



24 July 2016, Sunday

From 18:00: Welcome party in Uni CarlVogt

25 July 2016, Monday

9:00-9:30 Opening

9:30-10:15

Chairperson: **Montserrat Filella**

OPENING LECTURE

Microbes as geologic agents in the sedimentary equation

Judith Mckenzie, Switzerland

10:15-10:45

Coffee break

Session 1: DATA EVALUATION AND CONSISTENCY

Chairperson: **Dmitrii Kulik**

10:45-11:05

OC 1 George Dan Miron: Internally consistent thermodynamic data for hydrothermal mineral solubility equilibria in the system Ca-Mg-Na-K-Al-Si-O-H-C-Cl

11:05-11:25

OC 2 Cezary Gumiński: Remarks on the evaluation of complexation constants of cations with the sulfate anion

11:25-11:45

OC 3 Davide Costa: The NEA thermochemical database project: 30 years of accomplishments

11:45-12:05

OC 4 Ernst Gamsjäger: Heat capacities and entropies of molybdates and carbonates

12:05-12:25

OC 5 Simão P. Pinho: Quaternary ammonium-based deep eutectic solvents

12:25-14:00

Lunch break

Workshop: Technology-critical elements prone to hydrolysis in biological and environmental systems
(COST TD1470 workshop)

14:00-14:15

INTRODUCTION

Montserrat Filella, Switzerland

14:15-15:00

INVITED LECTURE

Learning from Ascidians about trafficking of hydrolysis-prone metals

Ann Valentine, USA

15:00-15:20

OC 6 Charlotte Ashworth: Speciation and electrochemistry of indium in aqueous sulfate and chloride solutions

15:20-15:45

Coffee break

15:45-16:30

INVITED LECTURE

Technology-critical elements Ga, In and Ln in medicinal inorganic chemistry

Chris Orvig, Canada

16:30-16:50

OC7 Montserrat Filella: Can we predict the behaviour of prone-to-hydrolysis TCEs in aqueous media of analytical, toxicological or environmental significance?

17:00-19:00 POSTER SESSION

26 July 2016, Tuesday

Session 2: IONIC LIQUIDS

Chairperson: **James Sangster**

8:30-9:15

KEYNOTE LECTURE

Gas solubility in ionic liquids: progress and prospects

Johan Jacquemin, UK

9:15-9:35

OC 8 Yizhak Marcus: Solubility parameters of room temperature ionic liquids and solubilities in them

9:35-9:55

OC 9 Takashi Makino: CO₂ absorption in ionic liquids under high-pressure conditions

9:55-10:15

OC 10 Xirong Huang: Microemulsification of hydrophobic ionic liquid to enhance enzyme solubility and catalytic performance

10:15-10:45

Coffee break

Chairperson: **Yizhak Marcus**

10:45-11:05

OC 11 Magdalena Bendová: Partition coefficients octanol-water of selected (-)-menthol-substituted chiral ionic liquids

11:05-11:25

OC 12 Jan Rotrekl: Structure-property relationships and the impact of impurities on the physico-chemical properties for novel oligoglyme-substituted ionic liquids

11:25-11:45

OC 13 Jean-Michel Andanson: Impact of the size and shape of ions on the ability of ionic liquids to dissolve cellulose

11:45-12:05

OC 14 Toshiyuki Shikata: Temperature dependent hydration behavior of chemically modified celluloses in aqueous solution

12:05-13:30

Lunch break

Workshop: Solubility in energy and waste issues of emerging concern

13:30-13:45

INTRODUCTION

Wolfgang Hummel, Switzerland

13:45-14:30

INVITED LECTURE

Fluid-rock interactions related to unconventional shale gas produced water and drilling waste

Rosemary Capo, USA

14:30-15:15

INVITED LECTURE

The effect of solubility decrease on geothermal power plant operation

Julia Scheiber, France

15:15-15:45

Coffee break

15:45-16:30

INVITED LECTURE

Numerical simulations of CO₂ sequestration in basaltic rock formations: Challenges for optimizing mineral-fluid reactions

Alexander Gysi, USA

16:30-17:15

INVITED LECTURE

Long-term behaviour of waste materials

Wolfgang Hummel, Switzerland

From 17:30 Geological excursion

27 July 2016, Wednesday

Session 3: MOLTEN SALTS AND HIGH-IONIC STRENGTH SOLUTIONS

Chairperson: **Marcelle Gaune-Escart**

8:30-9:15

KEYNOTE LECTURE

Solubility phenomena in molten salt reactor fuel

Rudy Konings, The Netherlands

9:15-9:35

OC 15 Maria Rosa González-Siso: Hydrolysis and solubility of Ni(II) under alkaline to hyperalkaline conditions and complex formation with ISA

9:35-9:55

OC 16 Glenn Hefter: Sulfur anions in alkaline solutions: some basic truths

9:55-10:15

OC 17 Olga Pestova: The scope on structure rearrangements in solution by vibration spectroscopy methods. Calcium perchlorate - water system

10:15-10:45

Coffee break

Chairperson: **Glenn Hefter**

10:45-11:05

OC 18 Artem V. Matyskin: Solubility of radium sulfate and carbonate in sodium chloride media

