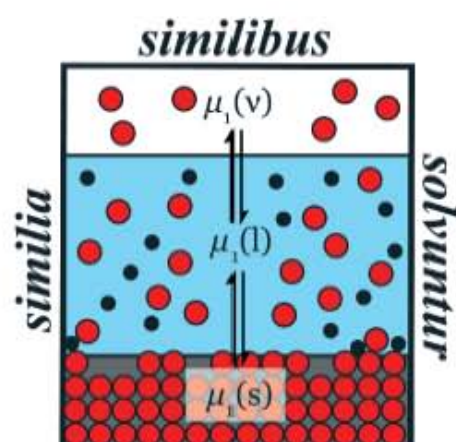


ISSP 2012



15th ISSP, Xining, 2012

Qinghai Institute of Salt Lakes, China
July 23th - 27th, 2012



Scientific Programme

SCIENTIFIC PROGRAMME

Monday, 23 July 2012

9:00-9:30 **Opening Ceremony:** Auditorium, Qinghai Institute of Salt Lakes
Vice Governor, Qinghai Province
Heinz Gamsjäger, IUPAC Representative
M. Clara Magalhães, Chair SSED (IUPAC)
Haizhou Ma, Director of Qinghai Institute of Salt Lakes
Dewen Zeng, Co-chair 14th ISSP

Chairperson: **Dewen Zeng**, Qinghai Institute of Salt Lakes, Xining, China

9:35-10:25 Plenary Lecture
Heinz Gamsjäger, Montanuniversität Leoben, Leoben, Austria
“SOLUBILITY PHENOMENA IN SCIENCE AND EDUCATION–EXPERIMENTS,
THERMODYNAMIC ANALYSES AND THEORETICAL ASPECTS”

10:25-10:45 *Coffee break*

Chairperson: **Wolfgang Voigt**, TU Bergakademie Freiberg, Germany

10:45-11:35 Plenary Lecture
Erich Königsberger, Murdoch University, Murdoch, Australia
“SOLID–SOLUTE PHASE EQUILIBRIA IN AQUEOUS SOLUTION –
FUNDAMENTALS AND APPLICATION”

11:35-12:15 Invited Lecture
Irina Zvereva, Saint-Petersburg State University, Saint-Petersburg, Russia
“SOLID SOLUTIONS OF LAYERED OXIDES WITH RARE EARTH ELEMENTS”

12:15-12:40 **Jianxin Chen**, Engineering Research Center of Seawater Utilization Technology,
Ministry of Education, Tianjin, China
“SOLUBILITY CHANGE OF THE TERNARY SYSTEM KCl–NH₄Cl–H₂O FROM
15 °C to 65 °C”

12:40-14:00 *Lunch break*

Chairperson: **Wolfgang Voigt**, TU Bergakademie Freiberg, Germany
Kaj Thomsen, Technical University of Denmark, Kongens Lyngby, Denmark

Peiming Wang, OLI Systems, Inc., Morris Plains, U.S.A.

“MODELING MIXED SOLVENT ELECTROLYTE SYSTEMS: PHASE BEHAVIOR, CHEMICAL EQUILIBRIA, AND TRANSPORT PROPERTIES”

14:40-15:05 **Alexander Toikka**, Saint-Petersburg State University, Russia

“SOLUBILITY, CRITICAL STATES AND THERMODYNAMIC PECULIARITIES OF MULTICOMPONENT REACTIVE LIQUID–LIQUID SYSTEMS”

15:05-15:30 **Kazuhiro Tamura**, Kanazawa University, Kanazawa, Japan

“SOLUBILITY OF THREE–PRIMARY–COLORS DISPERSE DYES AND THEIR BLENDS IN SUPERCRITICAL CARBON DIOXIDE”

15:30-15:55 **Igor Sedov**, Kazan Federal University, Kazan, Russia

“SOLUBILITY AND SOLVOPHOBICITY PHENOMENA IN SELF-ASSOCIATED SOLVENTS”

15:55-16:15 *Coffee break*

16:15-16:40 **Stefan Schlosser**, Slovak University of Technology, Bratislava, Slovakia

“PARTITIONING OF ORGANIC ACIDS INTO THE SOLVENTS WITH IONIC LIQUIDS AND THEIR RHEOLOGY”

16:40-17:05 **Ming-Jer Lee**, National Taiwan University of Science and Technology, Taipei, Taiwan

“PHASE BEHAVIOR OF AQUEOUS MIXTURES OF TETRAHYDROFURAN WITH BIOLOGICAL BUFFER HEPES”

17:05-17:30 **Simão Pinho**, Universidade de Aveiro, Aveiro, Portugal

“EXPERIMENTAL AND MOLECULAR DYNAMICS SIMULATION STUDIES ON THE SOLUBILITY OF AMINO ACIDS IN AQUEOUS ELECTROLYTE SOLUTIONS”

17:30-17:55 **Hiroyuki Matsuda**, Nihon University, Tokyo, Japan

“SOLUBILITIES OF POORLY WATER–SOLUBLE DRUGS AND ENHANCEMENT OF THEIR SOLUBILITIES BY ADDING CO-SOLVENTS”

17:55-18:20 **Ago Ken-ichi**, Hosei University, Tokyo, Japan

“PREDICABILITY OF SETCHENOV COEFFICIENTS IN FLUOROCARBON–ALCOHOL–NaOH SYSTEMS WITH THE GROUP CONTRIBUTION METHOD”

