

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY  
Analytical Chemistry Division  
SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA (SSED)

**Minutes**

**6<sup>th</sup> Annual Meeting of SSED (33<sup>rd</sup> overall)  
held in conjunction with the  
44<sup>th</sup> GA  
at the Università di Torino, Politecnico di Torino, Lingotto  
Complex, Torino, Italy  
6 August 2007**

The "List of Attendees" with complete addresses, telephone and fax numbers together with e-mail addresses is attached to these minutes (Appendix 1)

Monday, 6 August 2007

**Morning Session:** 9:00 - 12:00

- 1. Welcome of participants (Full List of Participants is in Appendix 1)** H. Gamsjäger  
Heinz Gamsjäger, Chairman of the SSED welcomed the participants. All of the participants were requested to introduce themselves together with their affiliation
- 2. In Memoriam Thedford Dirkse,** H. Gamsjäger  
Professor Gamsjäger presented a warm tribute to our former colleague Professor Thedford (Ted) P. Dirkse who passed away on October 23, 2006. Dr. Dirkse has been a long time contributor to the Solubility Project. An "In Memoriam" was published in *Chemistry International* 29, No.2, 2007 p.15. A copy of the slide used by Dr. Gamsjäger is given in Attachment A.2.
- 3. Approval of the Minutes of the 32<sup>nd</sup> Annual Meeting (5<sup>th</sup> of SSED) in conjunction with the 12<sup>th</sup> ISSP at the TU Bergakademe, Freiberg, Germany, 22-23 July 2006** R. Tomkins  
The minutes had been distributed by e-mail prior to the meeting and also distributed as hard copies at the meeting. The minutes were approved as presented.
- 4. Other Items for the Agenda** H. Gamsjäger  
It was suggested that discussions should take place on the Stability Constants Data Base concerning metal humic binding constants as 12 (a) on the Agenda. Also, a report on the Solution Chemistry Conference held in Perth, Australia in 2006 should perhaps be given by Earle Waghorne as part of item 14 on the Agenda.

## 5. Franzosini Award

H. Gamsjäger

Since the restructuring of IUPAC activities in 2001 the even year annual meetings of the Solubility Data Group have become better attended than the odd year ones. This is due to the fact that the even year meetings are organized in conjunction with the biennial ISSPs, the main scientific event of this group.

Therefore it has been proposed to award the Franzosini Prize also biennially at the even year meeting. The members of the Solubility Data Group present in Turin were in favor of the rearrangement to award 1 prize every two years. Daniela Freier (Freiberg, Germany) designed a certificate for the Franzosini Prize winner 2006, Prof. Dewen Zheng. It is recommended to use analogous certificates for future prize winners. A copy of the Award Certificate is in Attachment A.3.

### Action Item

It was recommended that a procedure for nomination should be formulated and the award nomination should be advertised appropriately. Both potential contributors to the Solubility project as well as contributors to the Equilibrium Data project should be targeted for nomination.

## 6. Chairman's Report for 2006 - 2007 (Full Report is in Appendix, Attachment A.4)

H. Gamsjäger

### a) Visibility of SSED within IUPAC 2006/2007

Dr. Gamsjäger cited several examples of items that have appeared in Chemistry International during the past year. In particular articles by Maria Clara Magâlhaes [Art and Science: Looking in the same direction] and Trevor Letcher [Solubility and Thermodynamic properties related to environmental issues] were highlighted.

### b) IUPAC Poster Prize Recipients

The three winners of the IUPAC Poster Prizes received at the 12<sup>th</sup> ISSP 2006 in Freiberg, Germany were noted. Details of the poster topics are given in the full report (Appendix 4) Dr. Margarida Costa Gomes indicated that she was one of the authors contributing to "Developments and Applications in Solubility", Trevor Letcher (editor).

### c) 12<sup>th</sup> ISSP

Four of the seven plenary and invited lectures as well as a summary report on the workshop given at the 12<sup>th</sup> ISSP in Freiberg, Germany have been published in Pure and Applied Chemistry, **79**, No. 5 (2007), pp. 825-894.

### d) Books

John Wiley has published two books edited by Trevor Letcher during 2006/2007. The titles are "Developments and Applications of Solubility" and "Thermodynamics, Solubility and Environmental Issues". Several active members of the SSED contributed to both books.

