

XXXIX Jeep – 39th Edition of the Joint European Days on Equilibrium Between Phases 2013

MATEC Web of Conferences Volume 3 (2013)

**Nancy, France
19-21 March 2013**

Editors:

**N. David
J.-N. Jaubert
R. Privat**

ISBN: 978-1-63266-272-9

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

This work is licensed under a Creative Commons Attribution license:

<http://creativecommons.org/licenses/by/2.0/>

You are free to:

Share – copy and redistribute the material in any medium or format.

Adapt – remix, transform, and build upon the material for any purpose, even commercial.

The licensor cannot revoke these freedoms as long as you follow the license terms.

Under the following terms:

You must give appropriate credit, provide a link to the license, and indicate if changes were made.

You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use. The copyright is retained by the corresponding authors.

Printed by Curran Associates, Inc. (2014)

For additional information, please contact EDP Sciences – Web of Conferences at the address below.

EDP Sciences – Web of Conferences
17, Avenue du Hoggar
Parc d'Activité de Courtabœuf
BP 112
F-91944 Les Ulis Cedex A
France

Phone: +33 (0) 1 69 18 75 75
Fax: +33 (0) 1 69 28 84 91

contact@webofconferences.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

Modeling Wax Formation with Predictive UNIQUAC: from Petroleum and Fuels to Biofuels	1
<i>J.A.P. Coutinho</i>	
Equilibrium Structure of Dense Gases.....	2
<i>B. Sedunov</i>	
Hydration Characteristics of Lithium, Zinc, Potassium and Sodium Salts	7
<i>E. Lefebvre, S. Bennici, E. Gagnière, D. Mangin, A. Auroux</i>	
Characterization and Optimization of a Novel Protein Refolding Methodology	10
<i>G. Roussel, S.L. Rouse, M. Sansom, E.A. Perpète, C. Michaux</i>	
Multi-Phases Problematic in the Oil \& Gas Industry: Solid Phases Combined to Fluid Phases	11
<i>P. Duchet-Suchaux</i>	
Thermodynamic and Structural Studies of the Solid Deposit Formation in Paraffinic Petroleum Cuts	12
<i>M. Dirand, D. Petitjean, M. Bouroukba</i>	
Misanthus Ash Melting: Comparison of Thermodynamic Calculation and Experiments in Thermal Processes.....	13
<i>J. Kaknics, R. Michel, M-L. Bouchetou, J. Poirier</i>	
Thermodynamic Assessments of the Fe-Y and Ni-Sc Systems.....	17
<i>S. Kardellass, C. Servant, N. Selhaoui, A. Iddaoudi, M. Ait Amari, L. Bouirden</i>	
On the Bi₂O₃-Al₂O₃-PbO System.....	23
<i>F. Oudich, N. David, J.M. Fiorani, M. Vilasi</i>	
Thermal Evolution of Solid-Liquid Equilibria in the Quaternary System: NaBH₄-NaBO₂-NaOH-H₂O	24
<i>T. Vilarinho-Franco, A. Teysier, R. Tenu, J. Delmas, P. Capron, J.J. Couniou, C. Goutaudier</i>	
Second Harmonic Generation: Applications in Phase Diagram Investigations.....	25
<i>F. Simon, J. Mahieux, S. Clevers, N. Couvrat, V. Dupray, G. Coquerel</i>	
The Effective Diffusion Coefficient of Boron in the Fe₂B Layers Formed on the Iron Substrate	27
<i>M. Keddam, B. Bouarour, Z. Nait Abdellah, R. Chegroune</i>	
On the Solid-Liquid Equilibrium Behavior of Fatty Acids with Ethanolamines.....	31
<i>G.J. Maximo, J.A.P. Coutinho, M.C. Costa, A.J.A. Meirelles</i>	
Modeling Phase Diagrams of Systems Containing Ionic Liquids Used in Different Applications	32
<i>Y.S. Chen, F. Mutelet, J-N. Jaubert</i>	
Thermodynamic Investigation of the Al₂O₃-M₂O \{M=K,Na\} Systems	36
<i>L. Zhang, S. Guhl</i>	
Self-Assembly of Organic-Inorganic Hybrid Nanolayers: Effect of Endgroup Polarity on Nanostructures.....	37
<i>A. Dhotel, Z. Xu, L. Delbreilh, B. Youssef, J.M. Saiter, L. Tan</i>	
Prevention of the Scaling in Water Distribution Systems	41
<i>M. Ben Amor, M. Tili</i>	
The Thermodynamics of Alcohols-Hydrocarbons Mixtures	44
<i>R. Privat, J.-N. Jaubert, M. Molière</i>	
Temperature-Resolved Second Harmonic Generation: A Tool Designed to Study Solid-Solid Transition.....	54
<i>S. Clevers, F. Simon, V. Dupray, G. Coquerel</i>	
Experimental Determination of the Critical Locus of Binary Systems Containing CO₂ and an Ethyl Ester	57
<i>N. Juntarachat, L. Coniglio, R. Privat, J.-N. Jaubert</i>	
Measurement of Vapor-Liquid Equilibria for Diethylamine + Methanol System Represented Double Azeotropy on Elevated Pressure	60
<i>T. Hiaki, K. Saida, T. Ishihara, T. Sato, M. Matsumoto, M. Okada</i>	
Growth and Characterization of New Borate-Based Crystal Fibers by the Micro-Pulling Down Technique	64
<i>M. Cochez, F. Assi, N. Kozhaya, M. Ferriol, M. Aillerie, G. Maxwell</i>	
FTIR Spectroscopy and X-Ray Powder Diffraction Characterization of Microcrystalline Cellulose Obtained from Alfa Fibers.....	65
<i>D. Trache, K. Khimeche, A. Donnot, R. Benelmir</i>	
Flow Calorimetry: A Technique for Caracterisation of Liquid-Liquid and Liquid-Gas Systems.....	67
<i>M.R. Simond, K. Ballerat-Busserolles, Y. Coulier, J-Y. Coxam</i>	
Contributions of Tzero™ Technology to Temperature Modulated Differential Scanning Calorimetry.....	71
<i>J. Loubens, F. Hoppenot</i>	

