasallo, *Universidad de la Habana, Habana, Cuba* and J.A.I.D. Gongora, A. Calderón* and E. Marín, *Instituto Politécnico Nacional, México, DF, México*

Thermal Conductivity and Interfacial Thermal Resistance Measurement of Thermally-Oxidized SiO₂ Films on a Silicon Wafer Using a Thermo-Reflectance Technique

R. Kato*, *Ulvac-Riko Inc., Yokohama, Japan* and I. Hatta, *Fukui University of Technology, Fukui, Japan*

Two Metrological Aspects of Auto-Normalized Front Photopyroelectric Method to Measure Thermal Effusivity in Liquids

G. Gutiérrez-Juárez*, *Universidad de Guanajuato, León, GT, México*, R. Ivanov, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México*, J.P. Pichardo-Molina, *Centro de Investigaciones en Optica A.C., León, GT, México*, M. Vargas-Luna, *Universidad de Guanajuato, León, GT, México*, J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México* and A. Camacho-Pérez, *Instituto Tecnológico de León, León, GT, México*

Properties at the Nanoscale

Appraising Nanofluid Cooled Microchannel Heat Sink Performance through Thermal Dispersion Model

H. Abbassi and M.H. Saidi*, *Sharif University of Technology, Tehran, Iran*

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Properties at the Nanoscale

Experimental Study of the Thermodynamic Properties of Microemulsions

N.G. Polikhronidi and G.V. Stepanov, *Institute of Physics of the Dagestan Scientific Center of the Russian Academy of Sciences, Makhachkala, Dagestan, Russia*, I.M. Abdulagatov*, *Russian Academy of Sciences, Makhachkala, Dagestan, Russia* and R.G. Batyrova, *Institute for Geothermal Problems of the Dagestan Scientific Center of the Russian Academy of Sciences, Makhachkala, Dagestan, Russia*

Molecular Dynamics Simulation of Effects of Atomic Vacancies on Thermal Conduction of Solid Argon

S. Fujiwara*, *Akashi National College of Technology, Akashi, Japan*, Xing Zhang, *Tsinghua University, Beijing, China* and M. Fujii, *Kyushu University, Kasuga, Japan*

Solvents and Weakly Coordinating Anions as Stabilizers for Transition-Metal Nanoclusters

L.S. Ott* and R.G. Finke, *Colorado State University, Fort Collins, CO, U.S.A.*

The Surface Pressure and the Fragmentation of a Nanocrystal

M.N. Magomedov*, *Daghestan Scientific Center of the RAS, Makhachkala, Dagestan, Russia*

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Properties at the Nanoscale

Thermal Conductivity of Solid Matrix Unit in Silica Aerogel

Yusong Liu, Xinxin Zhang* and Fan Yu, *University of Science and Technology Beijing, Beijing, China*, Y.Y. Zuo, *University of Toronto, Toronto, ON, Canada* and Z. Zhang, *University of Science and Technology Beijing, Beijing, China*

Thermal Properties of (Nano) ZnO-DMSO Colloidal Dispersions

E. Marín, A. Calderón* and D. Díaz, *Instituto Politécnico Nacional, México, DF, México*

Thermal Properties of Nanofluids Containing Polymer-Protected Au/Pd Bimetallic Clusters Suspended in Etilen Glycol

E. Marín, J.F. Sanchez Ramírez, J.L. Herrera Pérez and A. Calderón*, *Instituto Politécnico Nacional, México, DF, México*

Thermodynamic Properties and Melting of Nanoparticles

A.I. Karasevskii* and V.Y. Kapchynskyy, G. V. Kurdyumov *Institute for Metal Physics NASU, Kiev, Ukraine*

Thermodynamic Properties of Bi₂Te₃ Nanowire Arrays

C.L. Chen* and Y.Y. Chen, *Academia Sinica, Taipei, Taiwan*

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Afternoon 1 1:45 PM - 3:30 PM

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Properties of Polymers

Acoustic Emission During Loading of Carbon-Fibre-Reinforced and Glass Fibre-Reinforced Plastics

G.H. Narzullaev*, *Samarkand State University, Samarkand, Uzbekistan*

Dielectric Spectroscopy and Adiabatic Calorimetry During Early Stages of Polymer Crystallization

A. Wurm*, *University of Rostock, Rostock, Germany*, Y. Miyazaki, K. Miwa and A. Inaba, *Osaka University, Osaka, Japan* and C. Schick, *University of Rostock, Rostock, Germany*

Experimental Investigation on the Thermal Conductivity Measurement of the Fly Ash Dispersed Plastic Composite Using Guarded Hot Plate Apparatus

J. Fujino*, *Fukuoka University, Jonan-ku, Fukuoka, Japan* and T. Honda, *Fukuoka University, Fukuoka, Jonan-ku, Japan*

Modeling of Process Heat Transport in Abs-Plast

U.T. Khodjaeva, M.M. Safarov* and M.S. Saiduloeva, *Tajik Technical University named after M.S. Osimi, Dushanbe, Tajikistan*

Production of Microcellular Foam Plastics by Supercritical Carbon Dioxide

Hyo-Kwang Bae* and Yong-Kil Kwon, *Yeungnam University, Gyongsan, Korea*

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Properties of Polymers

Reliability of PMMA Measured by Guarded Hot Plate, Contact Pulse Transient Method, Hot Bridge Method and DSC

L. Kubicar*, *Institute of Physics SAS, Bratislava, Slovakia*,
U. Hammerschmidt, *Physikalisch-Technische Bundesanstalt, Braunschweig, Germany* and V. Bohac, *Institute of Physics SAS, Bratislava, Slovakia*

Rigid Amorphous Fraction in Polymer Nano-Composites

A. Sargsyan*, *University of Rostock, Rostock, Germany*, S. Thomas and S. Thomas, *Mahatma Gandhi University, Kottayam, Kerala, India*, A. Tonoyan and S. Davtyan, *State Engineering University of Armenia, Yerevan, Armenia* and C. Schick, *University of Rostock, Rostock, Germany*

Spectral and Thermal Studies of Zn(II) 1, 2 Naphthoquinone Oximates

S.P. Rasale and S.B. Jagtap, *Annasaheb Magar Mahavidyalaya Hadapsar, Pune, India*, V.V. Dhapte and E.H. Khan, *Bharati Vidyapeeth Deemed University, Pune, India* and P.S. Khandagale*, *Bharati Vidyapeeth, Deemed University, Pune, India*

Spectroscopic and Thermogravimetric Studies of Solid State Ligand to Metal Charge Transfer Complexes

M. Wadekar* and C.V. Rode, *National Chemical Laboratory, Pune, India*, B.M. Rawal, *Narmada College, Baroch, Gujarat, India* and A.P. Prabhune, *National Chemical Laboratory, Pune, India*

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Properties of Polymers

Synthesis and Thermal Decomposition Studies of Some Isonaphthazarin Chelates of Transition Metals

P.S. Khandagale*, *Bharati Vidyapeeth, Deemed University, Pune, India*, R.C. Chikate, *University of Pune, Pune, India*, R.G. Sarawadekar, *HEMRL, Pune, India* and V.D. Kelkar and M. Wadekar, *University of Pune, Pune, India*

Properties of Solids

About a Technique of Thermochemical Calculation of Crystals Dissolution Process

M.M. Asadov* and A.S. Abbasov, *National Academy of Sciences of Azerbaijan, Baku, Azerbaijan*

Application of Crystal Chemical Approach to Predicting the Thermal Expansion of Compounds in the NZP Family

V.I. Pet'kov and E.A. Asabina*, *Nizhni Novgorod State University, Nizhni Novgorod, Russia* and B.I. Lazoryak, *Moscow State University, Moscow, Russia*

Crystal Chemistry and Thermal Expansion of $\text{Mg}_{0.5}\text{Zr}_2(\text{PO}_4)_3$

E.R. Gobeच्या and Yu.K. Kabalov, *Moscow State University, Moscow, Russia* and M.V. Sukhanov, V.I. Pet'kov and E.A. Asabina*, *Nizhni Novgorod State University, Nizhni Novgorod, Russia*

Determination of the Thermal Conductivity and Thermal Diffusivity of Materials Using Fin Heat Transfer Theory

D. Hurley* and A. Campo, *The University of Vermont, Burlington, VT, U.S.A.*

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Afternoon 1 1:45 PM - 3:30 PM

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Properties of Solids

Energetics of High Temperature Phase Transitions of Rare Earth Oxides

P. Simoncic* and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.*

Equation of State for High-Pressure Polymeric Phase of Solid Nitrogen from Computer Simulation

L.N. Yakub*, *Odessa State Academy of Refrigeration, Odessa, Ukraine*

Experimental Measurement of the Thermal Conductivity of the NZP Compounds Family

V.I. Pet'kov, *Nizhni Novgorod State University, Nizhni Novgorod, Russia*, V.N. Loshkarev, *Russian Federal Nuclear Center, Sarov, Nizhni Novgorod, Russia* and E.A. Asabina*, *Nizhni Novgorod State University, Nizhni Novgorod, Russia*

Improvement of Mechanical and Thermal Properties of the Thermoplastics Reinforced with Natural Fibres by Electron Beam Processing

S.-W. Kim*, *University of Ulsan, Ulsan, Korea*, S.H. Lee, *Korea Research Institute of Standards and Science, Daejeon, Yuseong-Gu, Korea*, J.S. Kang, *Korea Institute of Construction Technology, Gyeonggi-Do, Korea* and Kweon-Ho Kang, *Korea Atomic Energy Research Institute, Daejeon, Yuseong-gu, Korea*

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Properties of Solids

Photoacoustic Characterization of Natural Mineral Pyrite (FeS₂)

P.M. Nikolić and D.T. Luković, *Institute of Technical Sciences SASA, Belgrade, Serbia*, M.V. Nikolić, *University of Belgrade, Belgrade, Serbia*, S. Djurić, *Institute of Technical Sciences SASA, Belgrade, Serbia*, L.S. Lukić*, *IRITEL, Belgrade, Serbia* and D. Urošević, *Mathematical Institute of SASA, Belgrade, Serbia*

Space Charge Limited Currents in TlInS₂ Single Crystal at Different Temperatures

S.N. Mustafaeva*, *National Academy of Sciences of Azerbaijan, Baku, Azerbaijan*

SRM for Calibration of a Laser Flash Instrument at High Temperatures

U.V. Mardolcar*, *Instituto Superior Técnico, Lisboa, Portugal* and C.A. Nieto de Castro, *Universidade de Lisboa, Lisboa, Portugal*

Temperature-Dependent Anisotropy of the Electric Conductivity of TlB^{III}C₂^{VI} Single Crystal

S.N. Mustafaeva and M.M. Asadov*, *National Academy of Sciences of Azerbaijan, Baku, Azerbaijan*

The Influence of Various Thermal Loadings on the Thermal Conductivity and Emissivity of Isotropic Graphite at High Temperatures

A.V. Kostanovskiy*, M.E. Kostanovskaya and M.G. Zeodinov, *Russian Academy of Sciences, Moscow, Russia*

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Properties of Solids

Thermal and Electrical Conductivities of Silicon in Solid and Liquid States

J.B. Magomedov* and G.G. Gadjiev, *Dagestan Scientific Center, Russian Academy of Sciences, Makhachkala, Dagestan, Russia*

Thermal Conductivity of Crystalline GaSb under Uniform Compression

N.L. Kramynina*, N.V. Lugueva and S.M. Luguev, *Russian Academy of Sciences, Makhachkala, Russia*

Thermal Conductivity of Solid Solutions of Gd-S System in Temperature Range 80 - 400 K

S.M. Luguev* and N.V. Lugueva, *Russian Academy of Sciences, Makhachkala, Russia*

Thermal Decomposition of Barium Bis-Oxalatodiaquaindate(III) Trihydrate

M.S. Prasada Rao*, T. Kebede and B.B.V. Sailaja, *Andhra University, Visakhapatnam, India*

Thermal Properties of TiLnC_2 Low-Dimensional Chalkogenides

E.M. Kerimova*, S.N. Mustafaeva, F.M. Seidov, S.M. Bidzinova and G. Akhmedova, *National Academy of Sciences of Azerbaijan, Baku, Azerbaijan*

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Properties of Solids

Thermophysical Properties and Structure Evolution of Mechanically Activated BaTiO₃

V.P. Pavlovic, *University of Belgrade, Beograd, Serbia*, M.V. Nikolic, *University of Belgrade, Belgrade, Serbia*, V.B. Pavlovic, *University of Belgrade, Beograd, Serbia*, L.S. Lukic*, *IRITEL, Belgrade, Serbia* and P.M. Nikolic and M.M. Ristic, *Institute of Technical Sciences SASA, Belgrade, Serbia*

Thermophysical Properties of Automobile Metallic Brake Disk Materials

S.-W. Kim* and K. Park, *University of Ulsan, Ulsan, Korea*, S.H. Lee, *Korea Research Institute of Standards and Science, Daejeon, Yuseong-Gu, Korea* and Kweon-Ho Kang, *Korea Atomic Energy Research Institute, Daejeon, Yuseong-gu, Korea*

Thermophysical Properties of Rare-Earth-Stabilized Zirconia and Zirconate Pyrochlores As Surrogates for Actinide-Doped Zirconia

K. Shimamura*, T. Arima, K. Idemitsu and Y. Inagaki, *Kyushu University, Fukuoka, Japan*

Thermophysical Properties of the Tungsten-Copper Alloys

S.H. Lee* and Hae-Man Choi, *Korea Research Institute of Standards and Science, Daejeon, Yuseong-Gu, Korea*, S.-W. Kim, *University of Ulsan, Ulsan, Korea* and Kweon-Ho Kang, *Korea Atomic Energy Research Institute, Daejeon, Yuseong-gu, Korea*

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Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Property Needs in Biothermophotonics

**Benefits of the Mycorrhizal Fungi in Tomato Leaves
Measured by Open Photoacoustic Cell Technique:
Interpretation of the Diffusion Parameters**

S. Sánchez-Rocha, *CINVESTAV Unidad Irapuato, Irapuato, GT, México*, M. Vargas-Luna*, H. Huerta-Franco and G. Gutiérrez-Juárez, *Universidad de Guanajuato, León, GT, México* and V. Olalde-Portugal, *CINVESTAV Unidad Irapuato, Irapuato, GT, México*

**Comparative Analysis of the Thermal Properties of Chitin of
Marine Invertebrates**

B.A. Juare Rosa*, *CINVESTAV-IPN, Unidad Merida, Mérida, YU, México*, P. Quintana Owen, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*, P-L. Ardisson, *CINVESTAV-IPN, Unidad Merida, Mérida, YU, México* and J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*

**Curing Evolution Inspection of Buried Epoxy Resin Using
Photothermal Radiometry**

M.A. Zambrano-Arjona*, *CINVESTAV-IPN, Unidad Merida, Mérida, YU, México* and J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*

**Measurement of Liquid to Gel Phase Transition
Temperature and Critical Exponents in Agar**

R.A. Medina-Esquivel*, *CINVESTAV-Queretaro, Queretaro, QT, México*, Y. Freile-Pelegrin, *CINVESTAV-IPN, Unidad Merida, Mérida, YU, México*, P. Quintana Owen, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*, J.M. Yáñez-Limón, *CINVESTAV-Unidad Querétaro, Queretaro, QT, México* and J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Property Needs in Biothermophotonics

Photothermal Radiometry Analysis of Teeth Heating for Short Periods of Time

M.A Conde-Contreras*, *Centro de Investigacion y de Estudios Avanzados del IPN, Mérida, YU, México, V.*
Tiessler, *Universidad Autonoma de Yucatan-Mérida, Mérida, YU, México*, A. Cucina, *Universidad Autonoma de Yucatan, Mérida, YU, México* and P. Quintana Owen and J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*

Thermal Diffusivity Determination of Protoporphyrin IX Solution Mixed with Gold Metallic Nanoparticles

R. Gutiérrez Fuentes, J.F. Sánchez Ramírez and J.L. Jiménez Pérez*, *CICATA-IPN, México, DF, México*, E. Ramón-Gallegos, *Escuela Nacional de Ciencias Biológicas del IPN, México, DF, México* and A. Cruz-Orea, *CINVESTAV-IPN, México, DF, México*

Subsecond Thermophysics

Absorption Flash in Laser Evaporation of Oxide Materials

T.P. Salikhov* and V.V. Kan, *Physical Technical Institute, Tashkent, Uzbekistan*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermochemistry and Molecular Energetics

Application of Direct Calorimetry in Studies of Intermolecular Interactions in Solutions of Linear and Cyclic Oligopyrroles

E.V. Antina*, *Institute of Chemistry of Solutions of the Russian Academy of Science, Ivanovo, Russia* and E.V. Balantseva and E.V. Rumyantsev, *Ivanovo State University of Chemistry and Technology, Ivanovo, Russia*

Application of Thermal Analysis Technique to New Ferrochrome Reduction Process with Aluminum Powder

T. Hashizume, A. Saiki and K. Terayama*, *University of Toyama, Toyama, Japan*

Calorimetry of Si-C-O Polymer Derived Ceramics

T. Varga*, J. Moats and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.* and A. Saha and R. Raj, *University of Colorado at Boulder, Boulder, CO, U.S.A.*

Confined Electrons and Exotic Ions in Microporous $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$ - Calorimetric Study

O. Trofymuk* and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.* and Y. Toda, K. Hayashi and H. Hosono, *Tokyo Institute of Technology, Yokohama, Japan*

Dehydration and Formation Enthalpy of Mg, Ca, Sr, Ba-exchanged Zeolite Beta

P. Sun*, S. Deore and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermochemistry and Molecular Energetics

Energetic Study of Six Aminomethylbenzoic Acids

C.F.R.A.C. Lima and L.M.N.B.F. Santos*, *Universidade do Porto, Porto, Portugal* and L.R. Gomes, *Universidade Fernando Pessoa, Porto, Portugal*

Energetics of Sedimentary Dolomites

H.W. Eng* and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.*, D.K. McCarty, *Chevron Texaco, Houston, TX, U.S.A.* and V.A. Drits, *The University of Texas at Austin, Austin, TX, U.S.A.*

Energetics of the Microporous Oxides, $\text{Na}_{2-y}\text{M}_y\text{Nb}_{2-x}$

$\text{Ti}_x\text{O}_{6-x}(\text{OH})_x \cdot \text{H}_2\text{O}$

(M = Li, Sr, Ca, Mg, Y, Cu, Ni)

R.G. Iyer* and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.* and J.D. Pless and T.M. Nenoff, *Sandia National Laboratories, Albuquerque, NM, U.S.A.*

Enthalpies of Solution and Protonation of Free-And Metallo-Porphyrins

M. Gamboa*, L.A. Torres, M. Campos and A. Rojas, *Centro de Investigacion Y de Estudios Avanzados (CINVESTAV), México, DF, México*

Fluororganic Derivatives of Elements II - VI Groups: Phase Transitions Thermodynamics and Nanocrystalline Films Deposition

L.N. Zelenina*, T.P. Chusova and Y.G. Stenin, *Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia* and V.V. Bakovetz and T. M. Levashova, *Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia*

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Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermochemistry and Molecular Energetics

Gas Phase Enthalpy of Formation of the 1-Acetylvinyl P-Nitrobenzoate

A. Rojas*, A. Valdes, L.A. Torres and M. Campos, *Centro de Investigacion Y de Estudios Avanzados (CINVESTAV), México, DF, México* and J. Tamariz, *Nacional De Ciencias Biologicas Del IPN, México, DF, México*

Molar Standard Enthalpies of Combustion and Formation of the Fullerene C₈₄

A. Rojas and Martínez-H Melchor*, *Centro de Investigacion Y de Estudios Avanzados (Cinvestav), México, DF, México*

NIST Computational Chemistry Comparison and Benchmark Database

R.D. Johnson III*, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Oxidation Behavior of the Simulated Fuel with Dissolved Fission Products in Air at 573 - 873 K

Kweon-Ho Kang*, *Korea Atomic Energy Research Institute, Daejeon, Yuseong-gu, Korea*, K.C. Song, M.S. Yang and S.H. Na, *Korea Atomic Energy Research Institute, Yuseong, Daejeon, Korea*, S.H. Lee, *Korea Research Institute of Standards and Science, Daejeon, Yuseong-Gu, Korea* and S.-W. Kim, *University of Ulsan, Ulsan, Korea*

Oxide Melt Solution Calorimetry of Sulfides

S. Deore* and A. Navrotsky, *University of California at Davis, Davis, CA, U.S.A.*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermochemistry and Molecular Energetics

Phase Modification of Potassium Nitrate by Potassium Salts

Xuejun Zhang*, *North University of China, Taiyuan, China*

The Mean Dissociation Enthalpy of the N-O Bond for 2,2'-Bipyridine N,N'-Dioxide

M.D.M.C. Ribeiro da Silva*, A.R. Monteiro and J.M. Gonçalves, *University of Porto, Porto, Portugal* and W.E. Acree, Jr., *University of North Texas, Denton, TX, U.S.A.*

Thermochemical Studies on N-Thenoylthiocarbamic-O-N-Alkyl Esters

B. Schröder*, I.M.M. Monteiro, L.M.N.B.F. Santos and M.A.V. Ribeiro da Silva, *Universidade do Porto, Porto, Portugal*

Thermodynamic of the Pt-Cl System

Z.I. Semenova, *Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia* and V.A. Titov* and T.P. Chusova, *Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia*

Thermodynamic Properties of the Crystalline Phosphate $\text{Ni}_{0.5}\text{Zr}_2(\text{PO}_4)_3$

V.I. Pet'kov, *Nizhni Novgorod State University, Nizhni Novgorod, Russia*, V.N. Loshkarev, *Russian Federal Nuclear Center, All-Russian Research Institute of Experimental Physics, Nizhni Novgorod, Sarov, Russia* and M.V. Sukhanov, I.A. Schelokov and E.A. Asabina*, *Nizhni Novgorod State University, Nizhni Novgorod, Russia*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamic Frontiers and Education

**An Introductory Experiment of Chemical Equilibrium:
Determination of Thermodynamic Parameters for the
Chemical Equilibrium Between Nitrogen Dioxide and
Dinitrogen Tetraoxide in a Syringe**

M. Tesaki, N. Koga* and Y. Furukawa, *Hiroshima University,
Higashi-Hiroshima, Japan*

**Forecast of the Chemical Aging and Relevant Color Changes
in Paintings**

B. Zilbergleyt*, *System Dynamics Research Foundation,
Chicago, IL, U.S.A.*

**Le Chatelier Response: a Quantitative Application of the Le
Chatelier Principle to Chemical Equilibria**

B. Zilbergleyt*, *System Dynamics Research Foundation,
Chicago, IL, U.S.A.*

**Strategies Using Lecture Demonstrations to Promote the
Learning of Thermodynamic Concepts**

L.M. Trejo*, T. Delgado and S. Flores, *Universidad Nacional
Autónoma de México (UNAM), México, DF, México*

Teaching Thermodynamics - A New Concept

R. Rüffler and G. Job*, *Institute of Physical Chemistry,
Hamburg, Germany*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

A Study of the Natural Dyes Destructive Oxidizing

Sh. Amonov* and A. Khololov, *Samarkand State University, Samarkand, Uzbekistan*

A Study on Acid-Base Equilibria in (n-Butylamine + Acetic Acid) Systems in Binary (Dimethyl Sulfoxide + 1,4-Dioxane) Solvent Mixtures

L. Chmurzynski*, M. Czaja and M. Makowski, *University of Gdansk, Gdansk, Poland*

Apparent Molar Volumes and Apparent Molar Heat Capacities of Aqueous Isoleucine and Threonine Species in Their Protonated Cationic, Zwitterionic, and Deprotonated Anionic Forms at T/K = (278.15 to 368.15) and at P = 0.35 MPa

S.P. Ziemer and E.M. Woolley*, *Brigham Young University, Provo, UT, U.S.A.*

Apparent Molar Volumes and Apparent Molar Heat Capacities of Aqueous N-Acetyl-D-Glucosamine at T/K = (278.15 to 368.15) and of Aqueous N-Methylacetamide at T/K = (278.15 to 393.15)

D.M. Swenson, S.P. Ziemer, M.B. Blodgett, J.S. Jones and E.M. Woolley*, *Brigham Young University, Provo, UT, U.S.A.*

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Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Batch Calorimetry with Solids, Liquids and Gases in Less than 1 mL Total Volume

L.D. Hansen*, *Brigham Young University, Provo, UT, U.S.A.* and D.J. Russell and D.W. Thomas, *Calorimetry Sciences Corporation, Lindon, UT, U.S.A.*

Bio-Physical Evaluation of Different Milks from Indian Animals

I. Johnson*, *St. Joseph's College, Trichy, India*

Bulk and Mesoscopic Thermodynamic Studies of Inorganic Biocompatible Materials Utilizable for Mimetic Bone Tissue Substitution in Dentistry

J. Sestak*, *Academy of Sciences of the Czech Republic, Prague, Czech Republic*, Z. Strnad and J. Strnad, *LASAK - Laboratory for Glass and Ceramics, Prague, Czech Republic* and N. Koga, *Hiroshima University, Higashi-Hiroshima, Japan*

Calorimetric Studies on Diclofenac Sodium, Diclofenac, and Sodium Bicarbonate Mixtures

I. Pasquali*, R. Bettini and F. Giordano, *University of Parma, Parma, Italy*

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Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Chemical Exergy of Canola Biomass Components