### e) Completed SDS volumes

Volumes 81 (parts 9-12), 82 (parts 1-5) and 83 have now been published

### f) Completed SDS Projects

The problem with the transfer from LaTeX to Word for the Hiroshi Miyamoto project [Project No. 2005-033-1-500] was discussed but no final recommendation for a quick resolution was forthcoming. Some attendees felt that this should not be a problem and wondered why the journal editors could not cope with this.

Action Item: A resolution to this problem is urgently needed.

### g) Current SDS Projects

Heinz Gamsjäger presented brief updates on 12 ongoing projects. For the project# 2006-032-1-500, Solubility data related to industrial processes. Mutual Solubility of ethers and ketones in water by Marian Góral a decision needs to be made as to whether it should be presented as 1 or 2 volumes. In general for large volumes the question was raised as to whether it is possible to submit in several parts or does it have to be one volume for one project.

Action item: The Editor-in-Chief [M. Salomon] needs to discuss this (splitting volumes into parts) with the journal editor.

Heinz Gamsjäger commented that all cases of volume splitting have to be discussed with the EIC and that one volume on ethers and one on ketones will almost certainly be acceptable. (In discussions between M. Salomon and the new editors of JPCRD, there is some reluctance on dividing large volumes into numerous parts. However, and particularly for very large volumes and upon recommendation of the Editor-in-Chief and the SSED, the editors of JPCRD have agreed to publish selected volumes in several parts. The decision to split volumes into several parts is thus the responsibility of the SSED. Authors should not enter into direct correspondence on this matter with the JPCRD editors. This would certainly result in delayed publication and possible changes in the peer reviewing procedures which are presently the responsibility of the SSED.)

**h) New SDS projects**

Three new projects were outlined.

**i) 13<sup>th</sup> ISSP [International Symposium on Solubility Phenomena and Related Equilibrium Processes]**

The 13<sup>th</sup> ISSP will be organized at the University College, Dublin, Ireland under the Chairmanship of Dr. Earle Waghorne. The conference is planned for July 27-31, 2008.

Action Item: The date needs changing from 2007 to 2008 in the Full Report [Appendix 4]. Also the conference should be listed in Chemistry International

## **7. SSED Officers**

Professor Gamsjäger announced that his term as Chairman of the SSED had expired and his replacement is Professor Dana E. Knox. In addition Dr. Earle Waghorne will replace Dr. Knox as the Secretary.

The makeup of the complete Subcommittee is given below:

Subcommittee on Solubility and Equilibrium Data (2008-2009)

Prof. Dana E. Knox (Chairman g-liq Chair)

Dr. Wolfgang Hummel (link to environmental applications)

Prof. Earle W. Waghorne (Secretary)

Prof. Erich Königsberger (link to industrial applications)

Prof. John W. Lorimer (Terminology, Nomenclature and Symbols)

Dr. Mark Salomon (EIC)

Prof. David G. Shaw (liq-liq Chair)

Prof. Wolfgang Voigt (sol-liq Chair)

Dr. Hans Wanner (link to former Com. V.6, Equilibrium Data)

Action Item:

(Dr. Hans Wanner resigned 11-01-2007, and no decision regarding a successor has yet been made.)

**8. - 10. Editor-in-Chief's Report for 2006-2007** M. Salomon

Dr. Salomon was unable to attend the meeting but submitted a report which is attached (Attachment A.5). The status of three manuscripts from 2006 is included in the report. New formatting guidelines for JPCRD are included in the report and examples of editorial changes made by the journal editor Dr. Malcolm Chase for three submitted 2007 articles are also part of Attachment A.5. These changes consisted of combining two small tables within a page; making the title part of the table and imbedding the references for a 'page' as part of the text in the Auxiliary Information section.

The key features (see attachment A.6) for new formatting guidelines for the journal are:

- AIP (American Institute of Physics) has switched to a portrait style publication
- Significant changes in reporting references to introduce a "cumulative set of References" is recommended
- The current electronic format that is being used is acceptable to AIP

Concerns were expressed about frequent changes in the format which involved extra work for those contributors who were in the middle of a volume preparation.

Action Item:

We need to know (via Mark Salomon) whether the proposed new formatting guidelines should only come into effect for future volumes and not for those currently in progress (at least for those volumes where a substantial amount of material has already been prepared (i.e. volumes submitted in 2005/2006). (M. Salomon subsequently noted that relative to agenda item 9 - Volumes for next year's SDS proposal - there were no firm commitments at this time. He also revised Attachment A.6, adding items 4 and 5, in response to this Action Item...)