18:20-20:00 *supper*

- O28 **L.I.N. Tomé¹, S.P. Pinho², M. Jorge³, J.R.B. Gomes¹, J.A.P. Coutinho¹**
¹Universidade de Aveiro, Aveiro, Portugal
²Instituto Politécnico de Bragança, Campus de Santa Apolónia, Bragança, Portugal
³Faculdade de Engenharia da Universidade do Porto, Porto, Portugal
- EXPERIMENTAL AND MOLECULAR DYNAMICS SIMULATION STUDIES ON THE SOLUBILITY OF AMINO ACIDS IN AQUEOUS ELECTROLYTE SOLUTIONS
- O29 **H. Matsuda**
Nihon University, Japan
- SOLUBILITIES OF POORLY WATER-SOLUBLE DRUGS AND ENHANCEMENT OF THEIR SOLUBILITIES BY ADDING CO-SOLVENTS
- O30 **K. Ago, H. Nishiumi**
Hosei University, Tokyo, Japan
- PREDICABILITY OF SETCHENOV COEFFICIENTS IN FLUOROCARBON-ALCOHOL-NaOH SYSTEMS WITH THE GROUP CONTRIBUTION METHOD
- O31 **W.E. Waghorne**
University College Dublin, Dublin, Ireland
- WHAT IS SOLVENT BASICITY?
- O32 **E. Furiá, A. Napoli, G. Sindona, A. Tagarelli**
University of Calabria, Arcavacata di Rende (CS), Italy
- SOLUBILITY MEASUREMENTS FOR DETERMINATION OF EQUILIBRIUM CONSTANTS IN AQUEOUS SOLUTION
- O33 **J. Jirsák^{1,2}, J. Škvor¹, I. Nezbeda^{1,2}**
¹J. E. Purkinje University in Ústí n. L., Ústí n. L., Czech Republic
²Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, Prague, Czech Republic
- A MOLECULAR MODEL FOR AQUEOUS SOLUTIONS OF NONPOLAR FLUIDS
- O34 **T.P. Krishna Murthy, B. Manohar**
Central Food Technological research Institute, Mysore, India
- SOLUBILITY OF BIOACTIVE COMPONENTS OF MANGO GINGER (CURCUMA AMADA ROXB) IN SUPERCRITICAL CARBON DIOXIDE

C: ORAL PRESENTATION

EXPERIMENTAL AND MOLECULAR DYNAMICS SIMULATION STUDIES ON THE SOLUBILITY OF AMINO ACIDS IN AQUEOUS ELECTROLYTE SOLUTIONS

Tomé¹ L.I.N., Pinho² S.P., Jorge³ M., Gomes¹ J.R.B. and Coutinho¹ J.A.P.

¹CICECO Departamento de Química, Universidade de Aveiro, 3810-193 Aveiro, Portugal, e-mail: jcoutinho@ua.pt

²LSRE/LCM-Laboratory of Separation and Reaction Engineering, Escola Superior de Tecnologia e de Gestão, Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5301-857, Bragança, Portugal, e-mail: spinho@ipb.pt

³LSRE/LCM-Laboratory of Separation and Reaction Engineering, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal, e-mail: mjorge@fe.up.pt

Separation and concentration of biological compounds are current subjects of interest due to their high cost in comparison to the total manufacture cost. For that purpose electrolytes may be employed as they can affect significantly biochemicals solubilities, a feature that has been used for salt-induced precipitation of proteins. Even if amino acids are among the simplest biochemicals they present many similarities with more complex molecules and are the building blocks of proteins [1]. Despite its importance, however, the experimental information available concerning salt effect on the amino acids solubilities is still very scarce and the molecular-level mechanisms for its theoretical interpretation are far from resolved [2].

In this work, the shake-flask method was combined with density measurements to provide new experimental data for the solubility of dl-alanine, l-isoleucine and l-valine in aqueous solutions of MgCl₂ or MgSO₄, at different electrolyte molalities and 298.15 K. Both salts showed to be salting-in agents, but a more pronounced effect was observed for MgCl₂. Regarding the magnitude of the salting-in in the whole salt molality range (up to 2 molal), for the same aqueous electrolyte solution, a definite trend was not possible to establish for the three different amino acids studied.

Aiming at further understanding the molecular interactions governing the behaviour of these systems, molecular dynamics simulations were performed for aqueous solutions of alanine, valine and isoleucine in the presence of MgCl₂, MgSO₄, NH₄Cl and (NH₄)₂SO₄, at T=298.15 K and different concentrations. The combined analysis of the thermodynamic data and of the radial distribution functions of the various groups and moieties, as well as of their respective energy of interaction, enabled to clarify the role of the cation on the solubility effects promoted by the salts, and to provide a molecular interpretation for the experimental data based on a balance between competitive interactions established by the ions and the other species present in solution.

References

- [1] Ferreira L.A., Macedo E.A., Pinho S.P., The Effect of Ammonium Sulfate on the Solubility of Amino Acids in Water at 298.15 and 323.15 K, *J. Chem. Thermodyn.*, **41**, (2009) 193–196.
- [2] Tomé L.I.N., Jorge M., Gomes J.R.B., Coutinho, J.A.P., Towards an understanding of the aqueous solubility of amino acids in the presence of salts: A molecular dynamics simulation study, *J. Phys. Chem. B*, **114**, (2010) 16450–16459.