Z.A. Antonava*, *Research Institute for Physical and Chemical Problems, Minsk, Belarus*, G.J. Kabo and L.S. Karpushenkova, *Belarusian State University, Minsk, Belarus*, Y.V. Maksimuk, *Research Institute for Physical and Chemical Problems, Minsk, Belarus*, A.V. Blokhin, *Belarusian State University, Minsk, Belarus* and A.A. Simirskii, *Research Institute for Physical and Chemical Problems, Minsk, Belarus*

Comparative Study by Differential Scanning Calorimetry and Gas Chromatography of the Fatty Acids Content in Different Brands of Milk

M.P.B. Portilla*, E.R.H. Reynoso Herrera, E.R.E. Rojas Escudero and P.E.G. Elizalde Galván, *UNAM, México, DF, México*

Determination and Modeling of Thermal Properties of Aloe Vera Exudate

P.A. Vargas* and A.L. López de Ramos, *Universidad Simón Bolívar, Caracas, Venezuela*

Differential Calorimetry of Natural Microbial Communities

E. Djamali, F. Rohwer, P. Salamon and P. Turner*, *San Diego State University, San Diego, CA, U.S.A.*

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Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Differential Scanning Calorimetry of Glycerinated Muscle Fibres Reveals Distinct Conformational States During the ATP Hydrolysis

Zs. Vertes*, T. Dergez, F. Konczol, N. Farkas, J. Belagyi and D. Lőrinczy, *University Pécs, Pécs, Hungary*

Effect of NaCl Concentration on Formation of Highly Crystalline Phase in DMPG Bilayers

M. Kinoshita*, H. Nakazawa and S. Kato, *Kwansei-Gakuin University, Sanda, Hyogo, Japan*

Fast Authentication of Edible Oils by DSC and TAM Calorimetry

M. Angiuli, C. Ferrari, L. Lepori, E. Matteoli*, M.C. Righetti, G. Salvetti and E. Tombari, *Istituto Processi Chimico-Fisici, CNR, Pisa, Italy*

Fatty Acid Composition, Thermal Characteristic and Spread Ability of Certain Margarines

S. Szakaly, *Hungarian Dairy Research Institute, Pécs, Hungary*, J. Csapo, *University of Kaposvár, Kaposvár, Hungary*, B. Schaffer, *Hungarian Dairy Research Institute, Pécs, Hungary* and D. Lőrinczy*, *University Pécs, Pécs, Hungary*

Gas Sorption in Poly(Lactic Acid)

N.S. Oliveira, *Universidade de Aveiro, Aveiro, Portugal*, J.R. Dorgan, *Colorado School of Mines, Golden, CO, U.S.A.* and A. Ferreira and I.M. Marrucho*, *Universidade de Aveiro, Aveiro, Portugal*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Heat Capacity and Derived Thermodynamic Properties of Rimantadine in the Condensed State Between T = (5 and 370) K

A.B. Bazyleva*, A.V. Blokhin and G.J. Kabo, *Belarusian State University, Minsk, Belarus*

Hydrolysis of Lecithin by PLA₂ in Model Bile

J. Bai, *Nanjing Normal University, Nanjing, China* and X.-Q. An*, *Nanjing Normal University, Nanjing, China*

Influence of Calcium Diffusion on Thermal and Optic Properties on Components of Corn Grains During Traditional Nixtamalization Process

J.L. Fernández-Muñoz*, E. San Martín-Martínez, J.A.I. Díaz-Góngora and A. Calderón, *Instituto Politécnico Nacional, México, DF, México*

Modeling of Solid Solubilities in Supercritical Fluid Using a Qausi-Chemical Nonrandom Lattice Fluid Equation of State

Moon Sam Shin*, Hong-Il Yoo, Youn-Woo Lee and Hwayong Kim, *Seoul National University, Seoul, Korea*

Molecular Mechanism of Cell Differentiation of Multi-Cellular Organism and Its Carcinogenic Transformation by Mutation Based on the Molecular Anvil Model of an Enzyme and Non-Equilibrium Thermodynamics

K. Amaya*, *Consultant of J.B.I. Company, Tokyo, Japan*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Photosynthesis Evolution in Aquatic Lirium (Eichhornia Crassipes) by Means of the Photoacoustic Technique

A.C. Ricalde, C.M. Barradas, J.L. Fernández Muñoz, E. Marín and A. Calderón*, *Instituto Politécnico Nacional, México, DF, México*

Solubility of Beta-Carotene in Binary Mixed Solvents

T. Treszczanowicz* and A.J. Treszczanowicz, *Polish Academy of Sciences, Institute of Physical Chemistry, Warsaw, Poland* and T. Kasprzycka-Guttman, *Warsaw University, Warsaw, Poland*

Sound Thermodynamic Properties Prediction for the Drug Design and Development in Pharmaceutical and Agrochemical Research Using COSMO-RS

A. Klamt*, *COSMOlogic GmbH&CoKG, Leverkusen, Germany*

Structural Function of Asymmetric Chain N-Lignoceroylsphingosylphosphocholine (C24:0-SM) As Studied by Microcalorimetry and Electron Microscopy

Y. Kawasaki* and M. Kodama, *Okayama University of Science, Okayama, Japan*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Study of Skin Phantoms by Photothermal Radiometry in Frequency Domain and Multivariate Methods

J.P. Pichardo-Molina*, *Centro de Investigaciones en Optica A.C., León, GT, México*, G. Gutiérrez-Juárez and H. Landa-Hernández, *Universidad de Guanajuato, León, GT, México*, R. Ivanov, *Universidad Autonoma de Zacatecas, Zacatecas, ZA, México* and O. Barbosa-García, *Centro de Investigaciones en Optica A.C., León, GT, México*

Study on Thermal Stability of Lysozyme Adsorbed on Hydrophobic Packing Surface

X.P. Geng*, M.R. Zheng, Y.N. Wu and Z.M. Lei, *Xi'an University of Engineering Science & Technology, Xi'an, Shaanxi, China* and X.D. Geng, *Northwest University, Xi'an, Shaanxi, China*

The Effect of Cholesterol Concentration on Preparation of Berberine Hydrochloride Liposomes

F. Zhang, *China* and X.-Q. An*, *Nanjing Normal University, Nanjing, China*

The Effect of Phalloidin on Actin Filaments in Complex with ADP.BeFx

J. Orban, F. Kelemen, S.Z. Barko and D. Lőrinczy*, *University Pécs, Pécs, Hungary*

Thermal Analysis of Collagen-Like Peptides Using MEMS Microcalorimetry

H. Tada*, P. Xu, D.L. Kaplan and P.Y. Wong, *Tufts University, Medford, MA, U.S.A.*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Thermal Analysis of the Samples of Tamra Bhasma Prepared by Different Ayurvedic Pharmacies

M. Wadekar*, *National Chemical Laboratory, Pune, India*
and R. Lad, S. Takale, R.D. Kankaria and B.A. Kulkarni,
Bharati Vidyapeeth Deemed University, Pune, India

Thermal Decomposition Patterns of Some Biosalts Isolated from Medicinal Plants

P.S. Khandagale*, P. Jadhav and D.G. Kanase, *Bharati Vidyapeeth, Deemed University, Pune, India* and S.H. Bhosale and S.S. Kadam, *Poona College of Pharmacy, Pune, India*

Thermal Kinetics Study for Prediction of Shelf Life of Drug

Fen Xu*, Li-Xian Sun, L.-N. Yang, Jian-Guo Liang and H.-T. Zhang, *Chinese Academy of Sciences, Dalian, China*

Thermochemistry of Heteroatomic Compounds: Enthalpy of Combustion and Formation of Organic Derivatives of P, As, Sb, and Bi

V.V. Ovchinnikov*, *Kazan State Architecture-Building University, Kazan, Russia*

Thermodynamic Properties of Liquid-Vapor Equilibrium and the Energies of Specific Intermolecular Interactions of Components of Vitamin "E" Synthesis

A.A. Baev and A.K. Baev*, *Russian Academy of Science, Ivanovo, Russia*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Thermodynamics and Properties in the Biological, Medical, Pharmaceutical, Agricultural, and Food Sectors

Thermogravimetric Investigations of Human Tooth Hard Tissues in Thermocycling

A.J. Panas*, *Military University of Technology Institute of Aviation Technology, Warsaw, Poland*, S. Cudzilo, *Military University of Technology, Warsaw, Poland*, S. Zmuda, *Military Medical Institute, Warsaw, Poland* and M. Preiskorn, *Dental Health Center, Warsaw, Poland*

Thermophysical and Thermochemical Characteristics of Biodiesel Fuels Produced from Belarusian Vegetable Oils

Y.V. Maksimuk, *Research Institute for Physical and Chemical Problems, Minsk, Belarus*, M.B. Charapennikau*, *Chemical Faculty of Belarusian State University, Minsk, Belarus* and Z.A. Antonava, *Research Institute for Physical and Chemical Problems, Minsk, Belarus*

Topical Permeation Characteristics of Ibuprofen from Poloxamer Gels with Chemical Promoters

N.T. González* and H. Sumano, *Nacional Autonomous University of Mexico (UNAM), México, DF, México*

Vapor-Liquid Equilibria of the Alkanes + 2 Butoxyethanol Systems

Moon Sam Shin*, Sunghyun Chang, Jihoon Im and Hwayong Kim, *Seoul National University, Seoul, Korea*

Posters 1

Chair: J.W. Magee and J.A. Widegren

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Wetting, Interfaces, and Membranes

Design of a System for Collection of Condensate Using Capillary Forces

S.W. Wilinski*, A. De Freitas and A.L. López de Ramos,
Universidad Simón Bolívar, Caracas, Venezuela

Determination of Superficial Dynamical Tension of CO₂ + Water from 293 K to 313 K With Pressures of 3, 4 and 5 MPa

J. Meléndez*, *Universidad Simón Bolívar, Caracas, Venezuela*, S. Zeppieri, *Universidad Simón Bolívar GFT-USB, Caracas, Venezuela* and A.L. López de Ramos, *Universidad Simón Bolívar, Caracas, Venezuela*

Interfacial Properties of Three Nonionic Surfactants in an Aqueous Amine Solution (N-Methyldiethanolamine + Diethanolamine)

J. Águila-Hernández*, B.E. García-Flores and A. Trejo,
Instituto Mexicano del Petróleo, México, DF, México

Reduced Capillary Length Scale in the Application of Ostwald Ripening Theory to the Precipitation of Charged Colloidal Particles in Electrolyte Solutions

J.D. Rowe and J.K. Baird*, *University of Alabama in Huntsville, Huntsville, AL, U.S.A.*

Software Demonstrations 1

Chair: A.I. Johns and M.L. Huber

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

1:50 PM An Automated System for Calculating Thermophysical Properties of Natural and Ozone-Safe Refrigerants and Their Mixtures

A.A. Vasserman* and V.P. Malchevsky, *Odessa National Maritime University, Odessa, Ukraine* and S.V. Bodyul, *Odessa State Academy of Refrigeration, Odessa, Ukraine*

1:50 PM Computer Packages for the Thermophysical Properties of Fluids and Solids

R.D. McCarty*, *Rimfire Consulting, Grand Junction, CO, U.S.A.*

1:50 PM Demonstration of Infotherm: Thermophysical Property Data of Mixtures and Pure Fluids

J. Homann*, *FIZ CHEMIE Berlin, Berlin, Germany*

1:50 PM Description of the Handbook of Thermodynamic Values Structure and of the Software for Dianik-Win Database and for Website Thermodynamics of Natural Processes

I.L. Khodakovsky*, *Dubna International University for Nature, Society and Man, Dubna, Moscow Region, Russia*

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Software Demonstrations 1

(continued)

Chair: A.I. Johns and M.L. Huber

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

1:50 PM Development of Program Package for Thermophysical Properties of Fluids: PROPATH- Availabilities of Dynamic Link Library (DLL) in Windows Applications

T. Yamaguchi*, *Nagasaki University, Nagasaki, Japan*, R. Akasaka, *Kyushu Lutheran College, Kumamoto City, Kurokami, Japan*, T. Honda, *Fukuoka University, Fukuoka, Jonan-ku, Japan*, S. Momoki, *Nagasaki University, Nagasaki, Japan*, T. Takata, *Kyushu University, Fukuoka, Nishi-ku, Japan* and T. Ito, *University of East Asia, Shimonoseki, Ichinomiya-gakuen, Japan*

1:50 PM DIPPR® 801 Database

J.R. Rowley*, W.V. Wilding, J.L. Oscarson and R.L. Rowley, *Brigham Young University, Provo, UT, U.S.A.*

1:50 PM Generating Reliable Thermodynamic Model Parameters with the help of DECHEMA Software Suite

R. Sass* and U. Westhaus, *DECHEMA e.V., Frankfurt am Main, Germany*

1:50 PM IVTANTHERMO Software for Users and Experts

V.S. Iorish*, *Glushko Thermocenter of Russian Academy of Sciences, Moscow, Russia*

1:50 PM NIST/TRC Databases and Software Tools for Chemistry and Engineering

M. Frenkel*, R.D. Chirico, V.V. Diky, C.D. Muzny, Q. Dong, X. Yan, A. Kazakov, I.M. Abdulagatov, B.A. Stevenson and G.R. Hardin, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

-continued on next page-

Software Demonstrations 1

(continued)

Chair: A.I. Johns and M.L. Huber

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

1:50 PM Property Libraries for Working Fluids for Calculating Heat Cycles, Turbines, Heat Pumps, and Refrigeration Processes

H.-J. Kretzschmar*, I. Stoecker, I. Jaehne, D. Seibt and M. Kunick, *Zittau/Goerlitz University of Applied Sciences, Zittau, Germany*

1:50 PM Software Demonstration of the Dortmund Databank (DDB) and its Application for Process Design

E.C. Ihmels*, J. Menke, K. Fischer, J. Rarey and J. Gmehling, *DDBST GmbH, Oldenburg, Germany*

1:50 PM The Network Database on Physical-Chemical Properties of Metals and Alloys

B.R. Gelchinski, *Institute of Metallurgy of the Ural Branch of the Russian Academy of Science, Ekaterinburg, Russia*, E.V. Dyuldina*, *Magnitogorsk State Technical University, Magnitogorsk, Chelyabinsk, Russia*, S.S. Les'kiv, *Southern Ural State University, Chelyabinsk, Russia*, S.V. Stunkus and K.Y. Shunyaev, *Institute of Thermophysics of the Siberian Branch of the Russian Academy of Science, Novosibirsk, Russia* and V.A. Titov, *Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia*

1:50 PM The REFPROP Database for the Thermophysical Properties of Fluids

E.W. Lemmon*, M.L. Huber and M.O. McLinden, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

-continued on next page-

Wednesday, August 02, 2006

Joint Session

Software Demonstrations 1

(continued)

Chair: A.I. Johns and M.L. Huber

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

**1:50 PM Using the PPDS Dataexpert Software to Provide
Thermodynamically Consistent Data for the Thermophysical
Properties of Pure Compounds**

A.I. Johns*, A.C. Scott, T. Brisbane and D.A.J. McGinnis, *TUV
NEL Ltd., Glasgow, East Kilbride, U.K.*

Wednesday, August 02, 2006

Joint Session

**Databases, Data Systems, Software Applications, and
Correlations 5**

Session 5

Chair: S.E. Quiñones-Cisneros and M.L. Huber

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-245

3:55 PM Correlations of the Solubility of Gases in Liquids

R. Battino*, P.G. Seybold, S. Sidigu, F. Campanell and J.N. Bohrer, *Wright State University, Dayton, OH, U.S.A.*

**4:15 PM Prediction of Solubilities of Medium-Sized Complex Chemicals
in Liquid Solvents: Retrieval, Reduction and Application**

J. Abildskov* and R. Gani, *Technical University of Denmark, Lyngby, Denmark* and R. Sass, *DECHEMA e.V., Frankfurt am Main, Germany*

4:35 PM Vapor-Liquid Equilibria of Alcohol-Chlorobenzene Mixtures

K.V. Rao*, R. Vijay Krishna, D.V. Pradeep Raju and A. Ravi Prasad, *Andhra University, Visakhapatnam, India*

**4:55 PM Correlation of Binary VLE by Ge Models: Comparison of
Unconstrained Optimization Methods**

A. Ravi Prasad*, A. Aravind Kumar and B. Uma Sankar Naidu Babu, *Andhra University, Visakhapatnam, India*

**5:15 PM Obtaining a Consistent Set of Thermodynamic Data: As an
Example Ge-I and Ga-Cl Systems**

L.N. Zelenina*, T.P. Chusova, Y.G. Stenin, I.E. Paukov, P.P. Semyannikov and V.A. Titov, *Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia*

Wednesday, August 02, 2006 19th ICCT / 61st CalCon

Electrolyte and Non-Electrolyte Solution Thermodynamics 6

Thermal Properties of Complex Mixtures

Chair: M.S. Gruszkiewicz and A.W. Hakin

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-5

- 3:55 PM Enthalpic Discrimination of Chiral Compounds of Electrolytes and Non-Electrolytes in Solution (Invited)**
T. Kimura*, *Kinki University, Kowakae, Higashi-osaka, Japan*
- 4:35 PM Interactions between the Tetrachloroaurate(III) Ion and Alkyltrimethylammonium Ions and Micelles**
T. Tominaga*, H. Iwata, T. Yasugi and M. Takezaki, *Okayama University of Science, Okayama, Japan*
- 4:55 PM Thermodynamic Modeling of the Rheological Behavior of PEG3000, PEG6000 and PEG10000 Aqueous Solutions**
R.C. Cruz*, R.J. Martins, M.J.E. Cardoso and O.E. Barcia, *Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil*
- 5:15 PM Solubility in Solvent-Antisolvent Mixtures: A Calorimetric Study of Solid-Liquid Phase Diagrams in Ternary Systems**
M.H. Hamed, *K.N. Toosi University of Technology, Tehran, Iran* and J.P.E. Grolier*, *Blaise Pascal University, Aubière, France*
- 5:35 PM Volumetric and Calorimetric Investigations of Aqueous Rare Earth Element Containing Triflate Salt Systems**
K.M. Erickson*, A.W. Hakin and J.L. Liu, *The University of Lethbridge, Lethbridge, AB, Canada*

Wednesday, August 02, 2006

16th Symposium

Fluid Property Measurements 4

Chair: R. Srivastava

Afternoon 2 3:50 PM - 4:55 PM

Room: Eng-1B40

3:55 PM Accurate Values of the Transport Properties of Argon

E.F. May*, *University of Western Australia, Crawley, WA, Australia* and M.R. Moldover, R.F. Berg and J.J. Hurly, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

4:15 PM Bulk Viscosity of Stirred Xenon near the Critical Point

K.A. Gillis*, I.I. Shinder and M.R. Moldover, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

4:35 PM Convective Stirring and Acoustic Spectra of Near-Critical Xenon

I.I. Shinder*, K.A. Gillis and M.R. Moldover, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Ionic Liquids 6

Polymers and Surface Properties

Chair: J.F. Brennecke

Afternoon 2 3:50 PM - 5:35 PM

Room: Coors-4

3:55 PM Magnetic Suspension Balance Study of Carbon Dioxide Solubility in Ammonium-Based Polymerized Ionic Liquids: Poly(P-Vinylbenzyltrimethyl Ammonium Tetrafluoroborate) and Poly([2-(Methacryloyloxy)Ethyl] Trimethyl Ammonium Tetrafluoroborate)

A.B. Blasig, *University of Wyoming, Laramie, WY, U.S.A.*,
J.B. Tang, *Zhejiang University, Hangzhou, China* and X.
Hu, Y.S. Shen and M.R. Radosz*, *University of Wyoming,
Laramie, WY, U.S.A.*

4:15 PM Polymerizable Ionic Liquids for Gas Separation Membranes

J.E. Bara*, D.E. Camper, A.K. Kaminski, D.L. Gin and R.D.
Noble, *University of Colorado, Boulder, CO, U.S.A.*

4:35 PM CO₂ Permeability, Diffusivity and Solubility in Polyethylene Glycol-Grafted Polyionic Membranes and CO₂ Selectivity Relative to Methane and Nitrogen

X.H. Hu*, *University of Wyoming, Laramie, WY, U.S.A.*, J.B.
Tang, *Zhejiang University, Hangzhou, China* and A.B.
Blasig, Y.S. Shen and M.R. Radosz, *University of Wyoming,
Laramie, WY, U.S.A.*

4:55 PM Surface Tension Measurements of Imidazolium Based Ionic Liquids

P.J. Carvalho, M.G. Freire*, A.J. Queimada, I.M. Marrucho and
J.A.P. Coutinho, *Universidade de Aveiro, Aveiro, Portugal*

5:15 PM Surface Properties of Ionic Liquids

V. Sokhan*, *National Physical Laboratory, Teddington,
Middlesex, U.K.*

Wednesday, August 02, 2006

Joint Session

***Molecular Modeling, Including Simulation 8
Theory***

Chair: J. Errington

Afternoon 2 3:50 PM - 5:35 PM

Room: Math-100

**3:55 PM Boundary Fluctuation Theory of Thermal Transport
Coefficients**

J. Petracic* and P. Harrowell, *The University of Sydney,
Sydney, NSW, Australia*

**4:15 PM Preferential Interactions in Biological Systems by
Kirkwood-Buff Theory and Computer Simulation**

P.E. Smith* and M. Kang, *Kansas State University,
Manhattan, KS, U.S.A.*

4:35 PM Thermal Conductivity in One-Dimensional Systems?

P. Tempatarachoke and D. Isbister*, *University of New
South Wales, Australia*

**4:55 PM Molecular Dynamics Simulations of a Chemical Reaction;
Conditions for Local Equilibrium in a Temperature Gradient -
IACT Doctorate Award Presentation -**

J. Xu*, S. Kjelstrup and D. Bedeaux, *Norwegian University of
Science and Technology, Trondheim, Norway*

**5:15 PM Normalized Free Energy and Normalized Entropy Applied to
Some Lambda-Transitions**

P. Love*, *University of Connecticut at Stamford, Stamford,
CT, U.S.A.*

Wednesday, August 02, 2006

16th Symposium

Optical and Thermal Radiative Properties of Materials 1

Radiative Properties of Microstructured Surfaces

Chair: L.M. Hanssen

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-200

3:55 PM Radiative Properties of Microrough and Nanostructured Surfaces - An Overview (Invited)

Z.M. Zhang*, *Georgia Institute of Technology, Atlanta, GA, U.S.A.*

4:35 PM Reflectivity of a Periodic Structure of Self-Assembled Silica Micro-Spheres

M. Kihara*, K. Miyazaki and H. Tsukamoto, *Kyushu Institute of Technology, Fukuoka, Japan*

4:55 PM Optical Absorption Study in Electrochemical Etching Porous Silicon

M. Godinez, A. Florido-Cuellar, R.A. Muno Hernández, E. Marín and A. Calderón*, *Instituto Politécnico Nacional, México, DF, México*

5:15 PM Radiative Properties of Gold Surfaces with One-Dimensional Microscale Gaussian Random Roughness

K. Fu and P.F. Hsu*, *Florida Institute of Technology, Melbourne, FL, U.S.A.*

Wednesday, August 02, 2006 19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 2***

Experimental, Mixtures I

Chair: R.P. Danner and T.W. de Loos

Afternoon 2 3:50 PM - 5:35 PM

Room: Coors-1

3:55 PM High Pressure Phase Behavior of Binary Systems of Carbon Dioxide and Propane with Hyperbranched Polymers

T.W. de Loos*, E.J.M. Straver and V. Munoz, *Delft University of Technology, Delft, Netherlands*

4:15 PM Determination of Dew Points, Gas Phase Densities and Liquid Volume Fractions of Gas Condensates

K.N. Marsh* and M. Kandil, *University of Canterbury, Christchurch, New Zealand* and A.R.H. Goodwin, *Schlumberger Technology Corporation, Sugar Land, TX, U.S.A.*

4:35 PM An Experimental Study of Vapor-Liquid Equilibrium for Ammonia + Propane Refrigerant Mixtures

J.O. Kang*, Y.M. Park, J. Yoo, H.J. Kim and J. Lee, *Ajou University, Youngtong-gu, Suwon, Korea*

4:55 PM Study of the Phase Diagram of the (Carbon Dioxide + Caffeine) System at High Pressures by Combined Transitiometry and Thermodynamic Modeling

U.K. Deiters*, *University of Cologne, Köln, Germany* and S.L. Randzio, *Polish Academy of Sciences, Warsaw, Poland*

5:15 PM Specific Partial Molar Volumes at Infinite Dilution and Volumes of Mixing for Athabasca Bitumen and Bitumen Vacuum Resid + Solvent Mixtures

Y. Maham, X. Zhang and J.M. Shaw*, *University of Alberta, Edmonton, AB, Canada*

Wednesday, August 02, 2006

16th Symposium

Photothermal and Photoacoustic Techniques 2

Chair: G.J. Diebold

Afternoon 2 3:50 PM - 5:15 PM

Room: Eng-155

3:55 PM Photothermal Measurements of Microcrystalline CdSSe Glasses (Invited)

S.E. Bialkowski and O. Dada*, *Utah State University, Logan, UT, U.S.A.*

4:35 PM Development of a High Speed Laser Flash Method Using a Sub-Nanosecond Thermoreflectance Technique