**Afternoon Session: 14:00 - 17:00**

**11. Status of NIST Funding**

H. Gamsjäger

Dr. Mark Salomon will be instrumental in negotiating a new contract with NIST. In order for the renewal of the contract to be successful certain guidelines must be established. The following are critical.

- SSED members must commit themselves to produce SDS volumes
- A need exists for a realistic estimation of how many volumes can be produced per year. In the past 9 years from 1998 through 2007 a total of 17 volumes (no. 66-83) have been published. Members felt that 2 volumes per year should be promised for the next 3 years [The Phantom proposals will then essentially be completed]
- Submissions to JPCRD must be in MS Word with the formats that are currently in place with JPCRD

**12. Solubility Constant Database Project**

H. Gamsjäger

Dr. Gamsjäger referred to the Metal Humic Binding Constants Database proposed by Dr. Filella (Switzerland). The Equilibrium group is looking for endorsement of this project from the SSED.

### Action Item

Dr. Wolfgang Hummel should be contacted with the recommendation that Dr. Filella prepare a project submission form indicating that the project contains worthwhile work concerning the absorption of trace metals in nature. The project needs to be well defined.

(Subsequent e-mails have been sent to Dr. Filella and Prof. Lobinski, 2 Oct, and PD Dr. Hummel, 13 Oct)

### **13. Report of Glossary Task Group**

Professors John W. Lorimer, David G. Shaw and Dr. Pirketta Scharlin were not present at the meeting and no discussion took place on this topic. H. Gamsjäger reported, however, that Provisional Recommendations to Glossary of terms related to solubility are under review by ICTNS and were open to comments until 31 July 2007.

### **14. Report on the 14<sup>th</sup> ISSP-Dublin, Ireland, 2008**

E. Waghorne

Dr. Waghorne reported that to date six invited/plenary lectures had been contacted. E Königsberger and J-P Grolier had made firm commitments. The cost of registration should not exceed 400 euros. Refurbishment of lecture halls at the university was on-going. A parallel workshop on Equilibrium Constant projects was planned. Some of the suggested topics were:

- Biological applications
- Modeling
- Interfacing with industry

### **15. Future International Symposia on Solubility Phenomena 2010, 2012.**

A suggestion for the next ISSP has been put forward by V. Valyashko to be held in Russia at a suburb of St. Petersburg called Repino, see Attachment A.11. Repino is located approximately 30 kilometers northwest of the main portion of Saint Petersburg. No details concerning traffic connections between Repino and St. Petersburg have been available so far. In addition a possibility exists to have the symposium in New Jersey if not in 2010 then in 2012. Both venue offers, which SSED is very grateful for, should be presented at the 7<sup>th</sup> AM in Dublin. There many more members of the group will be involved in the decision than was possible in Turin.

### **Other items:**

#### **1. Teamwork between ACD [Analytical Chemistry Division and SSED.**

One of the most important messages resulting from the discussion within ACD was that cooperation of SSED with the rest of Div. V should be intensified. It was strongly recommended that the incoming chairman of SSED, Dana Knox should attend the Division V meeting in February tentatively scheduled for a city in Austria. [Subsequent to the meeting in Turin it is now known that the ACD meeting will be held in Rome early in 2008] A workshop on "Traceability of Solubility and Equilibrium Data" plus a round table discussion will be organized by H. Gamsjäger. Several items of relevance to SSED should be discussed at the ACD meeting including:

- Funding
- Participation of ACD members in ISSP'S & SSED and vice-versa

- Visibility of membership within IUPAC
- Formation of Advisory groups
- A follow up on a Glossary of Supersaturation (Subsequent to the meeting it has turned out that a project "Updates and revisions of introductions to gas-liquid, liquid-liquid and solid-liquid solubility" would be more important and easier to devise.)
- New projects such as "analysis & solubility of inorganic compounds", for example, Solubility of inorganic arsenic compounds and their analysis.

#### Action Items

1. Need to firm up the attendance and invitation of Dr. Dana Knox to the ACD meeting.
2. We need to know the status of the proposal by Marian Góral on the project involving esters in water (update: the Project Submission Form sent on Sep 25, 2007)
3. We need to have a definite completion data for Project Number: 2002-036-1-500- Solubility of hydroxybenzoic acids and hydroxybenzoates, by A. Goto and H. Miyamoto. Dana Knox should look into this. (update: according to email from Sep 21, 2007 to H. Gamsjäger, A. Goto plans to finish this task by the end of Mar, 2008.)