X-Ray Structural Study of Aqua Bis \(\backslash\)(Thymine-N¹, N³) Ethylenediamine Copper \(\backslash\)(ii) Dihydrate.....	72
<i>R. Mokhtari, A. Adkhis, F. Michaud, S. Top</i>	
Oxygenated Additives in Bio-Fuels: Excess Enthalpies of Mixtures Di-Butyl Ether + 1-Propanol + Heptane Or + Cyclohexane at 298.15 and 313.15 K.....	74
<i>F.E.M. Alaoui, F. Aguilar, M.J. González-Fernández, A. El Amarti, E. Montero</i>	
Density, Speed of Sound and Refractive Index for the Binary Systems Dbe + 1-Hexene, Or Heptane, Or Cyclohexane, Or 2, 2, 4 Trimethyl-Pentane, Or Toluene, Or Methyl-Cyclohexane at 298.15 K.....	75
<i>C. Peral, A. Martínez-Terradillos, F. Aguilar, F.E.M. Alaoui, E. Montero</i>	
Specific Migration of Irgastab 17 MOK and DBP from Rigid and Plasticized Poly(Vinyl Chloride) Into Organic Liquids.....	76
<i>A. Amara, C. Zeddam, N. Belhaneche-Bensemra</i>	
Thermal Treatment of Moroccan Phosphogypsum	80
<i>S. El Issiouy, A. Atbir, S. Mançour-Billah, R. Bellajrou, L. Boukbir, M. El Hadek</i>	
Liquid-Liquid Equilibria in Demixing Amines: A Thermodynamic Approach.....	85
<i>K. Ballerat-Busserolles, Y. Coulier, V. Majer, J-Y. Coxam</i>	
Concentration of Zinc Ions in Perchlorate Medium by a Membrane-Gel Using an Acid Extractant \(\backslash\)DEHPA)	89
<i>L. Belhadji, F. Belkacemi, D.E. Hadj-Boussaad</i>	
Study of Binary Systems NdF₃-MF \(\backslash\)(M = Li, Na, K): Experimental, Modeling and Thermodynamic Computation	93
<i>M. Berkani, M. Gaune-Escard</i>	
Study of the Ternary System Water/Sodium Hydroxide/Hydrazine for the Extraction of Hydrazine.....	96
<i>C. Bettan, A. El Hajj, D.M. Le, A.J. Bougrine, H. Delalu</i>	
Re-Investigation of the Binary System Phenanthrene/Anthracene	98
<i>A. Burel, N. Couvrat, S. Tisse, Y. Cartigny, G. Coquerel</i>	
Stability of Solid Phases in the Dexamethasone Acetate/Water System.....	100
<i>S. Delage, N. Couvrat, M. Sanselme, Y. Cartigny, G. Coquerel</i>	
Measurement of Carbon Dioxide Solubility in Aqueous Solution of Sodium Hydroxide from 293 to 333 K Up to 5 MPa	104
<i>P. Cézac, F. Contamine, G. Bassil, J.P. Serin, F. Lucile, O. Baudoin, D. Houssin, P. Arpentinier</i>	
Estimation of Adhesion Energy of Alumina Scales on FeCrAl Alloys: Effect of the TiO₂ Sol-Gel Coating	105
<i>R. Chegroune, M. Keddam</i>	
Purification of Artemisinin Excerpt from Artemisia Annua L	108
<i>Z. Chemat-Djenni, A. Sakhr</i>	
Experimental Determination of Liquid-Liquid Equilibrium Data and Their Representation Using the UNIQUAC and NRTL Equations.....	110
<i>S. Ghizellaoui, C. Coquelet</i>	
Vapor-Liquid Equilibrium Data Concerning Refrigerant Systems \(\backslash\)(R3110+R365mfc)	111
<i>H. Madani, A. Valtz, C. Coquelet</i>	
SLE for the Carbon Dioxide +trans-1,3,3,3-tetrafluoropropene.....	112
<i>G. Di Nicola, I. Cacciatore, M. Pierantozzi, A. Arteconi</i>	
Prediction of Thermal Properties of Ternary Systems of 2,2'oxybis[propane]⁺ benzene, toluene, cyclohexane or n-heptane	115
<i>S. Didaoui, A. Ait-Kaci</i>	
Study of the Chemical Inhibition of the Scaling of Large Agadir Water	116
<i>A. Driouiche, A. Hadfi, H. Eddaoudi, M. El Hadek</i>	
New Process of Preparation of Pyrazolidine: Synthesis, Extraction and Flow-sheet	118
<i>A. El Hajj, A.J. Bougrine, H. Delalu</i>	
Ternary Critical Point Determination of Experimental Demixion Curve: Calculation Method, Relevance and Limits	121
<i>C. Goutaudier, F. Bonnet, R. Tenu, O. Baudoin, J.J. Couniou</i>	
Determination of Acid Dissociation Constants of Some Hydroxy Schiff Bases by Ph-metric Titration. Application of the Hammett Equation	124
<i>R. Hadjeb, A. Bara, D. Barkat</i>	
Thermodynamic Excess Properties of 3,5- and 2,6-dimethylpyridine with Cyclohexane Measurement and Prediction	128
<i>H. Ben-makhlouf-Hakem, A. Ait-kaci, J. Jose</i>	
The Pretreatment of Miscanthus Using Ionic Liquids\(); A Way for Biofuel Production.....	131
<i>El-S.R.E. Hassan, F. Mutelet, J.-C. Moïse</i>	