T. Yagi*, N. Taketoshi, H. Kato and T. Baba, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

4:55 PM Application of a Differential Photoacoustic Cell in the Study of *in-situ* Electrochemical Deposition of Zinc

K.M. Briño-Enríquez* and J.J. Perez-Bueno, *Centro de Investigacion y Desarrollo Tecnológico en Electroquímica, Queretaro, QT, México* and M.L. Mendoza-Lopez, R. Velazquez-Hernandez and M.E. Rodriguez-Garcia, *Universidad Nacional Autónoma de México, Queretaro, QT, México*

Wednesday, August 02, 2006

16th Symposium

Properties of Working Fluids, Including Refrigerants 3

Experimental Thermodynamics 1

Chair: R.A. Perkins and M.O. McLinden

Afternoon 2 3:50 PM - 5:15 PM

Room: Eng-265

3:55 PM Vapor-Liquid Equilibrium Measurements for the Binary and Ternary Mixtures of R290, R600a and R32 at Temperatures Between 260 K and 330 K

K. Tanaka and Y. Higashi*, *Iwaki Meisei University, Iwaki, Fukushima, Japan* and Y. Kayukawa and K. Fujii, *National Institute of Advanced Industrial Science and Technology (AIST), National Metrology Institute of Japan (NMIJ), Tsukuba, Japan*

4:15 PM Measurements of the Surface Tension for Some Alcohols

K. Tanaka*, *Iwaki Meisei University, Iwaki, Fukushima, Japan* and Y. Higashi, *Iwaki Meisei University, Fukushima, Japan*

4:35 PM Thermophysical Properties of a Refrigerant Mixture of R365mfc (1,1,1,3,3-Pentafluorobutane) and Galden HT 55 (Perfluoropolyether)

H. Kremer*, *ESYTEC Energie- und Systemtechnik GmbH, Erlangen, Germany*, A.P. Fröba, C. Botero and A. Leipertz, *Universität Erlangen-Nürnberg, Erlangen, Germany* and F. Flohr and C. Meurer, *Hannover, Germany*

4:55 PM Determination of Saturated Vapor Pressure of Freons for Entire Range of the Liquid Phase

R.M. Varushchenko* and A.I. Druzhinina, *Moscow State University, Moscow, Russia*

Wednesday, August 02, 2006

16th Symposium

***Theory of Thermophysical Properties, Including Statistical
Mechanics 4***

Chair: J. Kincaid

Afternoon 2 3:50 PM - 5:55 PM

Room: Eng-151

**3:55 PM Determination of Third Virial Coefficients: A Mandatory
Routine Test**

C.G. Olivera-Fuentes, *Simon Bolívar University, Caracas,
Venezuela* and C.M. Colina*, *Pennsylvania State
University, University Park, PA, U.S.A.*

**4:15 PM Theoretical Calculation of the Transport Properties of
Monatomic Silver Vapor**

L. Biolsi*, *University of Missouri-Rolla, Rolla, MO, U.S.A.*
and P.M. Holland, *Thorleaf Research, Inc, Santa Barbara,
CA, U.S.A.*

**4:35 PM Theoretical Models for the Evaluation of Liquid Thermal
Conductivity: Gas-Like Models vs Solid-Like Models**

G. Latini* and G. Passerini, *Universita' Politecnica delle
Marche, Ancona, Italy*

**4:55 PM Speeds of Sound and Isothermal Compressibility of Ternary
Liquid Systems at 298.15 K: A Comparison with Theory**

V. Vyas*, *University of Allahabad, Allahabad, India*

**5:15 PM Effective Thermal Conductivity of Two-Phase Systems
Using Green's Function with Spherical Inclusions**

R.V. Singh* and Jagjiwanram, *University of Rajasthan,
Jaipur, India* and S.K. Jain, *Engineering College, Kota,
India*

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Wednesday, August 02, 2006

16th Symposium

***Theory of Thermophysical Properties, Including Statistical
Mechanics 4***
(continued)

Chair: J. Kincaid

Afternoon 2 3:50 PM - 5:55 PM

Room: Eng-151

**5:35 PM Behavior of Thermal Transport Properties of Disordered
Alloys: A Theoretical Study**

A. Alam* and A. Mookerjee, *S.N. Bose National Centre for
Basic Sciences, Salt Lake City, Kolkata, India*

Wednesday, August 02, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 5
Natural Products and the Environment***

Chair: N. Wright

Afternoon 2 3:50 PM - 5:15 PM

Room: Coors-3

- 3:55 PM Investigations on Structural Characteristic, Thermal Stability and Hygroscopicity of Sisal Fibres at Elevated Temperatures**
D. Saikia, Duliajan College, Duliajan, Assam, India*
- 4:15 PM Solubilities and Densities of Capsaicin in Supercritical Carbon Dioxide**
O. Elizalde-Solis, L.A. Galicia-Luna and F.F. Betancourt-Cárdenas, Instituto Politécnico Nacional, México, DF, México*
- 4:35 PM Model and Analysis of Vacuum Membrane Distillation for the Recovery of Volatile Aroma Compounds from Black Currant Juice**
V. Soni, J. Abildskov, G.E. Jonsson and R. Gani, Technical University of Denmark, Lyngby, Denmark*
- 4:55 PM Can Thermodynamic Studies and Thermal Analysis be of a Help for Safe Keeping of Biological Germplasm When Exposed to Cryopreservation?**
J. Sestak, Academy of Sciences of the Czech Republic, Prague, Czech Republic and J. Zamecnik, Research Institute of Crop Production, Prague, Czech Republic*

Wetting, Interfaces, and Membranes 1

Chair: K. Binder and M. Müller

Afternoon 2 3:50 PM - 5:35 PM

Room: Bens-180

- 3:55 PM Momentum and Heat Transfer at the Solid Liquid Interface (Invited)**
J-L. Barrat*, *University of Lyon, Villeurbanne, France*
- 4:35 PM An Interface Delocalization (Wetting) Transition in a Single Crystal Tin Superconductor: Experimental Study**
V.F. Kozhevnikov*, M.J. Van Bael, K. Temst, C. Van Haesendonck and J.O. Indekeu, *Katholieke Universiteit Leuven, Leuven, Belgium*
- 4:55 PM Adsorption of Polymers on a Brush: Tuning the Order of the Wetting Phase Transition**
L.G. MacDowell*, *Universidad Complutense, Madrid, Spain* and M. Müller, *Georg August Universität, Göttingen, Germany*
- 5:15 PM Calculation of the Surface Pressure and the Contact Energy in the Adsorption of Alkanes on Aqueous Substrates**
V.C. Weiss*, *International University Bremen, Bremen, Germany*

Wednesday, August 02, 2006 19th ICCT / 61st CalCon

Colloid and Interface Science 1

Polymer-Surfactant Mixtures

Chair: L. Piculell and M. Bastos

Evening 7:30 PM - 9:15 PM

Room: Coors-5

7:35 PM Thermodynamics of Interaction in Polymer-Surfactant Systems (Invited)

H.K. Yan*, Y.L. Wang, J.B. Wang and G.Y. Bai, *Chinese Academy of Sciences, Beijing, China*

8:15 PM Random vs Block Copolymers of Polyethylene Oxide and Polypropylene Oxide in Aqueous Solutions: Interaction with Ionic Surfactants- Giaque Travel Award Presentation -

A. Niemiec* and W. Loh, *Universidade Estadual de Campinas, Campinas, SP, Brazil*

8:35 PM A Novel Method to Determinate Aggregation Number in Micelles from ITC Experiment

Á. Piñeiro, S. Concha-Santos, M. Estrada-Villegas, A. Vega-Rodríguez and S. Pérez-Casas*, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*

8:55 PM Calorimetric Investigations of the Interaction Between Non-Ionic Polymers and Ionic Surfactants

W. Loh*, D.A. Brasil, L.A.C. Teixeira, A. Niemiec and R.C. da Silva, *Universidade Estadual de Campinas, Campinas, SP, Brazil*

Wednesday, August 02, 2006

Joint Session

**Databases, Data Systems, Software Applications, and
Correlations 6**

Session 6

Chair: A.I. Johns and M.L. Huber

Evening 7:30 PM - 9:35 PM

Room: Eng-245

**7:35 PM A Correlation for C_p for Solid Hydrocarbons Based on
Elemental Composition**

V. Lastovka, *University of Alberta, Edmonton, AB, Canada*,
N. Sallamie, *University of Calgary, Calgary, AB, Canada*
and Y. Maham and J.M. Shaw*, *University of Alberta,
Edmonton, AB, Canada*

**7:55 PM Use of Transformed Correlations to Help Screen and
Populate Properties within Databanks**

D.L. Morgan*, *Dow Corning Corporation, Midland, MI,
U.S.A.*

**8:15 PM Practical and Philosophical Observations from a Review of
Vapor Pressures of Explosives and Related Compounds**

J. Wormhoudt*, *Aerodyne Research, Inc, Billerica, MA,
U.S.A.*

**8:35 PM Experimental and Computational Study of Thermochemistry
of Fluoro- and Chloro-Phenols**

S.P. Verevkin* and V.N. Emel'yanenko, *University of Rostock,
Rostock, Germany*

**8:55 PM Comparative Study on the Performance of Three- and Four-
Parameter Correlations of the Enthalpy of Vaporization for
Pure Substance Refrigerants**

K.K. Park*, *Kookmin University, Seoul, Korea*

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Wednesday, August 02, 2006

Joint Session

***Databases, Data Systems, Software Applications, and
Correlations 6***

Session 6

(continued)

Chair: A.I. Johns and M.L. Huber

Evening 7:30 PM - 9:35 PM

Room: Eng-245

**9:15 PM Prediction of the Vapor Pressure of Non-Electrolyte Organic
Compounds via Group Contributions and Group Interactions**

Y. Nannoolal*, D. Ramjugernath and J. Rarey, *University of
KwaZulu-Natal, Durban, South Africa*

Instrumentation and Measurement Techniques 4

Chair: T.J. Bruno

Evening 7:30 PM - 9:15 PM

Room: Eng-105

7:35 PM Advanced Electromechanical Model for Torsional Crystal Viscosity Sensors

A. Laesecke* and H.-D. Seelig, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

7:55 PM A New Apparatus for Simultaneous Measurements of Viscosity and Density over Wide Temperature and Pressure Ranges

D. Seibt*, E. Vogel, E. Bich and E. Hassel, *University of Rostock, Rostock, Germany*

8:15 PM Thermophysical Method for Monitoring of Water Traces in Oils

P.V. Skripov, A.A. Starostin and D.V. Volosnikov*, *Institute of Thermal Physics, Ekaterinburg, Russia*

8:35 PM Structure and Thermophysical Properties of Molten BaGe by Using Electrostatic Levitation Technique

M. Watanabe*, A. Ishikura and A. Mizuno, *Gakushuin University, Tokyo, Japan*, T. Masaki and T. Ishikawa, *Japan Aerospace Exploration Agency, Tsububa, Japan* and J. Kohara, *Japan Synchrotron Radiation Research Institute, Sayo-gun, Hyogo, Japan*

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Wednesday, August 02, 2006

16th Symposium

Instrumentation and Measurement Techniques 4

(continued)

Chair: T.J. Bruno

Evening 7:30 PM - 9:15 PM

Room: Eng-105

**8:55 PM A Microelectromechanical System (MEMS), for the
Measurement of the Complex Relative Permittivity: Results
for Methylbenzene, Octane, Argon, and an Ionic Liquid at
Temperatures between (323 and 423) K and Pressures in
the Range (0.1 to 68) MPa**

A.R.H. Goodwin*, *Schlumberger Technology Corporation,
Sugar Land, TX, U.S.A.*, K.N. Marsh, *University of
Canterbury, Christchurch, New Zealand*, E.P. Donzier and O.
Vancauwenberghe, *Schlumberger-Doll Research,
Ridgefield, CT, U.S.A.*, M. de Lara, *Schlumberger
Cambridge Research, Cambridge, U.K.* and M.B. Mercier,
*École Supérieure d'Ingénieurs en Électrotechnique et
Électronique, Noisy le Grand, France*

Ionic Liquids 7
Simulation and Theory

Chair: L. Rebelo

Evening 7:30 PM - 9:15 PM

Room: Coors-4

7:35 PM Atomistic Simulation of Pyridinium- and Triazolium-Based Ionic Liquids

E.J. Maginn* and C. Cadena, *University of Notre Dame, Notre Dame, IN, U.S.A.*

7:55 PM Ion-Pair Formation of the Ionic Liquid [EMIM][NTf₂] as Function of Temperature and Concentration

T. Koeddermann, Ch. Wertz, A. Heintz* and R. Ludwig, *University of Rostock, Rostock, Germany*

8:15 PM Nanostructuring in Pure Ionic Liquids Investigated by Molecular Simulation

A.A.H. Padua*, *CNRS/Université Blaise Pascal, Aubière, France*, J.N.A. Canongia Lopes, *Instituto Superior Tecnico, Lisboa, Portugal* and M.F. Costa Gomes, *CNRS/Université Blaise Pascal, Aubière, France*

8:35 PM Transport Properties of Room Temperature Ionic Liquids by Molecular Dynamics Simulations

C. Rey-Castro*, A.L. Tormo and L.F. Vega, *Consejo Superior de Investigaciones Científicas, Barcelona, Bellaterra, Spain*

8:55 PM Salt Ionic Crystal Packing: Deconvoluting the Factors That Make Ionic Liquids Liquid

W.A. Henderson*, *U.S. Naval Academy, Annapolis, MD, U.S.A.*, V.G. Youn, Jr., *University of Minnesota, Minneapolis, MN, U.S.A.*, S. Passerini, *Casaccia Research Center, Rome, Italy*, P.C. Trulove, *U.S. Naval Academy, Annapolis, MD, U.S.A.* and H. De Long, *Air Force Office of Scientific Research, Arlington, VA, U.S.A.*

Wednesday, August 02, 2006

Joint Session

***Molecular Modeling, Including Simulation 9
Potentials***

Chair: V. Shen

Evening 7:30 PM - 9:15 PM

Room: Math-100

**7:35 PM Development of a Universal m-6-8 United Atom Force Field
for Accurate Molecular Simulations**

D. R. Culley* and J.F. Ely, *Colorado School of Mines,
Golden, CO, U.S.A.*

7:55 PM Transferable Potentials for Perfluorocarbons

J.R. Elliott, Jr.* and A.D. Sans, *The University of Akron,
Akron, OH, U.S.A.*

8:15 PM Parameterization of H₂S, SO₂ and NO₂

S.L. Clifford* and D. Ramjugernath, *University of KwaZulu-
Natal, Durban, South Africa* and K. Bolton, *University
College of Boraas, Boraas, Sweden*

**8:35 PM Development of New Molecular Models for Applications in
Process Engineering on the Basis of Quantum Chemical
Calculations**

B. Eckl*, J. Vrabec and H. Hasse, *University of Stuttgart,
Stuttgart, Germany*

**8:55 PM Hexafluoroethane (C₂F₆, R116) Intermolecular
Interaction Potential and Thermophysical Properties**

L. Zarkova, *Institute of Electronics, Sofia, Bulgaria*, U.
Hohm*, *TU Braunschweig, Braunschweig, Germany* and
M. Damyanova, *Institute of Electronics, Sofia, Bulgaria*

Wednesday, August 02, 2006

16th Symposium

Optical and Thermal Radiative Properties of Materials 2

Emissivity Measurements

Chair: Z.M. Zhang

Evening 7:30 PM - 9:15 PM

Room: Eng-200

- 7:35 PM Temperature- and Angle-Resolved Infrared Spectral Directional Emissivity of SiC, Alumina and Pt for Temperatures Up to 1000 °C**
- C.P. Cagran*, L.M. Hanssen, M. Noorma and S.N. Mekhontsev, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*
- 7:55 PM Measurements of Total Hemispherical Emissivity and Specific Heat Capacity of Nonconducting Materials by a Transient Calorimetric Technique**
- S. Sasaki, *Ichinoseki National College of Technology, Hagisho, Ichinoseki, Japan*, H. Kou*, *Daebul University, Jeonnam, Korea*, A. Hoshi, *Ichinoseki National College of Technology, Hagisho, Ichinoseki, Japan*, H. Masuda, *Tohoku University, Sendai, Japan* and H. Kiyohashi, *Sendai Digital Technical College, Sendai, Japan*
- 8:15 PM Measurement and Modeling of the Emittance of Silicon Wafers with Anisotropic Roughness**
- H.J.L. Lee, A.C. Bryson* and Z.M. Zhang, *Georgia Institute of Technology, Atlanta, GA, U.S.A.*
- 8:35 PM About the Proper Wavelength for Pyrometry on Shock Physics Experiments**
- A. Seifter* and A.W. Obst, *Los Alamos National Laboratory, Los Alamos, NM, U.S.A.*
- 8:55 PM Use of a High Temperature Reflectometer for Surface Temperature Measurements**
- L.M. Hanssen*, M. Noorma, A.V. Prokhorov, S.N. Mekhontsev and C.P. Cagran, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Wednesday, August 02, 2006 19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 3***

Experimental, Mixtures II

Chair: T.W. de Loos and U.K. Deiters

Evening 7:30 PM - 9:15 PM

Room: Coors-1

**7:35 PM Inverse Gas Chromatography Studies of Polymer-Solvent
Systems with High Pressure Carrier Gases (Invited)**

A.T. Jones, J.L. Duda and R.P. Danner*, *The Pennsylvania
State University, University Park, PA, U.S.A.*

**8:15 PM Light Scattering Study of Tricritical Phenomena in
Quaternary Solutions of Water, n-Decane, n-Undecane and
tert-Butanol**

N. Wang, *Lanzhou University, Lanzhou, Gansu, China*, X.-
Q. An, *Nanjing Normal University, Nanjing, China* and W.-
G. Shen*, *East China University of Science and Technology,
Shanghai, China*

**8:35 PM Measurement of Critical Microemulsion Concentration of
Supercritical Carbon Dioxide Microemulsion Using UV-Vis
Spectroscopy**

Y.-S. Zhou, *Lanzhou University, Lanzhou, Gansu, China*,
X.-Q. An*, *Nanjing Normal University, Nanjing, China* and
W.-G. Sheng, *Lanzhou University, Lanzhou, Gansu, China*

**8:55 PM Excess Molar Volumes and Spectroscopic Studies for the
Binary Mixtures of Alkoxyethanols with Amides/Amines at
298.15 K**

R. Kumar*, *Dyal Singh College, Karnal, Haryana, India*
and A. Pal, *Kurukshetra University, Kurukshetra, Haryana,
India*

Photothermal and Photoacoustic Techniques 3

Chair: G.J. Diebold

Evening 7:30 PM - 9:15 PM

Room: Eng-155

- 7:35 PM Thermal Diffusivity of Materials by Imaging of Lateral Thermal Diffusion**
G. Kalogiannakis, *Vrije Universiteit, Brussels, Belgium*, A. Okasha, *National Research Center, Cairo, Egypt*, S. Longuemart, *Université du Littoral Côte d'Opale, Dunkerque, France* and D. Van Hemelrijck and C. Glorieux*, *Katholieke Universiteit, Leuven, Belgium*
- 7:55 PM Development of Soret Forced Rayleigh Scattering Method for Mass Diffusion Coefficient of Methanol/Water Solutions in Polymer Electrolyte Membrane**
O. Kamita*, Y. Yamamoto and Y. Nagasaka, *Keio University, Yokohama, Kanagawa, Japan*
- 8:15 PM Measurement of Thermophysical Properties of Spherical Samples Using Photothermal Radiometry**
C. Wang*, *Suzhou University, Suzhou, Jiangsu, China*, Y. Liu and A. Mandelis, *University of Toronto, Toronto, ON, Canada* and J. Shen, *National Research Council of Canada, Vancouver, BC, Canada*
- 8:35 PM Photoacoustic Thermoelastic Imaging of Vickers Indented Solids Without and Under External Loading**
K.L. Muratikov* and A.L. Glazov, *A.F. Ioffe Physical-Technical Institute of RAS, St. Petersburg, Russia*

-continued on next page-

Wednesday, August 02, 2006

16th Symposium

Photothermal and Photoacoustic Techniques 3

(continued)

Chair: G.J. Diebold

Evening 7:30 PM - 9:15 PM

Room: Eng-155

**8:55 PM Nondestructive Characterization of Microstructures in
Titanium Modified 20% Cold Worked 316 Type Austenitic
Stainless Steel Using Photoacoustic Spectroscopy**

P. Palanichamy* and P. Kalyanasundaram, *Indira Gandhi
Centre for Atomic Research, Kalpakkam, India, C.*
Sanjeeviraja, *Alagappa University, Karaikkudi, India* and K.
Ramachandran, *Madurai Kamaraj University, Madurai,
India*

Properties of Aqueous Systems 1

Aqueous Electrolytes

Chair: A.H. Harvey

Evening 7:30 PM - 9:15 PM

Room: Eng-1B40

7:35 PM High Temperature Thermodynamics of Phosphoric Acid in Aqueous Solution

K. Ballerat-Busseroles, *Université Blaise Pascal/CNRS, Aubière, France*, J. Sedlbauer, *Technical University of Liberec, Liberec, Czech Republic* and V. Majer*, *Université Blaise Pascal/CNRS, Aubière, France*

7:55 PM Modeling Phase Separation in Water-Solvent-Electrolyte Mixtures

T.N. Rogers*, D.J. Wiegand and M.E. Mullins, *Michigan Technological University, Houghton, MI, U.S.A.*

8:15 PM Modeling Acid-Base Equilibria and Phase Behavior in Mixed-Solvent Electrolyte Systems

P. Wang, J.J. Kosinski, R.D. Springer and A. Anderko*, *OLI Systems Inc., Morris Plains, NJ, U.S.A.*

8:35 PM Equations of State for Multi-Component Solutions of Electrolytes Using Ion-Specific Parameters

Y. Lin* and K. Thomsen, *Technical University of Denmark (DTU), Lyngby, Denmark* and J.C. de Hemptinne, *Institut Français du Pétrole, Rueil Malmaison, France*

8:55 PM Pitzer pH Scale - Implication for pH Determination in Estuarine Waters

C.S. Wong, *Institute of Ocean Sciences, Sydney, BC, Canada*, P.Y. Tishchenko*, *V.I. Il'ichev Pacific Oceanological Institute, Vladivostok, Russia* and W.K. Johnson, *Institute of Ocean Sciences, Sydney, BC, Canada*

Wednesday, August 02, 2006

16th Symposium

Properties of Working Fluids, Including Refrigerants 4

Transport Properties

Chair: A. Laesecke and M.O. McLinden

Evening 7:30 PM - 8:55 PM

Room: Eng-265

7:35 PM Corresponding States for Transport Properties

R.D. McCarty*, *Rimfire Consulting, Grand Junction, CO, U.S.A.*

7:55 PM Transport Property Equations-of-State for HFC-245fa

K. Zou and A.S. Lawal*, *Texas Tech University, Lubbock, TX, U.S.A.*

8:15 PM Viscosity Measurements of Refrigerant Blend R-507A (50 wt% HFC-143a, 50 wt% HFC-125) in the Temperature Range 254 to 293 K and Pressures up to 10 MPa

H.M.N.T. Avelino, *Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal*, J.M.N.A. Fareleira*, *Centro de Química Estrutural, Lisboa, Portugal* and C.M.B.P. Oliveira, *Universidade Técnica de Lisboa, Lisboa, Portugal*

8:35 PM Thermophysical Properties of a Quaternary Refrigerant Mixture: Comparison of Dynamic Light Scattering Measurements with a Simple Prediction Method

C. Botero*, A.P. Fröba and A. Leipertz, *Universität Erlangen-Nürnberg, Erlangen, Germany*

Wednesday, August 02, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 6***

Thermodynamics of Biological Systems

Chair: R.D. Sheardy and N. Wright

Evening 7:30 PM - 9:15 PM

Room: Coors-3

**7:35 PM A Thermodynamic Investigation of Reactions Catalyzed by
D-Hydantoinase and N-Carbamoyl-D-Amino Acid Hydrolase**

Y.B. Tewari, *National Institute of Standards and Technology,
Gaithersburg, MD, U.S.A.*, N. Kishore, *Indian Institute of
Technology Bombay, Powai, Mumbai, India*, B.E. Lang,
*National Institute for Standards and Technology, Rockville,
MD, U.S.A.* and R.N. Goldberg*, *National Institute of
Standards and Technology, Gaithersburg, MD, U.S.A.*

**7:55 PM Computer-Aided Pure Component Property Prediction for
Isomers**

H.E. González-Villalba, J. Abildskov* and R. Gani, *Technical
University of Denmark, Lyngby, Denmark*

**8:15 PM Complex Heat Capacity of Non-Debye Process in
Saccharides**

Y. Ike*, Y. Seshimo and S. Kojima, *University of Tsukuba,
Tsukuba, Ibaraki, Japan*

**8:35 PM Thermodynamic Molecular Switch Controls Chemical
Equilibrium in Interacting Biological Systems**

P. W. Chun*, *University of Florida College of Medicine,
Gainesville, FL, U.S.A.*

**8:55 PM Kinetics and Thermodynamics of Enzymatic Reactions from
Spectrophotometric *in Situ* Measurements**

R. Patiño*, *Cinvestav - Unidad Mérida, Mérida, YU, México*

Wetting, Interfaces, and Membranes 2

Chair: M. Müller

Evening 7:30 PM - 9:15 PM

Room: Bens-180

7:35 PM Investigating Odd-Even Behavior in Wetting by Molecular Dynamics Simulation