#### Discussion of Subcommittees

##### **Subcommittee: Gas Solubilities**

D. Knox

Dr. Knox provided a written report on the status of three projects. A summary is attached [Attachment A.8]

##### **Subcommittee: Liquid Solubilities**

D. Shaw

Report is attached [Attachment A.9]

##### **Subcommittee: Solid Solubilities**

W. Voigt

Report is attached [Attachment A.10]

**Attachment  
A.1**

Attendees at the Meeting

**AKHYAR Farrukh, Dr. N.**

Pakistan Council for Science and Technology, Shahrah-e-Jamhuriat G-5/2, Islamabad, Pakistan

T: +92 51 9205157

F: + 92 519205171

EMAIL: akhyar100@yahoo.com

**BALAREW, Prof. Christo**

Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G.

Bonchevistr Bl 11, 1113 Sofia Bulgaria

Tel: +359 (2) 979-3925

Fax: +359 (2) 870-5024

Email: [balarew@svr.igic.bas.bg](mailto:balarew@svr.igic.bas.bg)

**COSTA GOMES, Dr. Margarida**

Laboratoire Thermodynamique des Solutions et Polymères, CNRS/ Université Blaise Pascal,  
Clermout-Ferraud, France

T: +33473407205

F: +33473405328

Email: [margarida.c.gomes@univ-bpclermont.fr](mailto:margarida.c.gomes@univ-bpclermont.fr)

**EYSSELTOVA, Dr. Jitka**

Department of Inorganic Chemistry, Charles University, Faculty of Science, Albertov 2030

Prague 12840, Czech Republic

Tel: 420 (2) 8198-2637

Email: [jeyss@seznam.cz](mailto:jeyss@seznam.cz)

**GAMSJÄGER, Prof. Heinz**

Lehrstuhl für Physikalische Chemie, Montanuniversität, Leoben, Franz-Josef-Strasse 18, Leoben  
8700, Austria

Tel: +43 (3842) 402-4804

Fax: +43 (3842) 402-4802

Email: [gamsjaeg@unileoben.ac.at](mailto:gamsjaeg@unileoben.ac.at)

**GÓRAL, Dr. Marian**

Institute of Physical Chemistry, Polish Academy of Sciences, 44/52 Kasprzaka, 01-224 Warsaw,  
Poland

Tel: +48 509 301559

Email: [mgoral@ichf.edu.pl](mailto:mgoral@ichf.edu.pl)

**GUMINSKI, Dr. Cezary**

Department of Chemistry, University of Warsaw, Pasteura 1, 02093 Warszawa, Poland

Tel: +48 (22) 8220211, ext. 331

Fax: +48 (22) 8225996

Email: [cegie@chem.uw.edu.pl](mailto:cegie@chem.uw.edu.pl)

**MACZYNSKI, D. Andrzej**

Institute of Physical Chemistry, Polish Academy of Sciences, 44/52 Ksaprza, 01-224 Warsaw, Poland

Tel: 48 608033360

Email: [macz@ichf.edu.pl](mailto:macz@ichf.edu.pl)

**MAKINO, Dr. Masakazu**

Institute for Environmental Sciences, University of Shizuoka, 52-1 Yada Suruga, Shizuoka 422-8526, Japan

Tel: +81 (54) 264 5785

Fax: + 81 (54) 264-5785

Email: [makinom@u-shizuoka-ken.ac.jp](mailto:makinom@u-shizuoka-ken.ac.jp)

**TOMKINS, Prof. Reginald**

Department of Chemical Engineering, New Jersey Institute of Technology, University Heights, Newark, NJ 07102

Tel: 973 596 5656

Fax: 973 596 8436

Email: [tomkinsr@njit.edu](mailto:tomkinsr@njit.edu)

**VOIGT, Prof. Wolfgang**

Institut für Anorganische Chemie, TU Bergakademie Freiberg, Leipziger Strasse 29, D-09596 Freiberg, Federal Republic of Germany

Tel: +49 (3731) 394338

Fax: + 49 (3731) 394058

Email: [wolfgang.voiqt@chemie.tu-freiberg.de](mailto:wolfgang.voiqt@chemie.tu-freiberg.de)

**WAGHORNE, Prof. Earle W.**

School of Chemistry and Chemical Biology, University College Dublin, Belfield, Dublin 4, Ireland

Tel: +353 (1) 706-2132

Fax: +353 (1) 706-2415

Email: [earle.waghorne@ucd.ie](mailto:earle.waghorne@ucd.ie)



## Attachment

### A.2

#### Item 2 on the Agenda

#### In Memoriam: Prof. Thedford P. Dirkse

##### **In memoriam Prof. Thedford P. Dirkse**

Jitka Eysseltova told me the sad news that our colleague and friend, Professor Thedford Dirkse, died on October 23, the previous year.