Physical and Chemical Stability of Triethylenetetramine Dihydrochloride, an API Against Wilson's Disease	134
<i>T. Henriet, R. Rotival, C. Ghaddar, M. Choquet, Y. Cartigny, I.B. Rietveld, B. Do</i>	
Thermodynamic Optimization of the Ho-Sn System	135
<i>A. Iddaoudi, N. Selhaoui, S. Kardellass, M. Ait Amar, R. Karioui, K. Mahdouk, H. Najih, L. Bouirden</i>	
Biomass Gasification in Bubbling Fluidized Bed: Behaviour of Inorganics at High Temperature and Their Interaction with Bed Material	137
<i>J. Kaknics, R. Michel, M-L. Bouchetou, J. Poirier</i>	
Extraction of Polyphenols	138
<i>L. Loucif Seiad, R. Derriche</i>	
A Thermodynamic Analysis of the Ge-Ru System	140
<i>K. Mahdouk, A. Iddaoudi, M. Ait Amar, N. Selhaoui</i>	
Thermodynamic Assessment of the Al-Re System	141
<i>H. Najih, K. Mahdouk, A. Iddaoudi, N. Selhaoui</i>	
Enhanced Production of Unstable Polymorph by Antisolvent Crystallization Supplying Minute-Bubbles	142
<i>M. Matsumoto, Y. Wada, K. Onoe</i>	
Modeling of the Solubility of Naproxen and Trimethoprim in Different Solvents at Different Temperature	146
<i>Y. Moudjari, W. Louaer, A-H. Meniai</i>	
Determination of Experimental Excess Molar Properties for Mixtures of Carboxylic Acids	152
<i>A. Attia, F. Mutelet, R. Solimando, M. Jeday, S. Tretjak</i>	
Determination of the Surface Tension of Mixtures with Molecular Simulation	153
<i>J.C. Neyt, A. Wender, V. Lachet, P. Malfreyt</i>	
Thermodynamics Conditions for Guerbet Ethanol Reaction	154
<i>R. Olcese, M.M. Bettahar</i>	
Global Thermodynamic Behaviour of Supercritical Fluids: Example of Methane and Ethane	158
<i>A. Rizi, S. Ladjama, A. Abbaci</i>	
Nanosized Objects in Equilibrium Supercritical Fluids	162
<i>B. Sedunov</i>	
Thermodynamic Description of the Ga-Yb Binary System	168
<i>M. Idbenali, C. Servant</i>	
The Conformational Polymorphism of 1,1,2,2-tetrachloroethane ($\text{C}_2\text{H}_2\text{Cl}_4$)	172
<i>Ph. Negrier, M. Barrio, M. Zuriaga, S.C. Pérez, J.-Ll. Tamarit, D. Mondieig</i>	
Extraction of Copper and Zinc by Liquid-Membrane-Gel	173
<i>N. Taoualit, I. Abidet, D.E. Hadj-Boussaad</i>	
Experimental Determination and Prediction of Solid-Liquid Phase Equilibria for Binary $(\text{N}-\text{(2-acetoxyethyl)})-\text{p-nitroaniline}$ (1) + $\text{N-ethyle-4-nitroaniline}$ (2) Mixture	177
<i>D. Trache, K. Khimeche, R. Benelmir</i>	
Thermal Analysis of Microcrystalline Cellulose Prepared from Esparto Grass	179
<i>D. Trache, K. Khimeche, A. Donnot, R. Benelmir</i>	
Experimental Determination and Prediction of Liquid-Solid Equilibria for Binary $(\text{Methyl Palmitate} + \text{Naphthalene})$ Mixture	181
<i>M. Benziane, K. Khimeche, A. Dahmani, D. Trache</i>	
Stable, Metastable and Unstable Phases of Halogen Methane Derivatives	184
<i>J.-Ll. Tamarit</i>	
Simultaneous Thermal Analyses Under High Pressure and High Temperature: A Precious Tool for Investigation of Hydrogen Storage and Biomass Gasification	185
<i>H.-W. Marx, H. Rädel</i>	
Optimisation of the Preparation of a Phosphomagnesium Cement Based on Struvite and K-Struvite	186
<i>H. Hamm, A. Mnif</i>	
Measurement of Local Composition of Organic Materials Within Porous Inorganic Media Using Two-Dimensional Acoustic Mapping	187
<i>M. Cassiede, J.M. Shaw</i>	
Prediction of the Permeability of Polymers to Gases and Condensable Vapors	188
<i>M. Kréa, H. Hasnaoui, N. Terkmane, L.Gheraba</i>	
Relationship of Thermodynamic Properties Between Solid and Liquid States in $\text{A}^{\text{III}}\text{-B}^{\text{V}}$ Systems	189
<i>N.I. Ilinykh, V.P. Vassiliev</i>	
Heat Transfer Enhancement by Spinodal Decomposition in Micro Heat Exchangers	193
<i>S. Farisè, P. Poesio, G.P. Beretta</i>	
Modelling the Sigma Phase	199
<i>R. Mathieu, N. Dupin, J.-C. Crivello, J.-M. Joubert, K. Yaqoob, A. Breidi, J.M. Fiorani, N. David</i>	