P. Srivastava* and W.G. Chapman, *Rice University, Houston, TX, U.S.A.* and P.E. Laibinis, *Vanderbilt University, Nashville, TN, U.S.A.*

7:55 PM Pattern Formation and Morphology Evolution in Langmuir Monolayers

A. Flores, E. Corvera-Poire, C. Garza and R. Castillo*, *UNAM, México, DF, México*

8:15 PM Surface Phase Diagram of Water

I. Brovchenko* and A. Oleinikova, *University of Dortmund, Dortmund, Germany*

8:35 PM Thermomechanical Treatment of Fluid-Fluid Interfaces within Density Gradient Theory - A Review

K. Meier* and S. Kabelac, *Helmut-Schmidt-University, Hamburg, Germany*

8:55 PM Phase Equilibrium and Interface Properties in Binary Mixtures: Molecular Dynamics and Density Gradient Theory Predictions

A. Mejia*, *Universidad de Concepcion, Concepcion, Chile*, L.F. Vega, *Consejo Superior de Investigaciones Cientificas, Barcelona, Bellaterra, Spain* and H. Segura, *Universidad de Concepcion, Concepcion, Chile*

Instrumentation and Measurement Techniques 5

Chair: T. J. Bruno

Morning 1 8:30 AM - 10:15 AM

Room: Eng-151

8:35 AM Applications of an Optical Method for Relative Pressure and Density Characterization on SF₆ Near Its Critical Point

Y. Garrabos, C. Lecoutre-Chabot*, F. Palencia and D. Beysens, *CNRS, Pessac Cedex, France*

8:55 AM Dynamic Light Scattering (DLS) for the Determination of Thermophysical Properties of Ionic Liquids

A.P. Fröba and C. Botero, *Universität Erlangen-Nürnberg, Erlangen, Germany*, H. Kremer, *ESYTEC Energie- und Systemtechnik GmbH, Erlangen, Germany* and A. Leipertz*, *Universität Erlangen-Nürnberg, Erlangen, Germany*

9:15 AM Multiple Scattering in Turbid Liquids: Theory, Simulation and Experiments

W. Schröer*, J. Köser and F. Kuhnert, *University Bremen, Bremen, Germany*

9:35 AM A New Method for the Measurement of the Water Enhancement in Compressed Air

G. Koglbauer and M. Wendland*, *University of Natural Resources and Applied Life Sciences, Vienna, Austria*

9:55 AM A New Apparatus for the Measurement of Polymer-Solvent-Monomer Phase Equilibria at Process Conditions

L.C. Wilson*, *The Dow Chemical Company, South Charleston, WV, U.S.A.*

Optical and Thermal Radiative Properties of Materials 3

Radiative Properties of Metals and Oxides

Chair: Z.M. Zhang

Morning 1 8:30 AM - 10:15 AM

Room: Eng-200

8:35 AM On the Classification of Skin Effect Regions of Pure Metals I: Diagram of Incident Frequency vs Relaxation Time of Metal

Y. Zheng*, *Victoria, BC, Canada*

8:55 AM On the Classification of Skin Effect of Pure Metals II: Thermal Radiative Absorption and Emission

Y. Zheng*, *Victoria, BC, Canada*

9:15 AM Thermal Radiative Properties of Oxides, An Overview

P. Echegut*, J.F. Brun, D. De Sous Meneses and B. Rousseau, *Centre de Recherches sur les Matériaux à Haute Températures – CNRS, Orléans, France*

9:35 AM Effect of the Scattering of Light on the Thermal Radiative Properties of a Nearly Black Body Coating

H. Gomart*, *Centre de Recherches sur les Matériaux à Haute Températures – CNRS, Orléans, France*, S. Schelz and E. Véron, *CEA / Le Ripault, Monts, France* and B. Rousseau and P. Echegut, *Centre de Recherches sur les Matériaux à Haute Températures – CNRS, Orléans, France*

9:55 AM Oxidation Effect on Spectral Emissivity of Ni-Based Alloys, Iron and Tungsten Carbide/Cobalt

L. del Campo*, R.B. Perez-Saez and M.J. Tello, *Universidad del País Vasco, Leioa, Bizkaia, Spain*

Photothermal and Photoacoustic Techniques 4

Chair: G.J. Diebold

Morning 1 8:30 AM - 10:15 AM

Room: Eng-155

8:35 AM Thermophysical Characterization of Liquid Mixtures using a Thermal-Wave Cavity

A. Matvienko* and A. Mandelis, *University of Toronto, Toronto, ON, Canada*

8:55 AM High Precision Measurements of Thermal Diffusivity for Binary Liquid Mixtures by Using the Photoacoustic Phase in the Transmission Mode

J.A. Balderas-López*, *UPIBI-IPN, Madero, México*

9:15 AM Spectrometer System for Characterization of Thermo-reflectance of Metals

J. Ishii* and Y. Shimizu, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

9:35 AM Photothermal and Structural Characterization of $\text{Cu}_x(\text{CdTe})_y\text{O}_z$ Films Grown by Reactive RF Cosputtering

J. Garcia-Rivera* and R. Velazquez-Hernandez, *Universidad Nacional Autonoma de Mexico, Queretaro, QT, México*, J. Carmona-Rodriguez, *Unidad Queretaro, Queretaro, QT, México*, S. Jimenez-Sandoval and R. Lozada-Morales, *Centro de Investigacion y de Estudios Avanzados del I.P.N., Queretaro, QT, México* and M.E. Rodriguez, *Universidad Nacional Autonoma de Mexico, Queretaro, QT, México*

9:55 AM Thermal Diffusivity Studies on Ge-Te-I Glasses Using Photothermal Deflection Spectroscopy

P. Pattanayak, N. Manikandan*, M. Paulraj and S. Asokan, *Indian Institute of Science, Bangalore, India*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

Plenary 19ICCT/61CalCon 2

Chair: W. Loh and M.A.V. Ribeiro da Silva

Morning 1 8:30 AM - 10:15 AM

Room: UMC Ballroom

Colloid and Interface Science

8:35 AM Controlling Structure in Associating Polymer-Surfactant Mixtures (Invited)

L. Piculell*, *Lund University, Lund, Sweden*

Thermochemistry and Molecular Energetics

9:25 AM Energetics of Free Radicals: Bridges Between Gas-Phase and Solution Data (Invited)

J.A. de Sousa Martinho Simões*, *Universidade de Lisboa, Lisboa, Portugal*

Properties at the Nanoscale 1
Measurement Techniques of Nanoscale Materials

Chair: P. Norris and R. Stevens

Morning 1 8:30 AM - 10:35 AM

Room: Eng-245

8:35 AM Development of Photothermal-Resistance Technique to Characterize the Thermophysical Properties of One-Dimensional Micro/Nanoscale Structures

J. Hou and X. Wang*, *University of Nebraska-Lincoln, Lincoln, NE, U.S.A.*, C. Liu, *Chinese Academy of Sciences, Shenyang, China* and H. Cheng, *Institute of Metal Research, Shenyang, China*

8:55 AM Nanometer Thin Films - Investigations by AC-Chip Calorimetry

H. Huth*, A. Minakov and C. Schick, *University of Rostock, Rostock, Germany*

9:15 AM Development of Nanoscale Temperature Measurement Technique Using Near-Field Fluorescence

M. Kobayashi, T. Jigami*, Y. Taguchi and Y. Nagasaka, *Keio University, Yokohama, Kanagawa, Japan*

9:35 AM Thermophysical Properties of Metal Films in Nanometer Scale

F. Takahashi, *Nagoya Municipal Industrial Research Institute, Nagoya, Atsuta-ku, Japan*, R. Kato, *Ulvac-Riko Inc., Yokohama, Midori-ku, Japan* and I. Hatta*, *Fukui University of Technology, Fukui, Japan*

9:55 AM Study of Thermal and Optical Properties of Opals by Photothermal Deflection Technique

G. Leahu, R. Li Voti*, C. Sibilia and M. Bertolotti, *Università degli Studi di Roma, Rome, Italy* and V.G. Golubev and D.A. Kurdyukov, *Russian Academy of Sciences, St. Petersburg, Russia*

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Thursday, August 03, 2006

16th Symposium

Properties at the Nanoscale 1
Measurement Techniques of Nanoscale Materials
(continued)

Chair: P. Norris and R. Stevens

Morning 1 8:30 AM - 10:35 AM

Room: Eng-245

**10:15 AM Peculiarities of Electric Current Propagation in Silicon
Samples with Quantum Dots**

E.U. Arzikulov*, J.T. Ruzimurodov, O.P. Usmonkulov and S.B.
Isamov, *Samarkand State University, Samarkand,*
Uzbekistan

Thursday, August 03, 2006

16th Symposium

Properties of Aqueous Systems 2

Thermodynamic Properties of Hydration 1

Chair: A.H. Harvey

Morning 1 8:30 AM - 10:15 AM

Room: Eng-1B40

8:35 AM Thermodynamic Properties of Hydration for Organic Solutes: Data Needs and Determination (Invited)

V. Majer*, *Université Blaise Pascal/CNRS, Aubière, France*

9:15 AM What Additional Measurements Are Necessary to Improve the Usefulness of Group Contribution Methods for the Thermodynamic Functions of Hydration of Aliphatic Ethers, Nitriles, and Amines?

A.V. Plyasunov*, *Arizona State University, Tempe, AZ, U.S.A.*, N.V. Plyasunova, *CrystalTech Web Hosting, Inc., Phoenix, AZ, U.S.A.* and E.L. Shock, *Arizona State University, Tempe, AZ, U.S.A.*

9:35 AM Limiting Activity Coefficients of Semihydrophobic Volatile Organic Compounds in an Extended Environmental Temperature Range

V. Dohnal*, *Institute of Chemical Technology, Prague, Czech Republic*

9:55 AM Application of Group Additivity Approach to Polyfunctional Aqueous Organic Solutes

J. Sedlbauer*, *Technical University of Liberec, Liberec, Czech Republic*

Thursday, August 03, 2006

16th Symposium

Properties of Fuels, Including Natural Gas Systems 1

Chair: K.R. Hall

Morning 1 8:30 AM - 10:15 AM

Room: Eng-105

8:35 AM A New Wide-Range Reference Equation of State for Natural Gases and Other Mixtures

O. Kunz*, *Ruhr-Universitaet Bochum, Bochum, Germany*,
W. Wagner, *Ruhr-Universität Bochum, Bochum, Germany*
and M. Jaeschke, *E.ON Ruhrgas AG, Dorsten, Germany*

8:55 AM Helmholtz Energy Model for Fluid Mixtures

J.F. Estela-Uribe* and A. De Mendoza, *Universidad Javeriana Cali, Cali, Colombia* and J.P.M. Trusler, *Imperial College London, London, U.K.*

9:15 AM Application of the Group Contribution SAFT (GC-SAFT) Equation of State to Polyaromatic Hydrocarbons

M. Benamira, J.P. Passarello and P. Tobaly, *Université Paris Nord, Villetaneuse, France* and J.C. de Hemptinne*, *Institut Francais du Petrole, Rueil Malmaison, France*

9:35 AM A Component Based EOS for Compressibility Factor of Natural and Sour Gases

N. Kumar and A.S. Lawal*, *Texas Tech University, Lubbock, TX, U.S.A.*

9:55 AM Direct Prediction of Cricondentherm and Cricondenbar Coordinates of Natural Gas Mixture using Cubic Equation of State

R. Taraf and R. Behbahani, *Petroleum University of Technology, Ahwaz, Iran* and M. Moshfeghian*, *J.M. Campbell & Company, Norman, OK, U.S.A.*

Thursday, August 03, 2006

16th Symposium

Properties of Working Fluids, Including Refrigerants 5

Experimental Thermodynamics 2: pVT and Calorimetry

Chair: R.R. Singh and M.O. McLinden

Morning 1 8:30 AM - 10:15 AM

Room: Eng-265

8:35 AM Study of the Isochoric Specific Heat Capacity of Liquid R32 and R410a

A. Matsuguchi*, K. Yamaya and N. Kagawa, *National Defense Academy, Hashirimizu, Yokosuka, Japan*

8:55 AM Measurements of Specific Heat Capacity of R143a by Using a Precision Flow Calorimeter

N. Kagawa* and A. Matsuguchi, *National Defense Academy, Hashirimizu, Yokosuka, Japan* and K. Watanabe, *Keio University, Hiyoshi, Yokohama, Japan*

9:15 AM Second and Third Virial Coefficients of R32 and R125 Based on Gaseous PVT-Measurements Near Saturation

K. Ichikura and M. Mukoubayashi*, *Keio University, Kohoku-ku, Yokohama, Japan* and H. Sato, *Keio University, Yokohama, Kohoku-ku, Japan*

9:35 AM The p-p-T Behavior of Propane from 265 to 500 K with Pressures to 36 MPa

M.O. McLinden*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

9:55 AM Specific Heat Capacity at Constant Volume of Propane at Temperatures from 85 K to 345 K with Pressures to 35 MPa

R.A. Perkins*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*, J.C. Sanchez Ochoa, *Instituto Politecnico Nacional, México, DF, México* and J.W. Magee, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Thursday, August 03, 2006

16th Symposium

Wetting, Interfaces, and Membranes 3

Chair: J.L. Barrat and M. Müller

Morning 1 8:30 AM - 10:15 AM

Room: Bens-180

8:35 AM Wetting Phase Transitions in Bose-Einstein Condensate Mixtures (Invited)

J.O. Indekeu* and B. Van Schaeybroeck, *Katholieke Universiteit Leuven, Leuven, Belgium*

9:15 AM Interaction Between Nanoparticles Mediated by Grafted Chains

D. Duque, *Universidad Autonoma de Madrid, Madrid, Spain* and L.F. Vega*, *Consejo Superior de Investigaciones Cientificas, Barcelona, Bellaterra, Spain*

9:35 AM Interface-Controlled Phase Transitions in Nanosystems: Phenomenological Theory and Monte Carlo Simulations

K. Binder*, *Johannes Gutenberg University, Mainz, Germany*, D.P. Landau, *The University of Georgia, Athens, GA, U.S.A.*, A. Milchev, *Bulgarian Academy of Sciences, Sofia, Bulgaria* and M. Müller, *Georg August Universität, Göttingen, Germany*

9:55 AM Capillary Evaporation in Nonwetable Grooves

M. Schoen* and H. Bohlen, *Technische Universität Berlin, Berlin, Germany*

Ionic Liquids 8
Transport and General

Chair: A. Heintz

Morning 2 10:35 AM - 12:20 PM

Room: Coors-3

10:40 AM Electrolytic Conductivities and Viscosities of Hydrophobic Room-Temperature Ionic Liquids

J.A. Widegren* and J.W. Magee, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*, K.N. Marsh, *University of Canterbury, Christchurch, New Zealand* and E.M. Saurer, *University of Notre Dame, Notre Dame, IN, U.S.A.*

11:00 AM Viscosity and Surface Tension of the Ionic Liquids [EMIM][EtOSO₃], [EMIM][NTf₂], [EMIM][N(CN)₂], and Their Binary Mixtures with Water, Methanol, and Ethanol by Surface Light Scattering (SLS)

A.P. Fröba*, *Universität Erlangen-Nürnberg, Erlangen, Germany*, H. Kremer, *ESYTEC Energie- und Systemtechnik GmbH, Erlangen, Germany* and C. Botero, A. Leipertz, D. Gerhard and P. Wasserscheid, *Universität Erlangen-Nürnberg, Erlangen, Germany*

11:20 AM The NdBr₃-MBr Ionic Mixtures: A Case Discussion of Thermodynamics and Transport Properties of Lanthanide (III) - Alkali Metal Halide Systems

M. Gaune-Escard*, *Ecole Polytechnique, Marseille, France*, L. Rycerz and E. Ingier-Stocka, *Wroclaw University of Technology, Wroclaw, Poland*, S. Gadzuric, *University of Novi Sad, Novi Sad, Serbia* and W. Gong, *Institute of Huizhou University, Huizhou, Guangdong, China*

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Thursday, August 03, 2006

Joint Session

Ionic Liquids 8
Transport and General
(continued)

Chair: A. Heintz

Morning 2 10:35 AM - 12:20 PM

Room: Coors-3

11:40 AM Salting-Out Effects in Aqueous Solutions of [BMIM][BF₄]

Z.P. Visak*, *Universidade Nova de Lisboa, Oeiras, Portugal*, J.R. Trindade, *Universidade de Aveiro, Aveiro, Portugal*, M. Blesic, *Universidade Nova de Lisboa, Oeiras, Portugal*, I.M. Marrucho and J.A.P. Coutinho, *Universidade de Aveiro, Aveiro, Portugal* and L.P.N. Rebelo, *Universidade Nova de Lisboa, Oeiras, Portugal*

12:00 PM Ternary Liquid-Liquid Equilibrium Measurement and Modeling of Imidazolium and Pyridinium Ionic Liquids

L.D. Simoni* and A. Chapeaux, *University of Notre Dame, Notre Dame, IN, U.S.A.*, T.M. Manzano, *University of Puerto Rico at Mayagüez, Mayagüez, Puerto Rico* and M.A. Stadtherr and J.F. Brennecke, *University of Notre Dame, Notre Dame, IN, U.S.A.*

Thursday, August 03, 2006

Joint Session

Molecular Modeling, Including Simulation 10

Fundamental Methods

Chair: P. Smith

Morning 2 10:35 AM - 12:20 PM

Room: Math-100

10:40 AM COSMO-RS: The Bridge from Quantum Chemistry to Fluid Phase Thermodynamics (Invited)

A. Klamt*, *COSMOlogic GmbH&CoKG, Leverkusen, Germany*

11:20 AM Improved *Ab Initio* Values of the Thermophysical Properties of Helium as Standards

J.J. Hurly*, M.R. Moldover and J.B. Mehl, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

11:40 AM First-Principles Calculations for Humidity Standards

A.H. Harvey*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.* and P.H. Huang, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

12:00 PM *Ab Initio* Monte Carlo Simulations of Fluid Phase Equilibria at Extreme Conditions

L.D. Gelb*, *Washington University in St. Louis, St. Louis, MO, U.S.A.*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

New Experimental Techniques 1
Calorimetry

Chair: T. Atake and A.R.H. Goodwin

Morning 2 10:35 AM - 12:20 PM

Room: Coors-2

**10:40 AM Combined Ultra Fast Scanning and AC Calorimetry for Films
in the Nanometer Range (Invited)**

H. Huth and C. Schick*, *University of Rostock, Rostock,
Germany*

**11:20 AM A Fully Automated Adiabatic Calorimeter for Heat Capacity
Measurement Between 80 and 400 K**

Z.-C. Tan*, Bei-Ping Liu, H.-T. Zhang, D.-T. Yue, Z.-H. Zhang
and Li-Xian Sun, *Chinese Academy of Sciences, Dalian,
China*

11:40 AM Peltier Tip Microcalorimeter

Y.H. Jeong*, *Pohang University of Science & Technology,
Pohang, Korea*

**12:00 PM Stochastic Temperature Modulation: A New Technique in
Temperature-Modulated DSC**

J.E.K. Schawe* and T. Hütter, *Mettler-Toledo GmbH,
Schwerzenbach, Switzerland*

New Materials 1
Polymers and Membranes

Chair: R.N. Lichtenthaler and R. Burriel

Morning 2 10:35 AM - 12:40 PM Room: Coors-5

10:40 AM New Functionalized Polymers as Membrane Materials (Invited)

C. Staudt-Bickel*, *University of Düsseldorf, Düsseldorf, Germany*

11:20 AM Design of Stable Pd-Based Membranes for Hydrogen Gas Separation: A Statistical Thermodynamics Approach

D.E. Nanu and A.J. Böttger*, *Delft University of Technology, Delft, Netherlands*

11:40 AM Evaluation of the Micro-Phase Separated Interface Formed by the Amiphiphilic Di-Block Copolymer by Transition Entropy

T. Yamada*, S. Asaoka and C. Koyanagi, *Tokyo Metropolitan University and CREST-JST, Tokyo, Japan*, T. Iyoda, *Tokyo Institute of Technology and CREST-JST, Midori-ku, Yokohama, Japan* and H. Yoshida, *Tokyo Metropolitan University and CREST-JST, Tokyo, Japan*

12:00 PM A Kinetic Analysis of Thermal Decomposition of Polyaniline/ZrO₂ Composite

S.-X. Wang*, *Dalian Jiaotong University, Dalian, China*, Z.-C. Tan, *Chinese Academy of Sciences, Dalian, China*, Yan-Sheng Li, *Dalian Jiaotong University, Dalian, China* and Li-Xian Sun, *Chinese Academy of Sciences, Dalian, China*

12:20 PM Synthesis, Characterization and Thermal Analysis of Polyaniline/Co₃O₄ Composites

Z.-C. Tan*, *Chinese Academy of Sciences, Dalian, China*, S.-X. Wang and Yan-Sheng Li, *Dalian Jiaotong University, Dalian, China* and Li-Xian Sun, *Chinese Academy of Sciences, Dalian, China*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 4***

Experimental, Pure Compounds

Chair: T. Kraska and U.K. Deiters

Morning 2 10:35 AM - 12:40 PM

Room: Coors-1

**10:40 AM PVT Measurements of Ammonia and Its Aqueous Mixtures
in the Temperature Range from 350 K to 600 K at Pressures
Up to 200 MPa**

N. Sakoda*, A. Wachi, N. Masuda and M. Uematsu, *Keio
University, Kohoku-ku, Yokohama, Japan*

**11:00 AM Measurements of Vapor Pressures and PVT Properties for
n-Butane from 280 to 440 K at Pressures to 200 MPa**

H. Miyamoto* and M. Uematsu, *Keio University, Kohoku-ku,
Yokohama, Japan*

**11:20 AM Thermophysical Properties of Alternative Refrigerants for
R-22**

I. Kul*, *Widener University, Chester, PA, U.S.A.*

**11:40 AM Synthesis and Extraction of Anhydrous High Purity
Hydrazine (HPH) from the Hydrazine Hydrate**

A.J. Bougrine*, R. Tenu, J. Berthet, A. Dhenain, H. Delalu and
J.J. Counioux, *Université Claude Bernard - Lyon I,
Villeurbanne, France*

**12:00 PM Determination of Thermodynamic Properties of Some
Organic Compounds by Experimental and Calculation
Methods for the Wide Temperature Range**

R.M. Varushchenko*, A.I. Druzhinina and O.V. Dorofeeva,
Moscow State University, Moscow, Russia

-continued on next page-

Thursday, August 03, 2006 19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 4***

***Experimental, Pure Compounds
(continued)***

Chair: T. Kraska and U.K. Deiters

Morning 2 10:35 AM - 12:40 PM

Room: Coors-1

**12:20 PM Vapor Pressures, Enthalpies of Vaporization and Heat
Capacities of C1 to C5 Alkanols at Ambient and Subambient
Temperatures - IACT Doctorate Award Presentation -**

K. Ruzicka and M. Fulem*, *Institute of Chemical Technology,
Prague, Czech Republic*, V.V. Diky, *Boulder, CO, U.S.A.*
and V. Ruzicka, *Institute of Chemical Technology, Prague,
Czech Republic*

Photothermal and Photoacoustic Techniques 5

Chair: G.J. Diebold

Morning 2 10:35 AM - 12:00 PM

Room: Eng-155

10:40 AM Thermal-Pulse Tomography of Space-Charge and Polarization Distributions in Electret Polymers

A. Mellinger* and R. Flores Suárez, *University of Potsdam, Potsdam, Germany*, R. Singh, *University of Allahabad, Allahabad, India*, M. Wegener and R. Gerhard-Multhaupt, *University of Potsdam, Potsdam, Germany* and S.B. Lang, *Ben-Gurion University of the Negev, Beer Sheva, Israel*

11:00 AM Effective Thermal Conductivity in Quasistatic Photothermal Phenomena: The Case of the Bulk Light Absorption

Yu.G. Gurevich*, *Universidad Salamanca, Salamanca, Spain*, G.N. Logvinov, *Instituto Politécnico Nacional, Culhuacan, México* and I.M. Lashkevich, *Ternopil State Pedagogical University, Ternopil, Ukraine*

11:20 AM Photothermal Measurements of the Thermal Properties of Micro-Structured Materials Based on Magnetic Fluids

R.A. Medina-Esquivel*, *CINVESTAV-Queretaro, Queretaro, QT, México*, P. Quintana Owen, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*, J.M. Yáñez-Limón, *CINVESTAV-Unidad Querétaro, Queretaro, QT, México* and J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*

11:40 AM Monitoring of the Formation of Polymeric Films by Photothermal Techniques

P. Martinez-Torres* and R. Medina-Esquivel, *CINVESTAV-IPN, Unidad Merida, Mérida, YU, México* and J.J. Alvarado-Gil, *CINVESTAV-IPN, Unidad Mérida, Mérida, YU, México*

Thursday, August 03, 2006

16th Symposium

Properties for Sustainable Development 1

Chair: A.C. Rutz

Morning 2 10:35 AM - 12:00 PM

Room: Eng-265

10:40 AM How "Sustainability" is Changing How We Make and Choose Products (Invited)

C. O'Brien*, *Idaho National Laboratory, Idaho Falls, ID, U.S.A.*

11:20 AM Thermophysical Properties for Analysis and Design of Power Cycles with Capture of Carbon Dioxide