I still remember Ted as a very active participant of the 7th International Symposium on Solubility Phenomena 1996, which was held in Leoben, Austria. Only nine years ago he co-authored and co-edited with Jitka Solubility Data Series volume 66.

The Solubility Data Group deeply mourns the death of its most senior member. We remember Ted with great affection and admiration.

An "In memoriam" was published in *Chemistry International* **29**, No. 2, 2007 p. 15



May 11, 1999: Dirkse Honored at Calvin

Attachment  
A.3  
Certificate for Franzosini Award

*Franzosini Award*

FOR

**Prof. Dr. Dewen Zeng**

FROM





**Hunan University,  
China**

12<sup>th</sup> ISSP - Freiberg - Germany, 2006

Prof. Dr. Heinz Gamsjäger  
CHAIR OF SSED

*Heinz Gamsjäger*

الإغلاية  
Solubilität  
Löslichkeit  
Растворимость  
Solubilität  
溶解度  
растворимость  
Oploselijkheid  
الذوبانية  
Solubilité  
Löslichkeit  
Διολυτότητα  
растворимость  
الإغلاية  
Rozpuszczalność  
Solubilitate  
Растворимость  
- HALLENÉ  
قابلية الذوبان



## Attachment

### A.4

Chairman's Activity Report 2006-2007

## SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

Chairman's Activity Report 2006 - 2007

### 1. Visibility of SSED within IUPAC 2006/2007

CI, 28, No. 2, March-April 2006

#### Features

p. 4 Maria Clara F. Magalhães, Rosa Maria Oliveira, "Art and Science: Looking in the same direction" (Exhibition at 11<sup>th</sup> ISSP)

CI, 28, No. 5, September-October 2006

#### The Project Place

p. 23 Trevor M. Letcher, (Task Group Chairman, Interdivisional (I, V and VI project), Solubility and thermodynamic properties related to environmental issues. Many contributors are members of Solubility Data Group

CI, 28, No. 6, November-December 2006

#### IUPAC Wire

p. 23: Dewen Zeng (Hunan University, Changsha, China) receives the 2006 Franzosini Award.

CI, 28, No. 6, November-December 2006

#### Conference Call

p. 30: "Solubility Phenomena" (and workshop: Quality assurance in thermodynamic databases for performance assessment studies in waste disposal), Conference Report 12<sup>th</sup> ISSP by Heinz Gamsjäger and Wolfgang Voigt

IUPAC Poster Prize Recipients-12<sup>th</sup> SSP 2006-Freiberg, Germany

Alexander S. Lileev (N.S. Kurnakov Institute of General and Inorganic Chemistry of Russian Academy of Sciences, Russia) "Non-additivity of contributions into the dielectric constant of saturated solutions and ion-ion interactions in ternary water-salt systems".

Sven Hagemann (Gesellschaft für Anlagen- und Reaktorsicherheit, Germany) "A new simple method for the investigation of hydrogen sulfide solubilities in aqueous solution".

Georgia Wollmann (Institute of Inorganic Chemistry, TU Bergakademie Freiberg, Germany) "Solubilities related to substituted polyhalites"

CI, 29, No. 2, March - April 2007

#### In memoriam

p. 15 Prof. Thedford P. Dirkse (USA)—Member, Subcommittee on Solid Solubilities, 2000-2001 and 1981-1993; Associate Member, Commission on Solubility Data, 1987-1993. (Died on 23 October 2006.)

CI, 29, No. 3, May - June 2007

#### Provisional Recommendations

p. 24 "Glossary of terms related to solubility", Comments by 31 July 2007, David G. Shaw

#### Bookworm

p. 27 Trevor M. Letcher (editor) "Developments and applications in solubility", The Royal Society of Chemistry, 2006. Rubin Battino, Larry Clever, Glenn Hefter, Wolfgang Hummel, Erich Königsberger, Justin Salminen, Reg Tomkins, Wolfgang Voigt, and Earle Waghorne, members of the Solubility Data Group, contributed to this volume.