11:05-11:25

OC 19 Marcus Altmaier: Formation, stability and solubility of ternary Nd(III)-OH-Cl(s) phases in dilute to concentrated Na-Mg-Ca-Cl solutions

11:25-11:45

OC 20 Frank Bok: Oxygen solubility modelling in water and brines

11:45-12:05

OC 21 Ezgi Yalcintas: New comprehensive thermodynamic model for the solubility of $TcO_2 \cdot xH_2O(am)$ in the aqueous Tc^{4+} - Na^+ - Mg^{2+} - Ca^{2+} - H^+ - Cl^- - OH^- system

12:05-12:25

OC 22 Yongliang Xiong: Experimental determination of solubilities of brucite $[Mg(OH)_2(cr)]$ in Na_2SO_4 solutions with borate to high ionic strengths: formation constant for $MgSO_4(aq)$ and Pitzer interaction parameters for $MgB(OH)_4^+ - SO_4^{2-}$

From 12:25 Lunch break

From 14:00 Visit to CERN and Geneva. Informal dinner by the lake

28 July 2016, Thursday

Session 4: COMPUTER ASSISTED MODELLING

Chairperson: **Clara Magalhães**

8:30-9:15

KEYNOTE LECTURE

Computer assisted modelling (*ab initio*, molecular dynamics and Monte Carlo)

Sergey Churakov, Switzerland

9:15-9:35

OC 23 Frank Eckert: *In silico* rational solvent selection: COSMO-RS prediction of solubility, cocrystallization, and solvate formation

9:35-10:20

KEYNOTE LECTURE

An overview of novel computational methods for equilibrium and kinetic calculations

Allan Leal, Switzerland

10:20-10:45

Coffee break

Chairperson: **Wolfgang Voigt**

10:45-11:05

OC 24 Risto Pajarre: Use of kinetically constrained free energy models for concentrated aqueous systems at 25-100 °C

11:05-11:25

OC 25 Kaj Thomsen: Thermodynamic modeling of the solubility of silica

11:25-11:45

OC 26 Zdeněk Wagner: Advanced analysis of isobaric heat capacities by mathematical gnostics

11:45-12:05

OC 27 Earle Waghorne: Enthalpy – entropy compensation in solvation

12:05-12:25

OC 28 Bruno Thien: Kinetics of aqueous glass dissolution: effect of magnesium, secondary minerals and surface area

12:25-14:00

Lunch break

Session 5: SOLUBILITY AND NANOPARTICLES

Chairperson: **Dewen Zeng**

14:00-14:45

KEYNOTE LECTURE

Thermodynamics of oxide systems as a function of particle size and surface chemistry

Juro Majzlan, Germany

14:45-15:05

OC 29 Tobias Grünzel: Melting temperatures and solubilities of $\text{Zn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ nanocrystals confined in mesoporous materials

15:05-15:25

OC 30 Diana Carolina Figueroa: Solubility measurements and modeling of zinc, lead and iron sulfides at high temperatures and high pressures

15:25-15:55

Coffee break

Chairperson: **Marcus Altmaier**

15:55-16:15

OC 31 David Fellhauer: Solubility and speciation of neptunium(V) in alkaline, dilute to concentrated NaCl, MgCl_2 and CaCl_2 solutions

16:15-16:35

OC 32 Julia Sohr: Solubility of lithium sulfate and the effect of other electrolytes

16:35-16:55

OC 33 Dewen Zeng: Solubility phenomena of sparingly soluble fluoride salts in zinc hydrometallurgical systems

16:55-17:15

OC 34 Abhas Singh: Dissolution-precipitation kinetics of fluoride-bearing minerals in groundwater

17:15-17:35

OC 35 Sherali Tursunbadalov: Determination of phase equilibria in the quinary Na,K//SO₄,CO₃,HCO₃-H₂O system at 100°C

From 19:00 Gala dinner in Satigny

29 July 2016, Friday

Session 6: ORGANICS AND MIXED SOLVENTS

Chairperson: **Earle Waghorne**

8:30-8:50

OC 36 Alex De Visscher: Salting out of benzene in water: a consistency evaluation

8:50-9:10

OC 37 Mikhail Skripkin: Solid phase formation in ternary aqueous and aqua-organic saline systems

9:10-9:30

OC 38 Keith Lodge: The prediction of equilibrium and the studies of the rate of mass transfer of the solute, toluene, to and from a head space with constant composition to a stirred aqueous phase in a spectrophotometric cell

9:30-9:50

OC 39 Touba Taki: Liquid-liquid extraction of ethylene glycol from an aqueous solution with 1-hexanol alcohol

9:50-10:10

OC 40 Yan Wang: Solubility and stability of gabapentin anhydrate and hydrate in alcohol +water mixtures

10:10-10:30

Poster winner talk

10:30-11:00

Coffee break

11:00-11:45

Chairperson: **Wolfgang Hummel**

CLOSING LECTURE

Lead minerals change in pieces of art

M. Clara F. Magalhães, Portugal

11:45-12:00

Workshop closing