R. Span*, *University of Paderborn, Paderborn, Germany*

11:40 AM Silica-BPPO Nanocomposite Membranes for CO₂ Separation

X.H. Hu*, H.C. Cong, Y.S. Shen and M.R. Radosz, *University of Wyoming, Laramie, WY, U.S.A.*

Thursday, August 03, 2006

16th Symposium

Properties of Aqueous Systems 3

Thermodynamic Properties of Hydration 2

Chair: V. Majer and A.H. Harvey

Morning 2 10:35 AM - 11:40 AM

Room: Eng-1B40

10:40 AM Procedure for the Calculation of the Gibbs Energies of Hydration for Volatile Solutes from Solubility Data

J.L. Alvarez and R.J. Fernandez-Prini*, *UAQ, Buenos Aires, Argentina*

11:00 AM Hydration Properties of Low Molecular Weight Perfluorocarbons

M.F. Costa Gomes* and A.A.H. Padua, *CNRS/Université Blaise Pascal, Aubière, France*

11:20 AM Pure Component Property Data for the IUPAC Project: Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes

R.D. Chirico*, V.V. Diky and M. Frenkel, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Thursday, August 03, 2006

16th Symposium

Properties of Fuels, Including Natural Gas Systems 2

Chair: J. Holste

Morning 2 10:35 AM - 12:20 PM

Room: Eng-105

10:40 AM Potential Approaches Towards Characterization and Property Estimation of Heavy Petroleum Fluids and Natural Gas Systems

M.R. Riazi* and Y.A. Roomi, *Kuwait University, Safat, Kuwait*

11:00 AM Modeling and Characterization of Reservoir Fluids Based on the PC-SAFT EOS and the Friction Theory

S.E. Quiñones-Cisneros*, *University of Cologne, Köln, Germany*, K.A.G. Schmidt, *Schlumberger Reservoir Fluids Center, Edmonton, AB, Canada*, J. Creek, *ChevronTexaco Exploration and Production Technology Company, Houston, TX, U.S.A.* and U.K. Deiters, *University of Cologne, Köln, Germany*

11:20 AM Experimental Phase Envelopes for Two Synthetic Light Natural Gas-Like Mixtures

K.R. Hall, S. Ejaz, M. Atilhan and S. Aparicio-Martinez*, *Texas A&M University, College Station, TX, U.S.A.*

11:40 AM Calculation of Phase Equilibrium for Gas Hydrate Systems Using Monte Carlo Simulation and Theory

S.J. Wierchowski and P.A. Monson*, *University of Massachusetts, Amherst, MA, U.S.A.*

12:00 PM Examining Complex Tuning Mechanism Occurring in the Mixed Hydrates

Do-Youn Kim, Jeasung Park, Sun-Hwa Yeon*, Y.J. Park and H. Lee, *Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Yuseong-gu, Korea*

Properties of Solids 2

Techniques and Measurement Methods

Chair: J.J. Alvarado-Gil and A. Mandelis

Morning 2 10:35 AM - 12:40 PM

Room: Eng-200

10:40 AM Novel Heat Transfer Mechanisms Governing Thermal Conductivity of Porous Solid Materials and Actual Problems in the Database Development

E. Litovsky*, V. Issoupov and J. Kleiman, *Integrity Testing Laboratory Inc., Markham, ON, Canada*

11:00 AM Hygric Material Properties of Porous Building Materials

P. Häupl* and H. Fechner, *Dresden University of Technology, Dresden, Germany*

11:20 AM Thermal Diffusivity Measurements of Supergrowth Carbon Nanotube Using the Laser Flash Method

M.A. Akoshima*, K.H. Hata, D.F. Futaba, K.M. Muzuno, T. Baba and H. Kato, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

11:40 AM Harmonic and Subharmonic Generation Analysis on ADP and Rochelle Salt Piezoelectric Crystals

A. Garcia-Quiroz*, *CINVESTAV-IPN, México, DF, México* and C.A. Alves, J.C. Costa, S.G.C. Moreira and D.P. Pereira, *Universidade Federal do Pará, Belém, Pará, Brazil*

12:00 PM Calorimetric Study of the Glass Transition in Lithium Borate Glasses Over a Wide Composition Range by Modulated DSC

Y. Matsuda*, C. Matsui and Y. Ike, *University of Tsukuba, Tsukuba, Ibaraki, Japan*, M. Kodama, *Sojo University, Ikeda, Kumamoto, Japan* and S. Kojima, *University of Tsukuba, Tsukuba, Ibaraki, Japan*

-continued on next page-

Thursday, August 03, 2006

16th Symposium

Properties of Solids 2

Techniques and Measurement Methods

(continued)

Chair: J.J. Alvarado-Gil and A. Mandelis

Morning 2 10:35 AM - 12:40 PM

Room: Eng-200

12:20 PM Thermal Diffusivity of Sintered $12\text{CaO}-7\text{Al}_2\text{O}_3$

P.M. Nikolić, D.T. Luković and S.M. Savić, *Institute of Technical Sciences SASA, Belgrade, Serbia*, A.M. Milovanović, *University of Kragujevac, Čačak, Serbia*, M.V. Nikolić, *University of Belgrade, Belgrade, Serbia* and L.S. Lukić*, *IRITEL, Belgrade, Serbia*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

Thermodynamic Frontiers and Education 1

Removing the Sting

Chair: R. Weir and T.M. Letcher

Morning 2 10:35 AM - 12:40 PM

Room: Coors-4

10:40 AM Taking the "Sting" out of Teaching Chemical Thermodynamics (Invited)

R. Battino*, *Wright State University, Dayton, OH, U.S.A.*

11:20 AM Teaching Thermodynamics: Chemical Potential from the Beginning

G. Job and R. Rüffler*, *Institute of Physical Chemistry, Hamburg, Germany*

11:40 AM What Are the Modern Educational Trends in a More Widely Comprehended Field of Thermodynamics, Thermal Analysis and Applied Thermal Physics?

J. Sestak*, *Academy of Sciences of the Czech Republic, Prague, Czech Republic* and M. Holecek, *University of West Bohemia, Pilsen, Czech Republic*

12:00 PM CosmoTherm_Edu: A Tool for Turning Molecular Thermodynamics Into a Vivid Experience

A. Klamt*, *COSMOlogic GmbH&CoKG, Leverkusen, Germany*

12:20 PM The Second Law in Modern Thermodynamics

Ji-Tao Wang* and Peiju Zheng, *Fudan University, Shanghai, China*

Wetting, Interfaces, and Membranes 4

Chair: L.G. MacDowell and M. Müller

Morning 2 10:35 AM - 12:20 PM

Room: Bens-180

10:40 AM Corresponding-States Analysis of the Surface Tension of Simple, Polar, and Ionic Fluids

V.C. Weiss*, *International University Bremen, Bremen, Germany* and W. Schröder, *University Bremen, Bremen, Germany*

11:00 AM Prediction of the Interfacial Tension of Binary Systems Water + Hydrocarbon (A Formal Thermodynamic Model Together with the UNIFAC Model)

A. Romero-Martínez*, C.G. Aranda-Bravo and A. Trejo, *Instituto Mexicano del Petróleo, México, DF, México*

11:20 AM Equilibrium Surface Tension of 2-Amine-2-Methyl-1-Propanol in an Aqueous Mixture of N-methyldiethanolamine + Diethanolamine in the Range (303 to 333) K

J. Águila-Hernández*, B.E. García-Flores and A. Trejo, *Instituto Mexicano del Petróleo, México, DF, México*

11:40 AM Wetting of Cu Grain Boundaries in the Cu-Bi System

N. Tinet and D. Chatain*, *CNRS, Campus de Luminy, Marseille, France*

12:00 PM Factors Affecting Coverage Dependence of the Diffusivity of One Metal Over the Surface of Another

P. Wynblatt*, *Carnegie Mellon University, Pittsburgh, PA, U.S.A.*, D. Chatain, *CNRS, Campus de Luminy, Marseille, France*, A. Ranguis and J.P. Monchoux, *CRM-CNRS, Marseille, France*, J. Moon, *Carnegie Mellon University, Pittsburgh, PA, U.S.A.* and S. Garoff, *Electronica and Telecommunications Research Institute, Daejeon, Korea*

Thursday, August 03, 2006

Joint Session

Exhibitions 2

See Exhibitions 1

Chair: R.D. Chirico

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

1:50 PM ACS Publications

Anter Corp.

Calorimetry Sciences Corp.

Elsevier

JECC Torisha Co.

Mettler-Toledo

Netzsch Instruments Inc.

PerkinElmer

Rubotherm

Springer

TA Instruments

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Databases, Data Systems, Software Applications, and Correlations

A Method for Estimating Critical Pressures

M.F. Bolotnikov* and E.B. Postnikov, *Kursk State University, Kursk, Russia*

A New Generalized Alpha Function for Patel and Teja Cubic Equation

M. Joda*, *Tehran Oil Refining Company, Tehran, Iran* and M. Vafaie-Sefti, *Tarbiat Modarres University (TMU), Tehran, Iran*

An Automated System for Calculating Risk and Ecological Damage of Refrigerants

O.I. Bodyul, I.V. Dubro and E.S. Bodyul*, *The Odessa State Academy of Refrigeration, Odessa, Ukraine* and D.V. Shabadash, *Odessa National Polytechnical University, Odessa, Ukraine*

Automated System for Calculating Thermophysical Properties of Natural and Ozone-Safe Refrigerants and Their Mixtures

A.A. Vasserman* and V.P. Malchevsky, *Odessa National Maritime University, Odessa, Ukraine* and S.V. Bodyul, *Odessa State Academy of Refrigeration, Odessa, Ukraine*

General Equation of the Fluid Viscosity

A.B. Kaplun and A.B. Meshalkin*, *Russian Academy of Sciences, Novosibirsk, Russia*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Databases, Data Systems, Software Applications, and Correlations

Inconsistency of Thermodynamic Quantities Under Different Standard State Pressures

Y. Nagano*, *Osaka University, Osaka, Japan*, T. Atake, *Tokyo Institute of Technology, Midori-ku, Yokohama, Japan*, M. Sorai, *Osaka University, Osaka, Japan*, H. Yokokawa, *National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan*, H. Yoshida, *Tokyo Metropolitan University, Hachioji, Japan* and K. Saito, *University of Tsukuba, Tsukuba, Ibaraki, Japan*

Pareto-Optimum Parameter Estimation in Thermodynamic Correlations

S.V. Artemenko* and V.A. Mazur, *Academy of Refrigeration, Odessa, Ukraine*

Prediction of Critical Properties of Non-Electrolyte Organic Compounds via Group Contributions and Group Interactions

Y. Nannoolal*, D. Ramjugernath and J. Rarey, *University of KwaZulu-Natal, Durban, South Africa*

Simple Models for Shear Viscosity and Self-Diffusion of Liquid Metals

M.L. Mandler, E. Bihuna, G. Moro and L.A.F. Coelho*, *State University of Santa Catarina, Joinville, SC, Brazil*

The NIST Retention Index Database

P.J. Linstrom*, V.I. Babushok, R.L. Brown, I.G. Zenkevich and S.E. Stein, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Databases, Data Systems, Software Applications, and Correlations

The Wagner Equation and the Extrapolation of Vapor Pressure Data to the Triple Point

J.C. Sanchez Ochoa*, *Instituto Politécnico Nacional, México, DF, México* and M.B. Ewing, *University College London, London, U.K.*

Thermodynamic Modeling of Phase Equilibrium and Thermophysical Properties of Multicomponent Sub- and Supercritical Fluids

V.I. Anikeev* and A. Yermakova, *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

Thermodynamic Properties of the Green Solvents

S.P. Verevkin* and V.N. Emel'yanenko, *University of Rostock, Rostock, Germany*

Uncertainty Evaluation of Equations of State for Carbon Dioxide

Y. Kayukawa* and K. Fujii, *National Institute of Advanced Industrial Science and Technology (AIST), National Metrology Institute of Japan (NMIJ), Tsukuba, Japan*

Viscosity of Heavy Fractions of Petroleum

M.S. Gama* and C.A.D. Moura, *Petróleo Brasileiro S.A., Rio de Janeiro, Brazil*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Fluid Property Measurements

Acoustic-Optical Method for Studying of High-Frequency Acoustic Waves in Liquid Matters

F.R. Akhmedzhanov*, *Samarkand State University, Samarkand, Uzbekistan*

Activity Coefficient and Excess Gibbs Free Energies for the Binary Mixtures of Dimethylsulphoxide with Substituted Benzenes

M.V.P. Rao* and M. Radhamma, *Sri Venkateswara University, Tirupati, India* and D.H.L. Prasad, *Indian Institute of Chemical Technology, Hyderabad, India*

Behavior of Hypersonic Velocity in Aqueous Solution of Gamma-Picoline at Various Concentrations

H.S. Haydarov*, L.M. Sabirov and D.I. Semenov, *Samarkand State University, Samarkand, Uzbekistan*

Compressed Liquid Densities of Pentane, Hexane, and Nonane at Temperatures from (313 to 363) K and Pressures up to 25 MPa

A. Zúñiga-Moreno and L.A. Galicia-Luna*, *Instituto Politécnico Nacional, México, DF, México*

Critical Constants of Two Isomers of Triacontane: n-Triacontane and Squalane

E.D. Nikitin* and A.P. Popov, *Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Fluid Property Measurements

Densities, Speeds of Sound and Isentropic Compressibilities of Mixtures of 2-Methoxyethanol + 2-Ethoxyethanol at 293.15, 298.15 and 303.15 K

I. Mozo*, I. Garcia de la Fuente, J.A. Gonzalez and J.C. Cobos,
Universidad de Valladolid, Valladolid, Spain

Densities, Viscosities, and Refractive Indices for Binary and Ternary Mixtures of N,N-Dimethylacetamide, 2-Methylbutan-2-ol, and Ethyl Acetate at 298.15 K for the Liquid Region and at Ambient Pressure

H. Iloukhani* and K. Khanlarzadeh, *Bu Ali Sina University, Hamadan, Iran*

Density and Viscosity of Aqueous Blends of Three Alkanolamines: N-Methyldiethanolamine, Diethanolamine, and 2-Amino-2-Methyl-1-Propanol in the Range (303 to 358) K

M.E. Rebolledo-Libreros*, R.E. Ortega-Urquiza and A. Trejo,
Instituto Mexicano del Petróleo, México, DF, México

Evaluation of Thermo-Acoustical Parameters of Some Binary Liquid Mixtures from Volume Expansivity Data - Part II

I. Johnson*, *St. Joseph's College, Trichy, India*

Excess Enthalpies and Vapor-Liquid Equilibrium Data for the Binary Mixtures of Dimethyl Sulphoxide with Ketones

M. Radhamma and M.V.P. Rao*, *Sri Venkateswara University, Tirupati, India* and Y.V.L. Havi Kumar, *Indian Institute of Chemical Technology, Hyderabad, India*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Fluid Property Measurements

Excess Molar Volume and Viscosity Study of Ternary Mixtures: 1-Propanol (1) + Triethylamine (2) + Cyclohexane (3) and 1-Propanol (1) + Tributylamine (2) + Cyclohexane (3) at 303.15 K

R.L. Gardas*, *University of Aveiro, Aveiro, Portugal* and S.L. Oswal, *Veer Narmad South Gujarat University, Gujarat, India*

Experimental High Pressure Vapor-Liquid Equilibria for the Ethane + 1-Propanol, and Propane + 1-Propanol Systems

R. Jiménez-Gallegos, L.A. Galicia-Luna*, C. Bouchot and O. Elizalde-Solis, *Instituto Politécnico Nacional, México, DF, México*

High Pressure Compressed Liquid Densities of Heptane: Comparison Between Experiments, Molecular Simulation and Equation of State

A. Zúñiga-Moreno, J.L. Rivera-Rojas, L.A. Galicia-Luna* and F.F. Betancourt-Cárdenas, *Instituto Politécnico Nacional, México, DF, México*

High Pressure Vapor-Liquid Equilibrium of the Binary Systems of Carbon Dioxide + Acetates

C.H. Kwon*, M.D. Seo, S.W. Kim and Jeong Won Kang, *Korea University, Seoul, Korea*

Investigation of Ultrasound and Hypersound Propagation Velocity and Absorption Coefficient in Several van der Waals and Associated Liquids

Sh.F. Fayzullaev* and Sh.F. Fayzullaev, *Samarkand State University, Samarkand, Uzbekistan*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Fluid Property Measurements

Measurement and Correlation of Binary Vapor-Liquid Equilibria of Isomeric Butanols with 1, 4 - Dioxane

B. Sambi Reddy, A. Ravi Prasad and K.V. Rao*, *Andhra University, Visakhapatnam, India*

Method of Measuring Heat of Transport and Coefficient of Gas Diffusion in Porous Media

L. Minkin*, *Portland Community College, Portland, OR, U.S.A.* and A.S. Shapovalov, *Saratov State University, Saratov, Russia*

On Surface Tension Effects in Suspended-Level Capillary Viscometers

F.J.P. Caetano, *Universidade Técnica de Lisboa, Lisboa, Portugal*, J.M.N.A. Fareleira, *Centro de Química Estrutural, Lisboa, Portugal*, C.M.B.P. Oliveira*, *Universidade Técnica de Lisboa, Lisboa, Portugal* and W.A. Wakeham, *University of Southampton, Southampton, Highfield, U.K.*

PVTx Behavior of the N-Methyl-2-Pyrrolidone/ Carbon Disulfide Mixed Solvent

S. Aparicio*, M.J. Davila, R. Alcalde, B. Garcia and J.M. Leal, *Universidad de Burgos, Burgos, Spain*

Studies on the Thermodynamics of Ion-Associated Extraction of ReO₄ in Hydrochloric Acid System with TiOA

X. Liu*, *Liaoning University, Shenyang, Liaoning, China* and D. Fang, C. Li, F. Nan and S. Zang, *West Virginia University, Morgantown, WV, U.S.A.*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Fluid Property Measurements

Study of the Enthalpy, Entropy and Free Energy Changes of Relaxation Processes in Some Organic Liquids of Aromatic Row

Sh.F. Fayzullaev* and Sh.F. Fayzullaev, *Samarkand State University, Samarkand, Uzbekistan*

The Isobaric Heat Capacity of Ethanol + Water Solutions

E.I. Hanifayeva, M.A. Talybov and A.N. Shahverdiyev*, *Azerbaijan Technical University, Baku, Azerbaijan*

Thermodynamic Properties of 1-Alkenes in the Liquid State

T.S. Khasanshin*, O.G. Poddubskij and A.P. Shchamialiou, *Mogilev State University of the Foodstuffs, Mogilev, Belarus*

Thermodynamic Properties of NMP/Methanol Over a Wide Temperature and Pressure Range

M.J. Davila*, *Universidad de Burgos, Burgos, Spain*, J.P.M. Trusler, *Imperial College London, London, U.K.* and S. Aparicio, R. Alcalde, B. Garcia and J.M. Leal, *Universidad de Burgos, Burgos, Spain*

Thermodynamics of Mixtures Containing a Strongly Polar Compound - Part VIII: Liquid-Liquid Equilibria for N,N-Dialkylamide + Selected N-Alkanes

J. Lobos, I. Mozo*, M.F. Regulez, J.A. Gonzalez, I. Garcia de la Fuente and J.C. Cobos, *Universidad de Valladolid, Valladolid, Spain*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Fluid Property Measurements

Thermophysical Properties of n-Cyclohexylpyrrolidone + n-Methyl-2-Pyrrolidone + Water Solvent Mixtures at 298.15 K

R. Alcalde*, S. Aparicio, M.J. Davila, B. Garcia and J.M. Leal,
Universidad de Burgos, Burgos, Spain

Thermophysical Property Measurements in the System n-Tetradecane + 2-Propanol

A. Laesecke*, C. Brill and S. Triplett, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Ultrasonic and Hypersonic Studies of Complex Molecular Dynamics in the Isotropic Phase of a Cholesteric Liquid Crystal

L.M. Sabirov and D.I. Semenov*, *Samarkand State University, Samarkand, Uzbekistan*

Vapor - Liquid Equilibria of Alkanes + 2 Propoxyethanol Systems

Moon Sam Shin* and Seungho Jung, *Seoul National University, Seoul, Korea*, Ju Ho Lee and Chul Soo Lee, *Korea University, Seoul, Korea* and Hwayong Kim, *Seoul National University, Seoul, Korea*

Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Ethanol, 2-Butanone, and 2,2,4-Trimethylpentane at 101.3 kPa

C.C. Wen and C.H. Tu*, *Providence University, Shalu, Taichung, Taiwan*

Glass Transition and Dielectric Relaxation in Viscous Monohydroxy Alcohols

Li-Min Wang* and R.Richert, *Arizona State Univ., Tempe, AZ, U.S.A.*

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Room: Stadium Club

Ionic Liquids

A Novel Method of Chemical Processing: Miscibility Switches in Ionic Liquids

M.C. Kroon*, A. Shariati, J. van Spronsen, R.A. Sheldon, G.J. Witkamp and C.J. Peters, *Delft University of Technology, Delft, Netherlands*

An Application of the Interstice Model to Viscosity of Ionic Liquid BMIBF₄

Zhen-Xing Jin, *Bohai University, Jinzhou, China*, Feng Xue, *Liaoning University, Shenyang, China*, Qingguo Zhang, *Bohai University, Jinzhou, China* and Jia-Zhen Yang*, *Liaoning University, Shenyang, China*

Application of the Graph Theory to Ternary Excess Molar Volumes of (an Ionic Liquid + Methanol + Water)

N. Deenadayalu*, S. Kumar and P. Bhujrajh, *Durban Institute of Technology, Durban, KwaZulu-Natal, South Africa*

Broadband Dielectric Response of the Ionic Liquid N-Methyl-N-Ethylpyrrolidinium Dicyanamide

S. Schrödle, *Murdoch University, Murdoch, WA, Australia*, G. Annat, D.R. MacFarlane and M. Forsyth, *Monash University, Clayton, Victoria, Australia*, R. Buchner, *Universität Regensburg, Regensburg, Germany* and G. Hefter*, *Murdoch University, Murdoch, WA, Australia*

Decomposition of Ionic Liquids in Chemical Processing

M.C. Kroon*, W. Buijs, C.J. Peters and G.J. Witkamp, *Delft University of Technology, Delft, Netherlands*

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Ionic Liquids

Densities, Viscosities, Decomposition Temperatures, and Heat Capacities of Ionic Liquids

J.M. Crosthwaite*, J.K. Dixon, M.J. Muldoon, G.F. Grubb, D.G. Hert, D.J. Couling, K.E. Montalto, P.A. Jefson, G.J. Lim, J.L. Anderson, S.N.V.K. Aki and J.F. Brennecke, *University of Notre Dame, Notre Dame, IN, U.S.A.*

Excess Molar Volumes for Binary (Ionic Liquid + Methanol or Water) and Ternary (Ionic Liquid + Methanol + Water) Systems at T = 298.15 K, 303.15 K and 313.15 K and at Atmospheric Pressure

P. Bhujrajh and N. Deenadayalu*, *Durban Institute of Technology, Durban, KwaZulu-Natal, South Africa*

Fluid Phase Behavior of (Ionic Liquid + Alcohol) Binary Mixtures: 1-Hexyl-3-Methylimidazolium Bistrisflamides + C₂-C₈ n-Alcohols

J. Lachwa, *Universidade Nova de Lisboa, Oeiras, Portugal*, P. Morgado, *Instituto Superior Técnico, Lisboa, Portugal*, J.M.S.S. Esperança* and H.J.R. Guedes, *Universidade Nova de Lisboa, Oeiras, Portugal*, C. Lopes, *Instituto Superior Técnico, Lisboa, Portugal* and L.P.N. Rebelo, *Universidade Nova de Lisboa, Oeiras, Portugal*

Liquid-Liquid Phase Equilibria and Interfacial Tension Measurements of Mixtures Containing Ionic Liquids

A. Heintz, A. Tschersich* and Ch. Werts, *University of Rostock, Rostock, Germany*

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Ionic Liquids

**On the Properties of 1-Butyl-3-Methylimidazolium
Octylsulfate Ionic Liquid**

J.M. Leal*, M.J. Davila, S. Aparicio, R. Alcalde and B. Garcia,
Universidad de Burgos, Burgos, Spain

**Phosphonium Based Ionic Liquids and Water: Mutual
Solubilities**

M.G. Freire*, P.J. Carvalho, I.M. Marrucho, J.A.P. Coutinho and
A.M. Fernandes, *Universidade de Aveiro, Aveiro, Portugal*

**PVT-Properties and Viscosities of Mixtures of Imidazolium-
Based Ionic Liquids and Alcohols from Molecular Simulation**

G. Raabe* and J. Koehler, *TU Braunschweig,
Braunschweig, Germany*

**Solubility Measurements of Mixed Vapor Containing Carbon
Dioxide in Ionic Liquids and Predictions**

Y.S. Kim*, J.H. Jang, B.D. Lim, Jeong Won Kang and Chul
Soo Lee, *Korea University, Seoul, Korea*

**Solubility of Carbon Dioxide and Ethane in Ionic Liquids
Containing the Anion Bis(Trifluoromethylsulfonyl)Amide**

G. Hong, P. Husson and M.F. Costa Gomes*,
CNRS/Université Blaise Pascal, Aubière, France and M.
Deetlefs and C. Hardacre, *Queen's University of Belfast,
Belfast, Northern Ireland, U.K.*