**CI**, 29, No. 4, July - August 2007

**Provisional Recommendations**

p. 25 "Glossary of terms related to solubility", Comments by 31 July 2007, David G. Shaw

**Bookworm**

p. 30 Trevor M. Letcher (editor) "Thermodynamics, solubility and environmental issues", Elsevier, 2007. Erich Königsberger, Clara Magalhães and Justin Salminen, members of the Solubility Data Group, contributed to this volume.

**Pure and Applied Chemistry**, 79, No. 5 (2007)

**12th International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP-12), 23-28 July 2006, Freiberg, Germany**

Preface, Earle Waghorne, p. iv

(1) Solubility of salts in water: Key issue for crystal growth and dissolution processes, Petros G. Koutsoukos, Aikaterini N. Kofina, and Dimitra G. Kanellopoulou, p. 825

(2) Li-air batteries: A classic example of limitations owing to solubilities, Ian Kowalczyk, Jeffery Read, and Mark Salomon, p. 851

(3) High-pressure investigations of solubility, Seiji Sawamura, p. 861

(4) Solubility data in radioactive waste disposal, Hans Wanner, p. 875

(5) Quality assurance in thermodynamic databases for performance assessment studies in waste disposal, W. Voigt, V. Brendler, K. Marsh, R. Rarey, H. Wanner, M. Gaune-Escard, P. Cloke, Th. Vercouter, E. Bastrakov, and S. Hagemann, p. 883

**2. New Books**

**Biominerization - Medical Aspects of Solubility**, John Wiley & Sons, Ltd.

Erich Königsberger (editor), LanChi Königsberger (co-editor)

ISBN: 0-470-09209-2

Hardcover

302 pages

September 2006

Chapter 1 "Solubility phenomena related to normal and pathological biominerization processes"

Erich Königsberger and LanChi Königsberger (authors)

Chapter 3 "Calcium and magnesium phosphates: normal and pathological mineralization"

M. Clara F. Magalhães, Paula A. A. P. Marques and R. N. Correia

**Developments and applications in solubility**, The Royal Society of Chemistry

Trevor Letcher (editor)

ISBN 0 85404 372 1; ISBN-13 978 085404 372 9

..... 20006

**Thermodynamics, Solubility and Environmental Issues**, Elsevier.

Trevor Letcher (editor)

ISBN-13: 978-0-444-52707-3; ISBN-10: 0-444-52707-9

..... 20007

### 3. Completed SDS Volumes

Volume **81**: Andrzej Maczynski, David G. Shaw (editors),

"**Hydrocarbons with Water and Seawater - Revised and Updated**,"

J. Phys. Chem. Ref. Data, **2006**, 35, No. 1, parts 9 and 10 (pp. 93-203).

J. Phys. Chem. Ref. Data, **2006**, 35, No. 2, parts 11 and 12 (pp. 785-838).

Volume **82**: Andrzej Maczynski, David G. Shaw (editors),

"**Alcohols with Water—Revised and Updated: C<sub>4</sub>- C<sub>7</sub> Alcohols with Water**,"

J. Phys. Chem. Ref. Data, **2007**, 36, No. 1, parts 1 and 2 (pp. 59-190).

J. Phys. Chem. Ref. Data, **2007**, 36, No. 2, parts 3 and 4 (pp. 399-484).

J. Phys. Chem. Ref. Data, **2007**, 36, No. 3, part 5 (pp. 685-731).

Volume **83**: Valerii Sazonov, David G. Shaw (editors),

" **Acetonitrile: Ternary and Quaternary Systems**,"

J. Phys. Chem. Ref. Data, **2007**, 36, No. 3, 733-1131.

### 4. Completed SDS Projects

Project number: 2002-025-1-500

Project Title: **Inorganic Actinide Compounds**

Task Group Leader: Jiri Hala

Starting date: 2002

Report: Project completed in November 2005, is at AIP, page proofs are not ready, SDS vol. 84

Project number: 2005-033-1-500

Project Title: **Transition and 12 to 14 Main Group Metals, Lanthanide, Actinide and Ammonium Halates**

Task Group Leader: Hiroshi Miyamoto

Starting date: 2002

Report: Project has been completed in December 2005, is being converted from LaTeX to Word, SDS vol. 85

### 5. SDS Projects in progress

Project number: 2002-031-1-500

Project Title: **Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates**

Task Group Leader: Alex De Visscher

Starting date: 2002

Report: Projected completion date (documents ready for external review): Spring 2008