Experimental Study of Group IVB Metals Oxicarbides.....	200
<i>F. Rejasse, O. Rapaud, N. Pradeilles, A. Maitre, G. Trolliard</i>	
New Correlative Method of Thermodynamic Analysis of the Inorganic Compounds	201
<i>V.P. Vasilyev, A.F. Taldrik, N.I. Ilinykh</i>	
On Transferring New Constant Pressure Heat Capacity Computation Methods to Engineering Practice	209
<i>S. Rajaeirad, N. Dadgostar, H. Loria, M. Satyro, J.M. Shaw</i>	
Heat Capacity Prediction of Complex Molecules by Mass Connectivity Index.....	211
<i>O. Koutchoukali, I. Haloui, M.S. Koutchoukali</i>	
Mass Transfer of Non-Polar Heavy Hydrocarbons in Aqueous Phase	215
<i>R. Nakhlé, R. Abou Naccoul, C. Goutaudier, R. Zaydan, J. Jose, J. Saab</i>	
Representation of Solid, Liquid, and Vapor Phases of Binary Lennard Jones Mixtures Using The SLV-EoS	218
<i>P. Stringari, M. Campestrini, C. Coquelet, P. Arpentinier</i>	
Phase Transitions in Porous Materials: Influence of Physico-Chemical Heterogeneities.....	224
<i>J. Puibasset</i>	
Predictive Thermodynamic Models and the Challenges of Bioprocesses.....	227
<i>J.C de Hemptinne, R. Lugo</i>	
Rimonabant Dimorphism, Much Ado About Almost Nothing.....	228
<i>M.-A. Perrin, M. Bauer, M. Barrio, J.-Ll. Tamarit, R. Céolin, I.B. Rietveld</i>	
Author Index	