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Ionic Liquids

Solubility of Hydrogen Sulfide in [BMIM][PF₆]

F.-Y. Jou and A.E. Mather*, *University of Alberta, Edmonton, AB, Canada*

Solution Enthalpies of Organic Solutes in the Ionic Liquids Butyl-Trimethyl-Ammonium (Trifluoromethylsulfonyl)Imide and 1-Ethyl-3-Methyl-Imidazolium Ethyl-Sulfate

A. Heintz*, *University of Rostock, Rostock, Germany*, E.V. Balantseva, *Ivanovo State University of Chemistry and Technology, Ivanovo, Russia* and J.K. Lehmann, *University of Rostock, Rostock, Germany*

Synthesis and Characterization of 1-(2-Hydroxyethyl)-3-Methyl Imidazolium and N-(2-Hydroxyethyl)-N-Methyl Morpholinium Ionic Liquids

S. Choi*, K.-S. Kim, J.-H. Cha and S.-H. Yoen, *Korea Advanced Institute of Science and Technology, Daejeon, Korea* and Huen Lee, *Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Yuseong-gu, Korea*

Thermodynamic Investigation on Intermediate of Room Temperature Ionic Liquid: The Heat Capacity and Thermodynamic Function of EMIC, BMIC and PMIC

Z.-H. Zhang, Li-Xian Sun*, Z.-C. Tan, Fen Xu and J.-L. Zeng, *Chinese Academy of Sciences, Dalian, China*

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Ionic Liquids

Thermodynamic Properties of [C6MIM][NTf2]

A.V. Blokhin, G.J. Kabo, Y.U. Paulechka* and Dz.H. Zaitsau, *Belarusian State University, Minsk, Belarus* and J.W. Magee, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Thermodynamic Property Screening of Ionic Liquids Using COSMO-RS

A. Klamt* and M. Diedenhofen, *COSMOlogic GmbH&CoKG, Leverkusen, Germany*

Thermophysical Properties of 1-Hexyl-3-Methylimidazolium Bis(Trifluoromethylsulfonyl)Imide

J.A. Widegren* and J.W. Magee, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*, K.N. Marsh, *University of Canterbury, Christchurch, New Zealand* and E.M. Saurer, *University of Notre Dame, Notre Dame, IN, U.S.A.*

Vapor Pressure for 1-Alkyl-3-Methylimidazolium Bis(Trifluoromethanesulfonyl)Imides

Dz.H. Zaitsau, G.J. Kabo and Y.U. Paulechka*, *Belarusian State University, Minsk, Belarus* and A. Heintz and S.P. Verevkin, *University of Rostock, Rostock, Germany*

Molecular Modeling, Including Simulation

Application of the Embedded Atom Model to Liquid Metals: Non-Crystalline Iron in Earth's Core

D.K. Belashchenko*, *Moscow Institute of Steel and Alloys, Moscow, Russia*

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Molecular Modeling, Including Simulation

Combination of Multi-Component Equilibria with CFD in Modeling Fast Reactive Processes

U. Ojaniemi, K. Penttilä, P. Koukkari* and M. Manninen, *VTT Process Chemistry, Finland*

Computer Simulation of Ionic Diffusion and Mobility in Molten Chlorides

E.S. Yakub*, *Odessa State Economic University, Odessa, Ukraine*

Corrected Diffusion Coefficient of Lithium in Helium and Helium in Lithium

K. Alioua and M. Bouledroua*, *Badji Mokhtar University, Annaba, Algeria*

Density Functional Theory for Polyelectrolytes Near Oppositely-Charged Surfaces

Z.D. Li* and J.Z. Wu, *University of California, Riverside, CA, U.S.A.*

Equilibrium and Non-Equilibrium Molecular Dynamics Simulations of Heat Conduction in Uranium Oxide and the Solid Solution with Plutonium Oxide

T. Arima*, S. Yamasaki, Y. Inagaki and K. Idemitsu, *Kyushu University, Fukuoka, Japan*

Evaluation of Thermal Conductivity of Hyperstoichiometric UO_{2+x} by Molecular Dynamics Simulation

T. Arima*, S. Yamasaki, Y. Inagaki and K. Idemitsu, *Kyushu University, Fukuoka, Japan*

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Molecular Modeling, Including Simulation

Excitation Transfer and Diffusion Property in a Very Weakly Excited Lithium Gas

L. Reggami and M. Bouledroua*, *Badji Mokhtar University, Annaba, Algeria*

Global Parameter Optimization for Equations of State

C.P. Emborsky, D.C. Miller and S.G. Sauer*, *Rose-Hulman Institute of Technology, Terre Haute, IN, U.S.A.*

Isotopic and Symmetry Effects in the Collision of Atomic Helium

F. Bouchelaghem, M. Bouledroua*, M.T. Bouazza and L. Reggami, *Badji Mokhtar University, Annaba, Algeria*

Modeling of POE Lubricants with Two Versions of the SAFT Model

J. Garcia*, *Universidad de Vigo, Vigo, Spain* and J. Fernández, *Universidad de Santiago de Compostela, Santiago de Compostela, Spain*

Molecular Dynamics Modeling of Liquid Iron-Sulphur Solutions Using the Embedded Atom Model

D.K. Belashchenko*, *Moscow Institute of Steel and Alloys, Moscow, Russia* and O.I. Ostrovski, *University of New South Wales, Sydney, NSW, Australia*

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Molecular Modeling, Including Simulation

Molecular Dynamics Simulation of Thermomechanical Properties of Pyrophyllite Nanoplate

N.K. Balabaev, *Russian Academy of Science, Pushchino, Russia*, M.A. Mazo, E.B. Gusarova, L.I. Manevitch* and A.A. Berlin, *Russian Academy of Science, Moscow, Russia* and G.C. Rutledge, *Massachusetts Institute of Technology, Cambridge, U.S.A.*

Multi-Scale Simulation for the Adsorption of Model Polymers and Proteins on Nano-Patterned Surfaces

A. Striolo*, *University of Oklahoma, Norman, OK, U.S.A.*

Mutual Diffusion Coefficients of Concentrated 1:1 Electrolyte from the Modified Mean Spherical Approximation

G.-H. Gao*, H.-B. Shi and Yang-Xin Yu, *Tsinghua University, Beijing, China*

Numerical Integration Techniques Based on a Geometric View for Molecular Dynamics Simulations

I. Fukuda*, S. Queyroy and M. Horie, *National Institute of Advanced Industrial Science and Technology, Tokyo, Japan* and H. Nakamura, *Osaka University, Osaka, Suita, Japan*

On the Validity of Stokes-Einstein Relation

M. Cappelezzo, S.H. Pezzin and L.A.F. Coelho*, *State University of Santa Catarina, Joinville, SC, Brazil*

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Molecular Modeling, Including Simulation

Simulating a Protein in a Non-Polar Solvent with Low Water Concentration

N. Diaz-Vergara and Á. Piñeiro*, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*

Structural Properties of Water and Solutions from Crystalline to Subcritical States Based on Computer Simulation Data

M.A. Zaripova, M.S. Muhamadiev, A.B. Badalov, Z.V. Kobuliev and M.M. Safarov*, *Tajik Technical University named after M.S. Osimi, Dushanbe, Tajikistan*

Structure and Energetics of Disordered Materials Using Darwin's Theory of Evolution

C.E. Mohn and S. Stølen*, *University of Oslo, Oslo, Blindern, Norway*

Surface Ordering and Capillary Phenomena of Confined Hard Cut-Sphere Particles

M.M. Piñeiro*, *Universidade de Vigo, Vigo, Spain* and A. Galindo and A.O. Parry, *Imperial College, London, U.K.*

Temperature Dependence of the Heat Capacity and Vapor Pressure of Pure Self-Associated Liquids: A New Correlation Based on a Two State Association Model

M. Medeiros*, *Universidad Nacional Autónoma de México, México, DF, México*, M. Costas, *Universidad Nacional Autónoma de México (UNAM), México, DF, México*, C.O. Armas-Alemán, *Universidad Nacional Autónoma de México, México, DF, México* and C. Cerdeiroña, *Universidad de Vigo, Ourense, Spain*

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Molecular Modeling, Including Simulation

The Virial Coefficients of Pure Gases and Mixtures: A Simple Additivity Scheme of Group Interactions

L. Lepori* and E. Matteoli, *Istituto Processi Chimico-Fisici, CNR, Pisa, Italy* and A. Spanedda and G.C. Bussolino, *Istituto Processi Chimico-Fisici, CNR, Pisa, Italy*

Thermodynamic Properties of the Gaussian Core Model Fluid

H.O. May*, *University of Applied Sciences Darmstadt, Darmstadt, Germany* and P. Mausbach, *University of Applied Sciences Köln, Köln, Germany*

Transport Properties of the Gaussian Core Model Fluid

P. Mausbach*, *University of Applied Sciences Köln, Köln, Germany* and H.O. May, *University of Applied Sciences Darmstadt, Darmstadt, Germany*

Use of the Trappe Model to Predict P-V-T Data at Extreme Conditions

B.L. Eggimann* and J.I. Siepmann, *University of Minnesota, Minneapolis, MN, U.S.A.* and L.E. Fried, *Lawrence Livermore National Laboratory, Livermore, CA, U.S.A.*

Vapor-Liquid Equilibria of Real Mixtures with Polar Two-Center Lennard-Jones Models

J. Vrabec*, Y.L. Huang and H. Hasse, *University of Stuttgart, Stuttgart, Germany*

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Molecular Modeling, Including Simulation

**Vapor-Liquid Phase Coexistence Properties for the
Triangular Well Fluid of Variable Width**

F.F. Betancourt-Cárdenas and L.A. Galicia-Luna*, *Instituto
Politécnico Nacional, México, DF, México*

**Verification of Onsager's Reciprocal Relations for
Evaporation and Condensation Using Non-Equilibrium
Molecular Dynamics**

J. Xu*, S. Kjelstrup, D. Bedeaux, A. Rosjorde and L. Rekvig,
*Norwegian University of Science and Technology,
Trondheim, Norway*

**Phase Equilibrium, Supercritical Fluids, and Separation
Technologies**

**Azeotropic and Heats of Mixing Data for Binary Organic
Systems Containing 1-Methoxy-2-Propanol and 2-Butoxy
Ethanol**

L. Negadi*, *University Aboubakr Belkaid of Tlemcen,
Tlemcen, Algeria* and J. Gmehling, *Carl von Ossietzky
Universität Oldenburg, Oldenburg, Germany*

**Comprehensive Study of Thermodynamic Properties for
Cyclohexanone Oxime**

G.J. Kabo, Dz.H. Zaitsau, Y.U. Paulechka* and A.V. Blokhin,
Belarusian State University, Minsk, Belarus and S.P.
Verevkin, A. Heintz and V.N. Emel'yanenko, *University of
Rostock, Rostock, Germany*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Critical Properties of Carbon Dioxide-Sulphur Hexafluoride-Trifluoromethane Systems

A.S. Lawal*, M. Lal and A. Ortiz, *Texas Tech University, Lubbock, TX, U.S.A.*

Derivative Properties of Pure Fluids and Binary Mixtures of N-Alkane and 1-Alkanols Through a Molecular-Based Equation of State

F. Llovel and L.F. Vega*, *Consejo Superior de Investigaciones Cientificas, Barcelona, Bellaterra, Spain*

Development of a Novel Apparatus for the Measurement of Vapor-Liquid Equilibria at Elevated Temperatures and Moderate Pressures

P. Reddy*, D. Ramjugernath and J.D. Raal, *University of KwaZulu-Natal, Durban, South Africa*

Effects of Free Fatty Acids on Phase Equilibrium of Model Bile

M.-Z. Ge and X.-Q. An*, *Nanjing Normal University, Nanjing, China*

Extraction of Monomethylhydrazine of Space Grade by Ternary Distillation: Modeling of Liquid/Vapor Equilibria

A.J. Bougrine*, R. Tenu, V. Goutelle, H. Delalu and J.J. Counioux, *Université Claude Bernard - Lyon I, Villeurbanne, France*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Initial Density Dependence of the Hydrogen Thermal Conductivity and Corresponding States Correlation for High Densities

H. Behnejad* and A. Pedram, *University of Tehran, Tehran, Iran*

Isobaric Vapor-Liquid Equilibria for the Systems of 2,3-Pentanedione with Ethanol, Cyclohexane, n-Hexane and Crotonaldehyde at 20 kPa

P. Moodley*, K.I. Ireland, D. Ramjugernath, P. Naidoo and J.D. Raal, *University of KwaZulu-Natal, Durban, South Africa*

Liquid-Liquid Equilibrium of Ternary Aqueous Solutions of α,α,α -Trifluorotoluene in 2,2,2-Trifluoroethanol at 298.2 K and 101 kPa

Z. Atik*, M. Chaou and A. Kritli, *University of Sciences and Technology Houari Boumediene, Bab-Ezzouar, Algeria*

Measurement and Correlation of Ternary Liquid-Liquid Equilibria of Acetonitrile and Water with n-Dodecane, 1-Dodecene, Nonanol and Heptanoic Acid at 323.15 K and 1 atm

C. Narasigadu*, D. Ramjugernath, J.D. Raal and P. Naidoo, *University of KwaZulu-Natal, Durban, South Africa*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Measurement of Vapor Pressure of Selected Organometallic Precursors by a Static Method

M. Fulem*, K. Ruzicka and V. Ruzicka, *Institute of Chemical Technology, Prague, Czech Republic* and E. Samochin, T. Simecek and E. Hulcius, *Academy of Sciences of the Czech Republic, Prague, Czech Republic*

Measurements of the Critical Parameters for Propane

T. Sato*, Y. Honda and A. Sakabe, *Keio University, Kouhoku-ku, Yokohama, Japan* and M. Uematsu, *Keio University, Kohoku-ku, Yokohama, Japan*

Measurements of the Isobaric Specific Heat Capacity For Aqueous Methanol Mixtures and Aqueous Ammonia Mixtures at High Pressures

I. Fujita*, *Keio University, Yokohama, Japan*, K. Tanaka, *Iwaki Meisei University, Iwaki, Fukushima, Japan* and M. Uematsu, *Keio University, Kohoku-ku, Yokohama, Japan*

Modeling the Liquid-Liquid Equilibria of Water + Perfluorocarbons with the Cubic-Plus-Association Equation of State

M.B. Oliveira, M.G. Freire and I.M. Marrucho, *Universidade de Aveiro, Aveiro, Portugal*, G.M. Kontogeorgis, *Technical University of Denmark, Lyngby, Denmark* and J.A.P. Coutinho and A.J. Queimada*, *Universidade de Aveiro, Aveiro, Portugal*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Peculiarities of Behaviour of Acoustic Absorption Coefficient in the Vicinity of Critical Point

O.I. Bilous*, *National Aviation University, Kiev, Ukraine*,
O.D. Alekhin, *Kyiv National Taras Shevchenko University, Kiev, Ukraine*, N.L. Kozlova, *National Aviation University, Kiev, Ukraine* and V.S. Sperkach, *National Taras Shevchenko University of Kyiv, Kiev, Ukraine*

Singular Diameters in Liquid-Liquid Critical Phenomena

G. Pérez-Sánchez*, P. Losada-Pérez, C.A. Cerdeiriña and L. Romani, *Universidad de Vigo, Ourense, Spain* and M.A. Anisimov and J.V. Sengers, *University of Maryland, College Park, MD, U.S.A.*

Solubilities of Solid Polycyclic Aromatic Hydrocarbons and Polycyclic Aromatic Heterocycles in Pressurized Hot Water

P. Karasek, J. Planeta and M. Roth*, *Academy of Sciences of the Czech Republic, Brno, Czech Republic*

Solubility of Carbon Dioxide in Pentaerythritol Ester Oils

O. Fandiño, E.R. López, L. Lugo and J. Fernández*, *Universidad de Santiago de Compostela, Santiago de Compostela, Spain*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Stereoisomeric Effects on Volumetric Properties Under Pressure for the System Cis- + Trans-Decalin

Y. Miyake, A. Baylaucq* and C.K. Zeberg-Mikkelsen, *Universite de Pau, Pau, France*, G. Galliero, *Universite de Marne-la-Vallee, Marne la Vallee, France*, H. Ushiki, *Tokyo University of Agriculture and Technology, Tokyo, Japan* and C. Boned, *Universite de Pau, Pau, France*

Temperature and Pressure Effect on PEG 1500-Supercritical CO₂ Phase Equilibria

I. Pasquali*, L. Comi, F. Giordano and R. Bettini, *University of Parma, Parma, Italy*

The Slope of the Critical Line and Excess Properties in Liquid-Liquid Phase Transitions

P. Losada-Pérez*, G. Pérez-Sánchez, J. Troncoso, C.A. Cerdeiriña and L. Romaní, *Universidad de Vigo, Ourense, Spain*

Thermodynamic Consistency Near the Liquid-Liquid Critical Point

P. Losada-Pérez*, G. Pérez-Sánchez, J. Troncoso, C.A. Cerdeiriña and L. Romaní, *Universidad de Vigo, Ourense, Spain*

Thermodynamic Properties of 1,1'-Biadamantane

L.S. Karpushenkava, Y.U. Paulechka*, A.V. Blokhin and A.G. Kabo, *Belarusian State University, Minsk, Belarus* and A.A. Pimerzin, *Samara State Technical University, Samara, Russia*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Thermodynamic Properties of Acetic Acid + Hydrocarbons Mixtures

L. Negadi*, *University Aboubakr Belkaid of Tlemcen, Tlemcen, Algeria*, N. Ainous, *University Claude Bernard-Lyon I, Villeurbanne, France*, A. Negadi, *University Aboubakr Belkaid of Tlemcen, Tlemcen, Algeria*, I. Mokbel, *University Claude Bernard-Lyon I, Villeurbanne, France*, A. Kaci, *USTHB, Dar El Beida, Algeria* and J. Jose, *University Claude Bernard-Lyon I, Villeurbanne, France*

Vapor-Liquid Equilibria of the Binary 1,1,2-Trifluoroethane (HFC-143a) + Propane (HC-290), + n-Butane (HC-600) Mixture Systems

J. Im*, G. Lee, Moon Sam Shin and Hwayong Kim, *Seoul National University, Seoul, Korea*

Vapor-Liquid Equilibria of the System Nitrogen-n-Octane Between 344.5 and 543.5 K and Pressures up to 50 MPa

G. Eliosa-Jiménez, *Universidad Autónoma Metropolitana-Azcapotzalco, México, DF, México* and G. Silva-Oliver and F. García-Sánchez*, *Instituto Mexicano del Petróleo, México, DF, México*

Vapor-Liquid Equilibrium for Binary Mixtures of Methanol with Other Alcohols

M.A. Siddiqi*, *University of Duisburg Essen, Duisburg, Germany*, M. Bashirov, *Azerbaijan Technical University, Baku, Azerbaijan* and B. Atakan, *University of Duisburg Essen, Duisburg, Germany*

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Phase Equilibrium, Supercritical Fluids, and Separation Technologies

Vapor-Liquid Equilibrium Measurements Using a Novel Static Total Pressure Apparatus

A.M. Motchelaho*, D. Ramjugernath and J.D. Raal,
University of KwaZulu-Natal, Durban, South Africa

Properties and Processes for a Hydrogen-based Economy

Use of Hydrogen for Economy of Fuel in Steam Turbine Plants

A.A. Vasserman and M. Shutenko*, *Odessa National Maritime University, Odessa, Ukraine*

Properties for Sustainable Development

A Search for Periodicities in the Solar Flux at 127 MHz

O.N.A. Fadipe*, *University Of Ado-Ekiti, Ekiti-State, Nigeria*

Properties of Aqueous Systems

A Design of New Equation for the Description of Temperature and Pressure Dependence of Standard Partial Molar Volume of Organic Solutes in Water

L. Hnedkovsky and I. Cibulka*, *Institute of Chemical Technology, Prague, Czech Republic*

Application of a Modified Regular Solution Model to Correlate the Solubilities of Phthalic Acid Isomers and Toluic Acid Isomers in Water

Bingwen Long*, Y. Wang, D. Zhao and ZuRong Yang,
China

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Properties of Aqueous Systems

**Calculation of Thermodynamic Properties of Water
Baipazine Reservior**

M.S. Makhmadiev, *Baipazine Hydroelectric Power Station, Tajikistan* and M.M. Safarov*, *Tajik Technical University named after M.S. Osimi, Dushanbe, Tajikistan*

**Determination of Temperature Dependence of Limiting
Activity Coefficients and Henry's Law Constants for MTBE in
Water**

P. Vrbka*, V. Dohnal and K. Rehak, *Institute of Chemical Technology, Prague, Czech Republic* and A. Boehme and A. Paschke, *Centre for Environmental Research, Leipzig, Germany*

**Experimental Study of Triflic Acid and Sodium Triflate in
Aqueous Solution: Standard Molar Volumes and Heat
Capacities Up to 573 K and 28 MPa**

E. Pourtier, K. Ballerat-Busseroles and V. Majer*, *Université Blaise Pascal/CNRS, Aubière, France*

**Extraction of Hydrophobic Compounds from Solid Matrixes
Using Subcritical Water**

E. Moreno, J. Reza* and A. Trejo, *Instituto Mexicano del Petróleo, México, DF, México*

**Gex-Model Using Local Area Fraction for Binary Electrolyte
Systems**

A. Haghtalab, *University of Qatar, Doha, Qatar* and M. Joda*, *Tehran Oil Refining Company, Tehran, Iran*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Aqueous Systems

Isotope Effects on Standard and Partial Molar Volumes of NaCl, HCl and NaOH Measured in Light and Heavy Water at 250 °C and 300 °C

E. Balodis*, L.N. Trevani and P.R. Tremaine, *University of Guelph, Guelph, ON, Canada*

Measurements of Dissociation Constants of Carbonic Acid in Synthetic Seawater by Means of a Cell without Liquid Junction

C.S. Wong, *Institute of Ocean Sciences, Sydney, BC, Canada*, P.Y. Tishchenko*, *V.I. Il'ichev Pacific Oceanological Institute, Vladivostok, Russia* and W.K. Johnson, *Institute of Ocean Sciences, Sydney, BC, Canada*

Molecular Mechanisms Underlying the Properties of Water

J. Jirsak and I. Nezbeda*, *Academy of Sciences, Prague, Czech Republic*

Nature of Phase Transitions: "Water - Ice" and "Ice - Water"

R.A. Medzhidov*, *Russian Academy of Science, Makhachkala, Dagestan, Russia*

Negative Dispersion of Hypersonic Velocity in Aqueous Solution of Gamma-Picoline

H.S. Haydarov, L.M. Sabirov and D.I. Semenov*, *Samarkand State University, Samarkand, Uzbekistan*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Aqueous Systems

PVT Properties and Phase Equilibria for the Binary n-Pentane + Water System

A.R. Rasulov* and S.M. Rasulov, *Institute of Physics of Dagestan Science Centre, Makhachkala, Dagestan, Russia*

Standard Partial Molar Volumes in Water of Oxygenated Aliphatic Compounds in Extended Ranges of Temperature and Pressure

L. Hnedkovsky, I. Cibulka* and T. Marek, *Institute of Chemical Technology, Prague, Czech Republic*

Thermodynamic Consideration of Equilibrium of CO₂-Hydrate in Seawater

C.S. Wong, *Institute of Ocean Sciences, Sydney, BC, Canada*, P.Y. Tishchenko*, *V.I. Il'ichev Pacific Oceanological Institute, Vladivostok, Russia* and W.K. Johnson, *Institute of Ocean Sciences, Sydney, BC, Canada*

Two-Phase and Three-Phase Equilibria in the Systems n-Pentane/Water and n-Hexane/Water; Correlation and Modeling

R.J. Perez* and R.A. Heidemann, *University of Calgary, Calgary, AB, Canada*

Viscosities and Densities of Binary Mixtures of Water with NaCl between 293.15 and 353.15 K

M.S. Muhamadiev*, D.I. Bobosherov, M.M. Safarov and A.B. Badalov, *Tajik Technical University named after M.S. Osimi, Dushanbe, Tajikistan*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Aqueous Systems

**What Quantum Chemists Owe to Molecular Physicists:
Aqueous Mixtures of Alcohols**

I. Nezbeda*, *Academy of Sciences, Prague, Czech Republic*

Properties of Fuels, Including Natural Gas Systems

**Alternative Antiknocking Liquid Biofuels: Thermodynamic
Properties of the Ternary Mixture ETBE + Toluene + Heptane
at 313.15 K**

R.M. Villamañán, J.J. Segovia, C.R. Chamorro, M.C. Martín
and M.A. Villamañán*, *Universidad de Valladolid, Valladolid,
Spain*

**Compositional Model for Predicting Asphaltene
Precipitation**

M.R. Omidkhah*, M. Nikookar and G.R. Pazuki, *Tarbiat
Modarres University (TMU), Tehran, Iran* and M.A. Emadi,
National Iranian Oil Company, Tehran, Iran

**Critical Phenomena at Hydrates Formation in Natural Gas -
Water System**

M.M. Asadov, *National Academy of Sciences of Azerbaijan,
Baku, Azerbaijan* and E.E. Ramazanova*, *Scientific
Research Institute, Baku, Azerbaijan*

**Densities of Ethylbenzene + n-Heptane Mixtures at High
Temperatures and High Pressures**

I.M. Abdulagatov*, *Russian Academy of Sciences,
Makhachkala, Dagestan, Russia* and N.D. Azizov,
Azerbaijan State Oil Academy, Baku, Azerbaijan