Project number: 2002-032-1-500

Project Title: **Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb)**

Task Group Leader: Heinz Gamsjäger

Starting date: September 2003

Report: Projected completion date (documents ready for external review), summer 2008

Project number: 2002-035-1-500

Project Title: **Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis**

Task Group Leader: E. Königsberger and L.-C. Königsberger

Starting date: 2002

Report: Projected completion date (documents ready for external review): mid-2008

Project Number: 2002-036-1-500

Project Title: **Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates**

Task Group Leader: Ayako Goto and Hiroshi Miyamoto

Starting Date: 2002

Report: Projected completion data(documents ready for external review: March 2008

Project Number: 2002-037-1-500

Project Title: **Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons**

Task Group Leader: Masakazu Makino and Ayako Goto

Starting Date: 2002

Report: Project completion date(documents ready for external review): end of 2007 or 2008.

Project number: 2002-044-1-500

Project Title: **Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions.**

Task Group Leader: Pirketta Scharlin

Starting date: September 16, 2002

Report: It is difficult to foretell completion date.

Project number: 2002-045-1-500

Project Title: **Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide.**

Task Group Leader: Dana Knox

Starting date: 2002

Report: earliest completion date would be early 2008.

Project number: 2005-006-1-500

Project Title: **Mutual Solubility of Alcohols and Water (update of SDS Vol 15)**

Task Group Leader: Andrzej Maczynski

Starting date: January 1, 2005



Report: Four articles (Parts 1- 4) have been published in the Journal of Physical and Chemical Reference Data, one (Part 5) is in print.

Project number: 2005-017-1-500

Project Title: **Glossary of terms related to solubility – Updates and revisions to the Orange Book**

Task Group Leader: DG Shaw

Starting date: July 2005

Report: Glossary under review by ICTNS: Comments by 31 July 2007

Project number: 2006-032-1-500

Project Title: **Solubility data related to industrial processes. Mutual solubility of ethers and ketones with water**

Task Group Leader: Marian Góral

Starting date: September 2006

Report: Projected completion date, end of 2007

Project number: 2006-033-1-500

Project Title: **Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems**

Task Group Leader: Cezary Guminski

Starting date: July 2005

Report: Assistance of a Chinese speaking scientist was absolutely necessary (ed.: perhaps 2006 Franzosini prize winner Dewen Zeng?!).

Projected completion date (documents ready for external review): end of this year

Project number: 2006-034-1-500

Project Title: **The solubility of oxygen in all solvents (update of SDS vol 7, 1981)**

Task Group Leader: H. Lawrence Clever

Starting date: September 2006

Report: personal communication

Projected completion date (documents ready for external review): December 31, 2007 at the earliest.

6. **New SDS Projects**, Phantom proposal, project submission forms sent:

**Peter G.T. Fogg**, Task Group Leader: **Solubility of Higher Alkynes in Liquids**

Complement to volume 76 of the Solubility Data Series entitled Solubility of Ethyne in Liquids, Peter G.T. Fogg (ed.).

Task Group Members: Mark Salomon

**Marian Góral**, Task Group Leader: **Mutual Solubility of Esters with Water**

Task Group Members: Andrzej Maczynski, Barbara Wisniewska-Gocłowska, David Shaw, Mark Salomon

**Valerii Sazonov**, Task Group Leader: **Nitriles C+3: Binary and Multicomponent Systems**

Task Group Members: David Shaw, Marian Góral, Mark Salomon

**Jitka Eyssełtova**, Task Group Leader: **Solubility in Systems with Lithium and/or Sodium Nitrates**

Task Group Members: Stefka Tepavitcharova, Vladimir Valyashko, Wolfgang Voigt, Mark Salomon

## 7. 13<sup>th</sup> ISSP

### **International Symposium on Solubility Phenomena and Related Equilibrium Processes**

The 13<sup>th</sup> ISSP will be organized at the University College Dublin, Ireland.

All interested Persons are invited to participate at the conference in Dublin, Ireland, July 27-31, 2008.

Parallel to the Symposium the Organization of a Workshop

### **SC-Database: project management, organization of data collection, entry and verification**

is being envisioned.



**Attachment A.5**  
**Editor-In-Chief's Report For 2006 - 2007**  
Submitted August, 2007

There are three manuscripts from 2006 still in progress.