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Fuels, Including Natural Gas Systems

Differential Scanning Calorimetry Studies of Gas Hydrate Inhibition

J. Lachance*, E.D. Sloan and S.F. Dec, *Colorado School of Mines, Golden, CO, U.S.A.*, J.L. Creek, *Chevron Energy Technology Company, Houston, TX, U.S.A.* and C.A. Koh, *Colorado School of Mines, Golden, CO, U.S.A.*

Generalized Virial Equation of State for Natural Gas Systems

J.F. Estela-Uribe* and J. Jaramillo, *Universidad Javeriana Cali, Cali, Colombia*

Instrumental Cross Calibration for Compositional Determination of Methane + Ethane Hydrates Using Raman and NMR Spectroscopy

K.C. Hester*, S.F. Dec, C.A. Koh and E.D. Sloan, *Colorado School of Mines, Golden, CO, U.S.A.*

MBWR-32 Equations of State for n-Hexane, n-Octane and n-Decane and Extension of the Multi-fluid Corresponding States Model for Natural Gas Properties

B.A. Dossey and J.F. Ely*, *Colorado School of Mines, Golden, CO, U.S.A.*

Methane Hydrate Heat Capacity and Enthalpy of Dissociation Measurements in Bulk and Sediment Systems

A. Gupta*, J. Lachance, E.D. Sloan and C.A. Koh, *Colorado School of Mines, Golden, CO, U.S.A.*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Fuels, Including Natural Gas Systems

Prediction of Natural Gas Mixtures Properties from Cubic and Molecular-Based Equations of State

K.R. Hall, S. Ejaz, M. Atilhan* and S. Aparicio-Martinez, *Texas A&M University, College Station, TX, U.S.A.*

Swapping Global Warming Gases for Methane in Gas Hydrate Layer

Youngjune Park*, Do-Youn Kim, Jeasung Park, Sun-Hwa Yeon, Kyuchul Shin and Jiwoong Seol, *Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Yuseong-gu, Korea*, Sung-oh Yang, *Korea National Oil Corporation, Anyang-si, Gyeonggi-do, Korea* and Huen Lee, *Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Yuseong-gu, Korea*

Properties of Mesoscopic, Self-Assembled, and Strongly Fluctuating Systems

Anomaly in the Heat Capacity of Triethylamine and Water

D.T. Jacobs*, R.A. Shewmon and R. Hartschuh, *The College of Wooster, Wooster, OH, U.S.A.*

Effects of Confinement on Self-Assembling Systems

A. Ciach*, *Polish Academy of Sciences, Warsaw, Poland*

Intensity Increasing of Light Beam Which Passes Across Inhomogeneous Medium Near the Critical Point

A.D. Alekhin*, *Kyiv National Taras Shevchenko University, Kiev, Ukraine*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Mesoscopic, Self-Assembled, and Strongly Fluctuating Systems

Thermal and Caloric Properties of Inhomogeneous Systems Under Gravity Near the Critical Point

A.D. Alekhin* and E.G. Rudnikov, *Kyiv National Taras Shevchenko University, Kiev, Ukraine*

Properties of Working Fluids, Including Refrigerants

A Combined Equation of State for HFC 218

V.A. Rykov, E.E. Ustjuzhanin*, I.V. Kudriavzeva and B.F. Reutov, *Moscow Power Engineering Institute, Moscow, Russia* and I.M. Abdulagatov, *Russian Academy of Sciences, Makhachkala, Dagestan, Russia*

An Improved He II State Equation

V. Arp*, *Cryodata Inc., Boulder, CO, U.S.A.*

Combined Models of Thermophysical Properties of HFC 236ea on the Coexistence Curve Including the Critical Point

E.E. Ustjuzhanin*, *Moscow Power Engineering Institute, Moscow, Russia*, I.M. Abdulagatov, *Russian Academy of Sciences, Makhachkala, Dagestan, Russia* and B.F. Reutov, *Moscow Power Engineering Institute, Moscow, Russia*

Experimental Study of Thermal Conductivity of R245fa

A.J. Grebenkov*, V.V. Saplitsa, O.V. Beliaeva and V.P. Petrushkevich, *Joint Institute of Power Engineering and Nuclear Research-Sosny, Minsk, Belarus*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Working Fluids, Including Refrigerants

Flammability Studies of Isomeric Structures of Ethane Derivatives and Percolation Theory

C. Blaszkowski* and I. Kul, *Widener University, Chester, PA, U.S.A.*

Investigation of Thermodynamic Activity in Multicomponent Alkali-Metal Liquids by a New Variant of the Effusion Method

D.N. Kagan*, G.A. Krechetova and E.E. Shpilrain, *Russian Academy of Sciences, Moscow, Russia*

Solid-Liquid Equilibria in the CO₂ + N₂O, CO₂ + R32, and N₂O + R32 Systems

G. Di Nicola*, G. Giuliani and S. Lioce, *Università Politecnica delle Marche, Ancona, Italy*, R. Stryjek, *Polish Academy of Sciences (PAN), Warsaw, Poland* and F. Polonara, *Università Politecnica delle Marche, Ancona, Italy*

Thermal Conductivity of Liquids Filled with Nano-Particles

S. Pittois, *Katholieke Universiteit, Leuven, Belgium*, S. George, *MAHE, Manipal, India* and J. Thoen and C. Glorieux*, *Katholieke Universiteit, Leuven, Belgium*

Thermal Conductivity of the Binary Refrigerant Mixtures (R125-R134a)

A.J. Grebenkov*, V.V. Saplitsa and Yu.G. Kotelevsky, *Joint Institute of Power Engineering and Nuclear Research-Sosny, Minsk, Belarus*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Properties of Working Fluids, Including Refrigerants

Thermophysical Properties of Some Nitrogen-Containing Working Fluids

A.J. Grebenkov*, V.P. Saplitsa, O.V. Beliaeva, V.P. Trubnikov and V.P. Tsurbelev, *Joint Institute of Power Engineering and Nuclear Research-Sosny, Minsk, Belarus*

Vapor Pressure of the (Lithium Bromide + Zinc Chloride + Methanol) System

J. Safarov*, *Friedrich - Alexander - Universität Erlangen - Nürnberg, Erlangen, Germany*

Theory of Thermophysical Properties, Including Statistical Mechanics

A Comparison of DHW Algorithm for Temperature Distribution Calculation with Fourier's Algorithm for Transmission of Heat Between Discrete Bodies

J. Gembarovic*, *TPRL, Inc., West Lafayette, IN, U.S.A.* and J. Gembarovic, Jr., *Purdue University, West Lafayette, IN, U.S.A.*

A New Statistical Mechanical Model for Calculating Kirkwood-Factors in Self-Associating Liquid Systems

A. Heintz and T. Vasiltsova*, *University of Rostock, Rostock, Germany*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Theory of Thermophysical Properties, Including Statistical Mechanics

A Quasi-Chemical Nonrandom Lattice Fluid Hydrogen Bonding Theory for Phase Equilibria of Associating Systems

Moon Sam Shin*, *Seoul National University, Seoul, Korea*,
Ki-Pung Yoo, *Sogang University, Seoul, Korea*, Chul Soo
Lee, *Korea University, Seoul, Korea* and Hwayong Kim,
Seoul National University, Seoul, Korea

About Aggregation of Acetonitrile Molecules in Pure Liquid State and in Solutions with Proton Donor Solvents

F.H. Tukhvatullin, A. Jumabaev, U.N. Tashkenbaev, H.
Hushvaktov, A. Absanov and M. Kuliyeva*, *Samarkand State
University, Samarkand, Uzbekistan*

Contradiction the Thermodynamic Properties of the Model sp^3 Hybridization and Unexplored Specific Intermolecular Interaction, Its Energies

A.K. Baev*, *Russian Academy of Science, Ivanovo, Russia*

Discrepancy Between Model sp^3 -Hybridization and Natural Chemical Interactions and the Chemistry of Liquid Non-Electrolytes

A.K. Baev*, *Russian Academy of Science, Ivanovo, Russia*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Theory of Thermophysical Properties, Including Statistical Mechanics

Equation of State of Liquids and Liquid Mixtures in Terms of Helmholtz Free Energy

V.I. Nedostup* and O.V. Nedostup, *National Academy of Sciences of Ukraine, Odessa, Ukraine*

Extended Carnot Theorem

Ji-Tao Wang* and Peiju Zheng, *Fudan University, Shanghai, China*

Ideal Gas Thermodynamic Functions of Organophosphorous Compounds from Density Functional Theory Calculations

O.N. Ryzhova*, V.G. Zverev and O.V. Dorofeeva, *Moscow State University, Moscow, Russia*

Intermolecular Hydrogen Bond and Orientational Correlation Times of Monomers and Associates in Pyridine Solutions

F.H. Tukhvatullin, A. Jumabaev*, U.N. Tashkenbaev and A. Omonov, *Samarkand State University, Samarkand, Uzbekistan*

Interpretation Excess Molar Thermal Expansion of the Binary Systems Formed by 1-Alkanols with 1-Alkenes in Terms of an Equation of State with Association

A.J. Treszczanowicz* and T. Treszczanowicz, *Polish Academy of Sciences, Institute of Physical Chemistry, Warsaw, Poland* and T.S. Pawlowski and T. Kasprzycka-Guttman, *Warsaw University, Warsaw, Poland*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Theory of Thermophysical Properties, Including Statistical Mechanics

Modeling the Vapor-liquid and Liquid-liquid Equilibria of Polymer Solutions

N. Pedrosa*, *University of Aveiro, Aveiro, Portugal*, L.F. Vega, *Consejo Superior de Investigaciones Cientificas, Barcelona, Bellaterra, Spain* and J.A.P. Coutinho and I.M. Marrucho, *Universidade de Aveiro, Aveiro, Portugal*

Phase Equilibrium Modeling of Intra- and Inter-Molecular Hydrogen-Bonding Ethylene Glycols Mixed with Nonpolar Solvents

J.H. Lee* and Chul Soo Lee, *Korea University, Seoul, Korea*

Self-Diffusion Coefficient of a Weakly Ionized Cesium Monatomic Gas: Symmetry Effects

M.T. Bouazza and M. Bouledroua*, *Badji Mokhtar University, Annaba, Algeria*

The Ellipsoid Model of Polyatomic Molecules and Its Use

V.I. Nedostup* and O.V. Nedostup, *National Academy of Sciences of Ukraine, Odessa, Ukraine*

The Equation for the Isochoric Heat Capacity of Water Vapor

R.A. Medzhidov*, *Russian Academy of Science, Makhachkala, Dagestan, Russia*

Posters 2

Chair: J.A. Widegren and J.W. Magee

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Theory of Thermophysical Properties, Including Statistical Mechanics

The Isotopic Sensitivities and Corresponding Uncertainties in Cryogenic Triple Point Realizations using Commercially Purified Gases

W.L. Tew*, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.*

The Spinodal Temperature of Binary Liquid Hydrocarbon Mixtures

J.G. Eberhart*, K. Lee, S. Gilkes, G. Gillette, A. Brennan and M. Mang, *University of Colorado at Colorado Springs, Colorado Springs, CO, U.S.A.*

The Thermodynamic Interrelationship Between Thermal and Elastic Properties of Condensed Phases: A Few Less-Well Known Scaling Relations and Their Applications

S. Raju* and E. Mohandas, *Indira Gandhi Centre for Atomic Research, Kalpakkam, India*

Thermodynamic Phase and Chemical Equilibrium of Involved Systems Aluminum Alkyls and Their Derivations

A.K. Baev*, *Russian Academy of Science, Ivanovo, Russia*

Thermodynamic Properties of a Dissociating Liquid in the Critical Region

A.J. Grebenkov* and V.P. Tsurbelev, *Joint Institute of Power Engineering and Nuclear Research-Sosny, Minsk, Belarus*

Thursday, August 03, 2006

Joint Session

Software Demonstrations 2

See Software Demonstrations 1

Chair: M.L. Huber and A.I. Johns

Afternoon 1 1:45 PM - 3:30 PM

Room: Stadium Club

Colloid and Interface Science 2
Biomimetic Systems

Chair: W. Loh and S. Pérez-Casas

Afternoon 2 3:50 PM - 5:35 PM

Room: Coors-2

- 3:55 PM Detergent-Like Membrane Disruption by Antimicrobial Peptides (Invited)**
K. Lohner*, *Austrian Academy of Sciences, Graz, Austria*
- 4:35 PM Interaction of Two Cecropin-Melittin Antimicrobial Peptides with Model Membranes: Calorimetric, Time Resolved Fluorescence Spectroscopy and Linear Dichroism Results**
G. Bai and P. Gomes, *University of Porto, Porto, Portugal*,
M. Hicks, *University of Warwick, Coventry, U.K.*, M. Prieto,
UTL, Lisboa, Portugal and M. Bastos*, *University of Porto, Porto, Portugal*
- 4:55 PM Studies on Interactions of Bovine Serum Albumin with Cationic Gemini and Single-Chain Surfactants**
Y.J. Li, X.Y. Wang and Y.L. Wang*, *Chinese Academy of Sciences, Beijing, China*
- 5:15 PM Thermodynamic and Structural Effects in Mixed Surfactant Solutions**
N.A. Smirnova*, *St. Petersburg State University, St. Petersburg, Russia*

Thursday, August 03, 2006

Joint Session

Molecular Modeling, Including Simulation 11

Thermal Properties 1

Chair: R. Sadus

Afternoon 2 3:50 PM - 5:35 PM

Room: Math-100

**3:55 PM Molecular Dynamics Simulation of the Metal Particle
Formation from Supersaturated Vapors**

T. Kraska* and N. Luemmen, *University Cologne, Köln,
Germany*

**4:15 PM Vapor Liquid Equilibrium of Linear Molecules with a Center
Shifted Point Dipole**

S. Lago* and M. Cortada, *Univ. Pablo de Olavide, Seville,
Spain*, B. Garzón, *Universidad San Pablo, Madrid, Spain*
and S. López-Vidal, F. Gámez and J.A. Anta, *Univ. Pablo de
Olavide, Seville, Spain*

**4:35 PM Development of a Molecular Model for the Prediction of
Phase Equilibria and Thermodynamic Properties of
Hydrofluorocarbons (HFC) and Their Mixtures**

J. Yustos, F. Llovel* and L.F. Vega, *Consejo Superior de
Investigaciones Científicas, Barcelona, Bellaterra, Spain*

**4:55 PM Interfacial Properties and Structure of Polymeric Blends
and Solutions from Interfacial-SAFT (iSAFT) Density
Functional Theory**

A. Dominik* and W.G. Chapman, *Rice University, Houston,
TX, U.S.A.*

**5:15 PM Investigation of Essentially Different Energy Distributions of
Molecular Orientations in Plastic Crystals**

A.B. Bazyleva*, G.J. Kabo and A.V. Blokhin, *Belarusian State
University, Minsk, Belarus*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

New Experimental Techniques 2

Viscosity and Calorimetry

Chair: A.R.H. Goodwin and T. Atake

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-105

3:55 PM Vibrating-Wire Sensors for Viscosity Measurements Under Extreme Conditions (Invited)

J.P.M. Trusler* and F. Peleties, *Imperial College London, London, U.K.*

4:35 PM Calorimetry and the 3ω Method and the Application to the Glass Transition Phenomena in 2-Butoxyethanol

T. Atake*, E. Osaki, Y. Yamada and H. Kawaji, *Tokyo Institute of Technology, Midori-ku, Yokohama, Japan*

4:55 PM TOPEM® - the Latest Innovation in Temperature Modulated DSC

S.R. Sauerbrunn*, *Mettler-Toledo, Inc., Newark, DE, U.S.A.*
and J.E.K. Schawe and T. Hütter, *Mettler-Toledo GmbH, Schwerzenbach, Switzerland*

5:15 PM Making Quartz Crystal Microbalance/Heat Conduction Calorimetry in Thin Films Reproducible, Precise, And Accurate

A.L. Smith*, *Masscal Corporation, Chatham, MA, U.S.A.*

New Materials 2

Magnetic and Superconducting Materials

Chair: Y.H. Jeong and R. Burriel

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-5

3:55 PM Ferromagnetic Shape Memory Alloys (Invited)

J. Pons*, E. Cesari, C. Segui, C. Picornell, R. Santamarta and
F. Masdeu, *Universitat de les Illes Balears, Palma de
Mallorca, Spain*

**4:35 PM Low-Temperature Relaxation Calorimetry of Some
Molecular Magnets**

Y. Nakazawa*, *Osaka University, Toyonaka, Osaka, Japan*
and S. Yamashita, *Tokyo Institute of Technology, Tokyo,
Japan*

4:55 PM Magnetocaloric Effect of a Molecular Nanomagnet

R. Burriel*, L. Tocado and E. Palacio, *CSIC - Universidad de
Zaragoza, Zaragoza, Spain* and R. Shaw and E.J.L.
McInnes, *University of Manchester, Manchester, U.K.*

**5:15 PM Particle Size vs Sample Quality As Factors Determining
Magnetic Properties in Nanoparticles**

B.F. Woodfield*, B. Lang, S. Liu, T.F. Walker, R. Stevens and J.
Boerio-Goates, *Brigham Young University, Provo, UT,
U.S.A.*, A. Navrotsky, *University of California at Davis,
Davis, CA, U.S.A.* and F. Hellman, *University of California
at Berkeley, Berkeley, CA, U.S.A.*

**5:35 PM Specific Heat As a Probe for Superconductivity in Pu-Based
Materials**

E. Colineau*, F. Wastin, P. Javorský, R. Jardin, P. Boulet and
J. Rebizant, *Institute for Transuranium Elements (ITU),
Karlsruhe, Germany*

Thursday, August 03, 2006

NIST/TRC Consortium Workshop 1

Open Session

Chair: M. Frenkel

Afternoon 2 3:30 PM - 5:00 PM

Room: Eng-151

3:30 PM Welcome and Introductions

M. Frenkel*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

3:35 PM Introductory Remarks

D.G. Friend*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

3:40 PM Overview of TRC Activities for the Period 2005-2006

M. Frenkel*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

4:00 PM TRC Data Collection Operation and Progress for the TRC Data Entry Facility

R.D. Chirico*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

4:15 PM Thermodata Engine (TDE): Version 2.0 for Pure Compounds

V.V. Diky*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

4:30 PM Web-ORACLE Dissemination Infrastructure and Thermoml Opener

C.D. Muzny*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

4:45 PM Further Development of the SOURCE Database and the IUPAC Ionic Liquids Database

A. Kazakov*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 5
Correlations***

Chair: P.M. Mathias and T.W. de Loos

Afternoon 2 3:50 PM - 5:35 PM

Room: Coors-1

3:55 PM Modeling of Supercritical Carbon Dioxide - Biopolymer Systems

A. Kasturirangan* and A.S. Teja, *Georgia Institute of Technology, Atlanta, GA, U.S.A.*

4:15 PM Rate-Based Distillation - Examples and Property Needs

P.M. Mathias*, *Fluor Corporation, Aliso Viejo, CA, U.S.A.*

4:35 PM The Use of Ionic Liquids As Solvents in Separating Organic Liquids and the Importance of Solubility in These Separations

T.M. Letcher* and P. Reddy, *University of KwaZulu-Natal, Durban, South Africa*

4:55 PM Modeling of the Solubility of Light Gases in Heavy Hydrocarbons and Their Mixtures

M.R. Riazi* and Y.A. Roomi, *Kuwait University, Safat, Kuwait*

5:15 PM Correlation and Prediction of the Solubility of CO₂ In Aqueous Solutions of n-Methyldiethanolamine + Piperazine

N.S. Matin*, M. Vahidi and M.H. Jenab, *National Iranian Oil Company, Tehran, Iran*, M. Goharrokhi, *Islamic Azad University, Tehran, Iran*, H. Najibi, *Petroleum University of Technology, Tehran, Iran* and A. Abdi, *Memorial University of Newfoundland (MUN), St. John's, NL, Canada*

Thursday, August 03, 2006

16th Symposium

Properties at the Nanoscale 2
Thermal Properties of Nanoscale Materials

Chair: R. Yang and R. Stevens

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-245

- 3:55 PM Thermoelectric Characterization of Nanostructured Bismuth Telluride and Carbon Nanotube Nanomaterials (Invited)**
T. Borca-Tasciuc*, *Rensselaer Polytechnic Institute (RPI), Troy, NY, U.S.A.*
- 4:35 PM Thermal Transport in MWNT Sheet**
A.E. Aliev*, M. Zhang, Sh. Fang, S.B. Lee, A.A. Zakhidov and R.H. Baughman, *University of Texas at Dallas, Richardson, TX, U.S.A.*
- 4:55 PM Temperature Dependence on Thermal Boundary Resistance at Metal-Dielectric Interfaces**
P.E. Hopkins* and R.N. Salaway, *University of Virginia, Charlottesville, VA, U.S.A.*, R.J. Stevens, *Rochester Institute of Technology, Rochester, NY, U.S.A.* and P.M. Norris, *University of Virginia, Charlottesville, VA, U.S.A.*
- 5:15 PM Thermal Conductivity of AlN Nanofluid**
P. Hu*, W.L. Shan, F. Yu and Z.S. Chen, *University of Science and Technology of China, Hefei, Anhui, China*

Thursday, August 03, 2006

16th Symposium

Properties for Sustainable Development 2

Chair: P. Wichlacz

Afternoon 2 3:50 PM - 5:15 PM

Room: Eng-200

3:55 PM Advanced Fuel Cycle Initiative Fuel Development Program Overview

W.J. Carmack*, *Idaho National Laboratory, Idaho Falls, ID, U.S.A.*

4:15 PM Chemical States of Volatile and Corrosive Fission Products in Thoria Based Fuels From Thermodynamic Studies

M. Ali (Basu), R. Mishra, S.R. Bharadwaj* and D. Das, *Bhabha Atomic Research Centre (B.A.R.C.), Trombay, Mumbai, India*

4:35 PM Quantitative Analysis of Engine Deposit Formation and Intensive Sustainability Study

Z. Ye*, *Southern University, Baton Rouge, LA, U.S.A.*, Q. Meng, *Toronto, ON, Canada*, H. Mohamadian and J. Wang, *Southern University, Baton Rouge, LA, U.S.A.* and L. Chen and L. Zhu, *Tianjin University, Tianjin, China*

4:55 PM Supercritical Fluid Extraction of Hydrocarbons from Both Spiked and Natural Polluted Soils Using Ethane

M.A. Avila-Chávez* and A. Trejo, *Instituto Mexicano del Petróleo, México, DF, México*

Thursday, August 03, 2006

16th Symposium

Properties of Aqueous Systems 4

Properties of Pure Water

Chair: C.J. Mundy and J.I. Siepmann

Afternoon 2 3:50 PM - 5:15 PM

Room: Eng-1B40

3:55 PM Formulation for the Viscosity of Water

M.L. Huber*, D.G. Friend, R.A. Perkins and A. Laesecke, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*, M.J. Assael and I.N. Metaxa, *Aristotle University, Thessaloniki, Greece*, E. Vogel, *University of Rostock, Rostock, Germany* and J.V. Sengers, *University of Maryland, College Park, MD, U.S.A.*

4:15 PM A Parametric Equation of State for the Liquid-Liquid Critical Point in Supercooled Water

D.A. Fuentevilla and M.A. Anisimov*, *University of Maryland, College Park, MD, U.S.A.*

4:35 PM Simulating Phase Equilibria of Water from First Principles

M.J. McGrath* and J.I. Siepmann, *University of Minnesota, Minneapolis, MN, U.S.A.* and I.F.W. Kuo and C.J. Mundy, *Lawrence Livermore National Laboratory, Livermore, CA, U.S.A.*

4:55 PM How H-Bond Network Leads to Anomalous Properties of Water?

N.P. Malomuzh*, *Odessa National University, Odessa, Ukraine*

Properties of Working Fluids, Including Refrigerants 6

Experimental Thermodynamics 3: Speed of Sound

Chair: E.W. Lemmon and M.O. McLinden

Afternoon 2 3:50 PM - 5:15 PM

Room: Eng-265

- 3:55 PM Speed of Sound and Ideal-Gas Heat Capacity Data of Selected Siloxanes from Acoustic Measurements: $[(\text{CH}_3)_2\text{SiO}]_4$ and $[(\text{CH}_3)_2\text{SiO}]_5$**
- R. Nannan*, *Delft University of Technology, Delft, Netherlands*, J.J. Hurly, *National Institute of Standards and Technology, Gaithersburg, MD, U.S.A.* and P. Colonna, *Delft University of Technology, Delft, Netherlands*
- 4:15 PM Measurements of the Speed of Sound in the Refrigerants 227ea and 365mfc in the Liquid Phase**
- K. Meier* and S. Kabelac, *Helmut-Schmidt-University, Hamburg, Germany*
- 4:35 PM Measurements of Sound Speed in Gaseous Ethane by a Spherical Resonator for Determination of Reliable Virial Coefficients**
- M. Yasui, S. Yamamoto* and H. Sato, *Keio University, Yokohama, Kohoku-ku, Japan*
- 4:55 PM Experimental Study of Thermodynamic Properties of R245fa**
- A.J. Grebenkov*, V.P. Tsurbelev, O.V. Beliaeva and B.D. Timofeyev, *Joint Institute of Power Engineering and Nuclear Research-Sosny, Minsk, Belarus*

Thursday, August 03, 2006

16th Symposium

Property Needs in Biothermophotonics 1

Chair: J.J. Alvarado-Gil

Afternoon 2 3:50 PM - 5:35 PM

Room: Eng-155

3:55 PM Optical Pathology of Photoacoustic Spectra of Ovarian Tissue: Classification Using Principal Component Analysis (PCA) and Artificial Neural Network (ANN) Analysis (Invited)

K.K. Mahato*, S.D. Kamath, D.V. Kamath, S. Ray and R.A. Bhat, *Manipal Academy of Higher Education, Manipal, India*

4:35 PM Characterization of Dental Demineralization Using a Biothermophotonic Technique (Invited)

A. Matvienko*, R. Jeon and A. Mandelis, *University of Toronto, Toronto, ON, Canada*, S. Abrams, *Four Cell Consulting, Toronto, ON, Canada* and G.V. Kulkarni, *University of Toronto, Toronto, ON, Canada*

5:15 PM The Effect of Hydration on Thermal Effusivity of Aqueous Solutions of Liquid Ethylene Glycol Polymers

A. Sikorska* and B.B.J. Linde, *University of Gdansk, Gdansk, Poland*

Thursday, August 03, 2006 19th ICCT / 61st CalCon

Thermodynamic Frontiers and Education 2

From Membranes to Diamonds

Chair: T.M. Letcher and R. Weir

Afternoon 2 3:50 PM - 5:55 PM

Room: Coors-4

3:55 PM Thermodynamics in Membrane Process Design (Invited)

R.N. Lichtenthaler*, *University of Heidelberg, Heidelberg, Germany*

4:35 PM The Constrained Free Energy Method for Multi-Phase Systems

P. Koukkari*, *VTT Process Chemistry, Finland* and R. Pajarre, *Technical Research Centre of Finland, VTT, Finland*

4:55 PM Discrete Thermodynamics of Chemical Equilibria

B. Zilbergleyt*, *System Dynamics Research Foundation, Chicago, IL, U.S.A.*

5:15 PM Modern Thermodynamics for Carat-size Synthetic Diamonds

Ji-Tao Wang* and Peiju Zheng, *Fudan University, Shanghai, China*

5:35 PM Heat and Energy Education in Secondary Schools in Japan - The Current Status and Perspective-

H. Tanaka* and N. Koga, *Hiroshima University, Higashi-Hiroshima, Japan*

Thursday, August 03, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 7***

Properties of Biological Solutions

Chair: P.W. Chun and D.P. Remeta

Afternoon 2 3:50 PM - 5:35 PM

Room: Coors-3

**3:55 PM Density Functional Study on the Osmotic Coefficient for the
DNA-Electrolyte Solutions**

K. Wang, *China* and Yang-Xin Yu* and G.-H. Gao,
Tsinghua University, Beijing, China

**4:15 PM Studies on Solvation Behavior of Some Amino Acids and
Lysozyme in Mixed Aqueous Solutions of Organic Salts**

T.S. Banipal and K. Singh, *Guru Nanak Dev University,
Amritsar, India*, G. Singh*, *C.T. Institute of Pharmaceutical
Sciences, Janadhar, Punjab, India* and P. Banipal, *Guru
Nanak Dev University, Amritsar, India*

**4:35 PM An Equation of State And Non-Linearity Parameter (B/A) of
Multicomponent Liquid Systems**

V. Vyas*, *University of Allahabad, Allahabad, India*

**4:55 PM Intermolecular / Interionic Interactions in L-Isoleucine-, L-
Proline-, and L-Glutamine- Aqueous Electrolyte Systems**

Riyazuddeen* and R. Basharat, *Aligarh Muslim University,
Aligarh, India*

**5:15 PM Specific Intermolecular Interactions of Pentacoordinated
Carbon Atom and Hydrogen-Bonding in Liquid Alcohols of
Acetylene Series and of Vitamin E Synthesis Components**

A.A. Baev and A.K. Baev*, *Russian Academy of Science,
Ivanovo, Russia*

Thursday, August 03, 2006

Joint Session

Plenary 7
Conference Banquet

Evening 6:00 PM - 10:00 PM

Room: NCAR

6:05 PM **Conference Banquet**

Friday, August 04, 2006

19th ICCT / 61st CalCon

Colloid and Interface Science 3

Polymer and Surfactant at Interfaces

Chair: H. Yan and W. Loh

Morning 1 8:30 AM - 9:55 AM

Room: Coors-2

8:35 AM Comparative Study of Mass Transfer in Oil-Water-Oil Multiple Emulsions Stabilized by Conventional and Gemini Surfactants by Differential Scanning Calorimetry

M. Nadeem* and I.B. Tan, *Universiti Teknologi PETRONAS, Perak, Malaysia*

8:55 AM Relaxation Processes in Semidilute and Dilute Solutions of Polymers in Liquid Crystal Solvents

S.A. Wieczorek*, *Polish Academy of Sciences, Warsaw, Poland*, E. Freyssingeas, *École Normale Supérieure de Lyon, Lyon, France* and R. Holyst, *Polish Academy of Sciences, Warsaw, Poland*

9:15 AM Polymer Adsorption on Silica Particles: Relation Between Kinks on Adsorption Isotherms and Bulk Phase Behavior

N. Derkaoui, *UBO, Brest, France*, S. Said and Y. Grohens, *UBS, Lorient, France* and R. Olier and M. Privat*, *UBO, Brest, France*

9:35 AM Calculation of Surface Tension by Direct Gibbs Energy Minimization

R. Pajarre*, *Technical Research Centre of Finland, VTT, Finland*, P. Koukkari, *VTT Process Chemistry, Finland* and T. Tanaka, *Technical Research Centre of Finland, VTT, Finland*

Friday, August 04, 2006

16th Symposium

Instrumentation and Measurement Techniques 6

Chair: L. Ott and T.J. Bruno

Morning 1 8:30 AM - 9:55 AM

Room: Eng-105

- 8:35 AM Two-Fluid Modification Into Monotonic Heating Regime Thermal Diffusivity Measurement**
A.J. Panas* and J. Sypek, *Military University of Technology
Institute of Aviation Technology, Warsaw, Poland*
- 8:55 AM Real-Time Sensing of Thermal Diffusivity for Dynamic Control on Anisotropic Heat Conduction of Liquid Crystal**
M. Motosuke* and Y. Nagasaka, *Keio University, Yokohama,
Kanagawa, Japan*
- 9:15 AM Steady State Hot Strip Method**
U. Hammerschmidt* and V. Meier, *Physikalisch-Technische
Bundesanstalt, Braunschweig, Germany*
- 9:35 AM Development of Thermal Properties Sensing Technique with 100 nm Spatial Resolution by Using Near-field Optics**
K. Ishikawa*, Y. Taguchi, T. Saiki and Y. Nagasaka, *Keio
University, Yokohama, Kanagawa, Japan*

Friday, August 04, 2006

16th Symposium

Inverse Problems and Non-Destructive Evaluation 1

Chair: R. Li Voti

Morning 1 8:30 AM - 10:15 AM

Room: Eng-155

8:35 AM Self-Regularizing Neural Network for Photothermal and Photoacoustic Depth Profiling (Invited)

G. Kalogiannakis, *Vrije Universiteit, Brussels, Belgium*, A. Okasha, *National Research Center, Cairo, Egypt*, J. Ravi, *Cochin University of Science and Technology, Kochi, India*, Y. Lu, *Katholieke Universiteit, Leuven, Belgium*, S. Longuemart, *Université du Littoral Côte d'Opale, Dunkerque, France* and C. Glorieux*, *Katholieke Universiteit, Leuven, Belgium*

9:15 AM Opto-Thermal Skin Hydration Depth Profiling Measurements Using Genetic Algorithm (Invited)

Y. Cui, P. Xiao* and R.E. Imhof, *London South Bank University, London, U.K.*

9:35 AM Thermal Diffusivity Effect in Opto-Thermal Skin Measurements

P. Xiao* and R.E. Imhof, *London South Bank University, London, U.K.*

9:55 AM Inversion Techniques Applied to Picosecond Acoustics

M. Tomoda, *Hokkaido University, Sapporo, Japan*, R. Li Voti*, *Università degli Studi di Roma, Rome, Italy* and O. Matsuda and O.B. Wright, *Hokkaido University, Sapporo, Japan*

Friday, August 04, 2006

Joint Session

Molecular Modeling, Including Simulation 12

Thermal Properties 2

Chair: S. Okazaki

Morning 1 8:30 AM - 10:15 AM

Room: Math-100

8:35 AM Molecular Dynamic Simulations and Global Equation of State of Square-Well Fluids with the Variable Well-Widths

S.B. Kiselev* and J.F. Ely, *Colorado School of Mines, Golden, CO, U.S.A.* and J.R. Elliot, Jr., *The University of Akron, Akron, OH, U.S.A.*

8:55 AM Molecular Modeling of Fluids: Simple Models of Polar and Associating Fluids and Their Applications

I. Nezbeda*, *Academy of Sciences, Prague, Czech Republic*

9:15 AM Linking Structure, Energetics and Fast-Ion Conduction

S. Stølen* and C.E. Mohn, *University of Oslo, Oslo, Blindern, Norway* and N.L. Allan, *University of Bristol, Bristol, Clifton, U.K.*

9:35 AM New Mixing Rules for High-Pressure Equilibrium Calculation of Water + Ethylene Glycol + Methane, Ethane and Acid Gases Systems using EOS/GE

A. Haghtalab*, *University of Qatar, Doha, Qatar* and S.H. Mazlomi, *Tarbiat Modarres University, Tehran, Iran*

9:55 AM Site-Site Potential Function and Second Virial Coefficients for Linear Molecules

L. Meng* and Y.-Y. Duan, *Tsinghua University, Beijing, China*

New Materials 3

Functional Materials

Chair: R. Burriel and R.N. Lichtenthaler

Morning 1 8:30 AM - 10:15 AM

Room: Coors-5

8:35 AM Thermodynamic Studies of Relaxor Ferroelectrics $\text{BaTi}_{1-x}\text{Zr}_x\text{O}_3$ - Giaque Travel Award Presentation -

M. Nagasawa*, H. Kawaji, T. Tojo and T. Atake, *Tokyo Institute of Technology, Midori-ku, Yokohama, Japan*

8:55 AM Nanocalorimetric Study of the Amorphous-to-Liquid Transition in Ultrathin Films of A-Ge

A.F. Lopeandía*, E. León-Gutierrez, G. Garcia, F. Pi, M.T. Clavaguera-Mora and J. Rodríguez-Viejo, *Universidad Autónoma de Barcelona, Bellaterra, Spain*

9:15 AM Thermodynamic Assessment of the La-Mn-Cr-O System for Applications on Solid Oxide Fuel Cell (SOFC) Materials Using the Calphad Approach

E. Povoden*, *ETH Zurich, Zürich, Switzerland*, A.N. Grundy, *École Polytechnique de Montreal, Montreal, QC, Canada* and L.J. Gauckler, *ETH Zurich, Zürich, Switzerland*

9:35 AM Studies on Thermodynamic Characteristics and Hydrogen Storage Performance of Metal Organic Frameworks

Jian Zhang, Ying-Ya Liu, Fen Xu, Li-Xian Sun*, Shiwei Zhang and H.-T. Zhang, *Chinese Academy of Sciences, Dalian, China*

9:55 AM Study of PCM Systems Containing Metal-Metal Oxide Particles

J.-L. Zeng*, Li-Xian Sun, Fen Xu, Z.-C. Tan and H.-T. Zhang, *Chinese Academy of Sciences, Dalian, China*

Friday, August 04, 2006

19th ICCT / 61st CalCon

***Phase Equilibrium, Supercritical Fluids, and Separation
Technologies 6***

Theory II

Chair: L.F. Vega and U.K. Deiters

Morning 1 8:30 AM - 10:15 AM

Room: Coors-4

**8:35 AM Stability Limits in Pure and Binary Fluid Mixtures Obtained
from Equations of State**

*A. Imre, KFKI Atomic Energy Research Institute, Budapest,
Hungary and T. Kraska*, University Cologne, Köln,
Germany*

**8:55 AM Van der Waals Theory is Correct: Selections of Cubic
Equations-of-State Are Problematic**

A.S. Lawal, Texas Tech University, Lubbock, TX, U.S.A.*

9:15 AM Onset of Convection in Supercritical Fluids

R. Bonnefoi, L. El Khouri and P. Carles, Universite Pierre et
Marie Curie, Case 162, Paris, France*

9:35 AM The Universal Triangle of Liquid - Gas States

V.S. Vorob'ev, G.A. Martynov and E.M. Apfelbaum, Russian
Academy of Science, Moscow, Russia*

**9:55 AM P-T-x Phase Diagram of the Ga-Se System:
Thermodynamics and Nonstoichiometry of Gallium Elenides**

V. Zlomanov, Moscow State University, Moscow, Russia,
A. Tyurin and K. Gavrichiev, Russian Academy of Sciences,
Moscow, Russia and A. Zavrazhnov, Voronezh State
University, Voronezh, Russia*

Friday, August 04, 2006

16th Symposium

Properties at the Nanoscale 3
Theory & Modeling of Transport in Nanoscale Materials

Chair: R. Stevens

Morning 1 8:30 AM - 10:15 AM

Room: Eng-245

8:35 AM Thermoelectric Transport in Nanocomposites

R.G. Yang*, *University of Colorado, Boulder, CO, U.S.A.*

**8:55 AM A Theoretical Study on Optical - Thermal Energy Conversion
in Metallic Nanoparticles**

Y. He and T. Zeng*, *North Carolina State University, Raleigh,
NC, U.S.A.*

**9:15 AM Thermal Properties of Nanoporous Zeolite MFI: Lattice
Dynamics Modeling and Experiments**

A.M. Greenstein*, Y.C. Hudiono, S. Graham and S. Nair,
Georgia Institute of Technology, Atlanta, GA, U.S.A.

**9:35 AM Temperature Dependence of Thermal Boundary
Conductance at FCC Embedded Atom Metal Interfaces: A
Molecular Dynamics Approach**

R.N. Salaway*, P.E. Hopkins and P.M. Norris, *University of
Virginia, Charlottesville, VA, U.S.A.*

9:55 AM Thermal Conductivity of a Gas in Nanoporous Structure

Yusong Liu, Xinxin Zhang* and Fan Yu, *University of Science
and Technology Beijing, Beijing, China*

Friday, August 04, 2006

16th Symposium

Properties of Aqueous Systems 5

Aqueous Interfaces

Chair: J.I. Siepmann

Morning 1 8:30 AM - 10:15 AM

Room: Eng-1B40

- 8:35 AM** **Structure and Dynamics of the Aqueous Liquid-Vapor Interface: a Comprehensive Particle-Based Simulation Study (Invited)**
- C.J. Mundy*, *Lawrence Livermore National Laboratory, Livermore, CA, U.S.A.* and I.F.W. Kuo, J.I. Siepmann and D.J. Tobias, *Lawrence Livermore National Laboratory, Livermore, CA,*
- 9:15 AM** **Effects of Size and Polarizability on Ion Partitioning at the Aqueous Liquid-Vapor Interface: A Molecular Simulation Perspective**
- B.L. Eggimann* and J.I. Siepmann, *University of Minnesota, Minneapolis, MN, U.S.A.*
- 9:35 AM** **Equilibrium and Interfacial Properties of Water + Alkanes: Measurements and Modeling**
- M.B. Oliveira, P.J. Carvalho, A.J. Queimada*, I.M. Marrucho and J.A.P. Coutinho, *Universidade de Aveiro, Aveiro, Portugal*
- 9:55 AM** **Experimental Study on the Interfacial Tension and Density of Water + Branched Hydrocarbon Systems as a Function of Temperature**
- C.G. Aranda-Bravo, A. Romero-Martínez* and A. Trejo, *Instituto Mexicano del Petróleo, México, DF, México*

Friday, August 04, 2006

16th Symposium

Properties of Fuels, Including Natural Gas Systems 3

Chair: J. Holste

Morning 1 8:30 AM - 9:55 AM

Room: Eng-200

- 8:35 AM ***Ab Initio* Calculations of Chemical Equilibria and Comparison with Experimental Data in the Vapor and the Liquid Phase Using the TAME-Synthesis Reaction As an Example**
A. Heintz*, S. Kapteina and S.P. Verevkin, *University of Rostock, Rostock, Germany*
- 8:55 AM **Measurement and Modeling of the Water Content of Sweet and Acid Natural Gas Systems**
M. Yarrison*, K.R. Cox and W.G. Chapman, *Rice University, Houston, TX, U.S.A.*
- 9:15 AM **Volumetric and Viscosity Modeling of Natural Gas Based on the Friction Theory**
S.E. Quiñones-Cisneros* and U.K. Deiters, *University of Cologne, Köln, Germany*
- 9:35 AM **High Accuracy Density Measurements for Two Light Synthetic Natural Gas-Like Mixtures Using a Single-Sinker, Magnetic-Suspension Densimeter**
K.R. Hall, S. Ejaz, M. Atilhan* and S. Aparicio-Martinez, *Texas A&M University, College Station, TX, U.S.A.*

Friday, August 04, 2006

16th Symposium

Properties of Working Fluids, Including Refrigerants 7

Properties and Working Fluids for Cycles

Chair: M.O. McLinden and R.R. Singh

Morning 1 8:30 AM - 9:55 AM

Room: Eng-265

8:35 AM Supplementary Backward Equations for the Industrial Formulation IAPWS-IF97 of Water and Steam for Fast Calculations of Heat Cycles, Boilers, and Steam Turbines

H.-J. Kretzschmar* and K. Knobloch, *Zittau/Goerlitz University of Applied Sciences, Zittau, Germany*, K. Miyagawa, *Tokyo, Japan* and W. Wagner, *Ruhr-Universität Bochum, Bochum, Germany*

8:55 AM Thermodynamic Analyses of Cycles by the Volume Translated Peng-Robinson Equation of State with g^E Mixing Rule

T. Yamaguchi*, K. Kanemaru, S. Momoki, T. Shigechi and T. Yamada, *Nagasaki University, Nagasaki, Japan*

9:15 AM Working Fluids for ORC Processes

B. Saleh, *Assiut University, Assiut, Egypt* and M. Wendland* and J. Fischer, *University of Natural Resources and Applied Life Sciences, Vienna, Austria*

9:35 AM 100 Years Third Law of Thermodynamics: Revisiting the Consequences for Temperature

A. Laesecke*, *National Institute of Standards and Technology, Boulder, CO, U.S.A.*

Friday, August 04, 2006

Joint Session

***Thermodynamics and Properties in the Biological, Medical,
Pharmaceutical, Agricultural, and Food Sectors 8
Calorimetry of Complex Systems***

Chair: N. Wright

Morning 1 8:30 AM - 9:55 AM

Room: Coors-3

**8:35 AM All Change Please: the Direct Measurement of Change in
Complex Systems -The Stig Sunner Memorial Award
Lecture- (Invited)**

S. Gaisford*, *University of London, London, U.K.*

**9:15 AM Thermodynamic Stability and Volumetric Characterization
of Molten Globule States of Cytochrome C Evaluated with
Differential Scanning, Isothermal Acid-Titration, and
Pressure Perturbation Calorimetry**

S. Kidokoro*, S. Nakamura and Y. Seki, *Nagaoka University
of Technology, Nagaoka, Niigata, Japan*

**9:35 AM Development of a Noninvasive Method for Measuring
Thermophysical Parameters and Blood Perfusion of Living
Tissues**

K. Yue, *China*, Xinxin Zhang*, *University of Science and
Technology Beijing, Beijing, China* and Y.Y. Zuo, *University
of Toronto, Toronto, ON, Canada*

Friday, August 04, 2006

16th Symposium

Instrumentation and Measurement Techniques 7

Chair: L. Ott and T.J. Bruno

Morning 2 10:35 AM - 12:00 PM

Room: Eng-105

10:40 AM Determination of Transient Thermal Interfacial Resistance Between Two Bonded Metal Bodies Using the Laser Flash Method and the Parameter Estimation Technique

N.D. Milosevic* and K.D. Maglic, *Vinca Institute of Nuclear Sciences, Belgrade, Serbia and Montenegro*

11:00 AM Development of High Speed Laser Flash Systems to Measure Thermophysical Properties of Thin Films

T. Baba*, N. Taketoshi and T. Yagi, *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan*

11:20 AM In-Depth and In-Plane Diffusivity Measurement of Thermal Barrier Coating by IR Camera: Evaluation of Aging

P.G. Bison*, *CNR-ITC, Padova, Italy*, F.M. Cernuschi, *CESI, Milano, Italy* and E. Grinzato and S. Marinetti, *CNR-ITC, Padova, Italy*

11:40 AM Structure in Microemulsions using Freeze-Fracture with Atomic Force Microscopy

C. Garza* and R. Castillo, *UNAM, México, DF, México*

Friday, August 04, 2006

16th Symposium

Inverse Problems and Non-Destructive Evaluation 2

Chair: R. Li Voti

Morning 2 10:35 AM - 12:20 PM

Room: Eng-155

10:40 AM Local Probing of Photothermally-Induced Surface Vibrations at Megahertz Frequencies (Invited)

M. Tomoda* and O.B. Wright, *Hokkaido University, Sapporo, Japan*

11:20 AM Development of Non-Destructive Remote Sensing Technique for Remaining Fluorocarbon in Insulations by Photothermal Radiometry

H. Ando* and Y. Nagasaka, *Keio University, Yokohama, Kanagawa, Japan*

11:40 AM An Operatorial Method for the Calculation of the Acoustic Field in a Shape Perturbed Resonator

P.A. Giuliano Albo*, *Istituto Elettrotecnico Nazionale Galileo Ferraris, Torino, Italy* and R.M. Gavioso and G. Benedetto, *Istituto Nazionale di Ricerca Metrologica, Torino, Italy*

12:00 PM Thermal Characterization of Multi-Layer Films by IR Thermography

J. Morikawa* and T. Hashimoto, *Tokyo Institute of Technology, Tokyo, Japan* and R. Li Voti, *Universita di Roma, La Sapienza, Rome, Italy*

Friday, August 04, 2006

19th ICCT / 61st CalCon

Plenary 19ICCT/61CalCon 3

Chair: R.N. Lichtenthaler and M. Frenkel

Morning 2 10:35 AM - 12:20 PM

Room: UMC Ballroom

New Materials

10:40 AM Structure, Magnetism and Thermodynamics of Novel Rare Earth Based Intermetallic Materials (Invited)

V.K. Pecharsky*, *Iowa State University, Ames, IA, U.S.A.*

11:30 AM 19ICCT/61CalCon Closing Ceremony

Friday, August 04, 2006

16th Symposium

Properties of Aqueous Systems 6

Phase Equilibria

Chair: A. Anderko and J.I. Siepmann

Morning 2 10:35 AM - 12:20 PM

Room: Eng-1B40

**10:40 AM Thermodynamic and Phase Behavior of Supercritical Water
- Organic Pollutant Mixtures**

V.A. Mazur* and S.V. Artemenko, *Academy of Refrigeration,
Odessa, Ukraine*

**11:00 AM Theoretical Derivation and Experimental Study of Ternary
Water-Salt Systems with Supercritical Fluid Equilibria**

V.M. Valyashko* and M.A. Urusova, *Russian Academy of
Sciences, Moscow, Russia*

11:20 AM Solubility of Copper Oxides in Water and Steam

D.A. Palmer*, *Oak Ridge National Laboratory, Oak Ridge,
TN, U.S.A.* and P. Benezeth, *L.M.T.G. CNRS, Toulouse,
France*

**11:40 AM Enthalpy of Solution and Solubility of CO₂ in Aqueous 2-
Amino-2-Methyl-1-Propanol (AMP)**

J.-Y. Coxam*, L. Rodier, D. Koschel and H. Arcis, *Université
Blaise Pascal / CNRS, Aubière, France*

**12:00 PM Experimental Study of the Thermophysical Properties of the
Binary System Hydrocarbon -Water (n-Heptane - Water)**

V.A. Mirskaya*, D.A. Nazarevich and R.O. Mirskaya,
*Dagestan Science Centre, Makhachkala, Dagestan,
Russia*

Friday, August 04, 2006

16th Symposium

***Theory of Thermophysical Properties, Including Statistical
Mechanics 5***

Chair: J.A. White and J. Kincaid

Morning 2 10:35 AM - 12:20 PM

Room: Eng-265

10:40 AM Helmholtz Type Equations of State - Some Practice Applications

E.C. Ihmels*, *DDBST GmbH, Oldenburg, Germany*

11:00 AM A Statistical Associating Fluid Theory for Strong Electrolyte Solutions

H. Zhao and C. McCabe*, *Vanderbilt University, Nashville, TN, U.S.A.*

11:20 AM A New Analytical Formulation for the Generalized Corresponding States Model for Thermodynamic and Surface Properties in Pure Fluids

S.B. Kiselev* and J.F. Ely, *Colorado School of Mines, Golden, CO, U.S.A.*

11:40 AM Adjusting the Parameters of the van der Waals Equation of State for Liquid-Phase p-v-T Predictions

J.G. Eberhart*, K. Townsend, E. Ingals, A. Brandin and R. Stamey, *University of Colorado at Colorado Springs, Colorado Springs, CO, U.S.A.*

12:00 PM Closed-Form Equations for the Van der Waals Gas-Liquid Critical Point

A.S. Lawal*, *Texas Tech University, Lubbock, TX, U.S.A.*

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