- 06-01            Jiri Hala, 'IUPAC-NIST Solubility Data Series. 84. Solubility of Inorganic Actinide Compounds'
- 06-05            Hiroshi Miyamoto, Ryo Miyamoto and Cezary Guminski, 'IUPAC-NIST Solubility Data Series. 85. Transition and 12 to 14 Main Group Metals, Lanthanide, Actinide and Ammonium Halates.'
- 06-07            Valerii P. Sazonov, David G. Shaw, and Adam Skrzecz (deceased), "IUPAC NIST Solubility Data Series. 83. Acetonitrile: Ternary and Quaternary Systems."

06-01 is at AIP, page proofs are not ready.

06-05 is being converted from LaTeX to Word, so that the cumulative index can easily be added.

06-07 is with the authors, the 2<sup>nd</sup> set of page proofs are being examined; when approved, conversion of the page numbers in the indices and be carried out.

Three 2007 articles were submitted in excellent shape. The journal editor, Dr. Malcolm Chase, made three types of changes to the articles. The changes consisted of combining the two small tables within a 'page,' making the title part of the table, and embedding the references for a 'page' as part of the text in the Auxiliary Information section. Lastly, a cumulative set of references was placed as the last section in the article. Please look at the next two pages of this attachment to see the type of changes that were made by Mal Chase.

The following three manuscripts will be submitted in August to the AIP for the preparation of the proof copy.

- 07-10            Andrzej Maczynski and David G. Shaw, "IUPAC-NIST Solubility Data Series. AA. Ethers with Water. Part 1. C<sub>2</sub>- C<sub>5</sub> Ethers with Water",
- 07-11            Andrzej Maczynski and David G. Shaw, "IUPAC-NIST Solubility Data Series. AA. Ethers with Water. Part 2. C<sub>6</sub> Ethers with Water",
- 07-12            Andrzej Maczynski and David G. Shaw, "IUPAC-NIST Solubility Data Series. AA. Ethers with Water. Part 3. C<sub>7</sub> - C<sub>14</sub> Ethers with Water",

<b>Components:</b> (1) Diethyl ether; C <sub>4</sub> H <sub>10</sub> O; [60-29-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>Original Measurements:</b> <sup>5</sup> W. D. Bancroft, Phys. Rev. <b>3</b> , 114 (1895).
<b>Variables:</b> One temperature: 20 °C	<b>Prepared by:</b> B. Wisniewska-Gocłowska

### Experimental values

TABLE 17. Solubility of diethyl ether/water system.<sup>5</sup>

Solubility of diethyl ether in water			
t (°C)	cm <sup>3</sup> (1) / 10cm <sup>3</sup> (2)	g (1) / 100 g sln (compiler)	x <sub>1</sub> (compiler)
20	1.03 - 1.04	6.86 - 6.92	0.0176 - 0.0177

Solubility of water in diethyl ether			
t (°C)	cm <sup>3</sup> (2) / 10cm <sup>3</sup> (1)	g (2) / 100 g sln (compiler)	x <sub>2</sub> (compiler)
20	0.08	1.10	0.0441

The assumptions 1 cm<sup>3</sup> (1) = 0.71352 g(1) and 1 cm<sup>3</sup> (2) = 0.9982323 g(2) at 20 °C by ref (1) were adopted in the calculations.

### Auxiliary Information

#### Method/Apparatus/Procedure:

The titration method was used. 10 cm<sup>3</sup> of solvent in a test tube was titrated with the another component till the solution clouded.

#### Source and Purity of Materials:

- (1) Source not specified; distilled over Na, change of boiling point 1 °C.  
 (2) Not specified.

#### Estimated Error:

Solubility: ±0.01 cm<sup>3</sup>.

#### References:

<sup>1</sup>International Critical Tables vol. 3, New York 1928.

<b>Components:</b> (1) Diethyl ether; $C_4H_{10}O$ ; [60-29-7] (2) Water; $H_2O$ ; [7732-18-5]	<b>Original Measurements:</b> <sup>5</sup> W. D. Bancroft, Phys. Rev. <b>3</b> , 114 (1895).
<b>Variables:</b> One temperature: 20 °C	<b>Prepared by:</b> B. Wisniewska-Gocłowska

### Experimental values

Table 17. Solubility of diethyl ether/water system. <sup>5</sup>			
Solubility of diethyl ether in water			
t (°C)	cm <sup>3</sup> (1) / 10cm <sup>3</sup> (2)	g (1) / 100 g sln (compiler)	x <sub>1</sub> (compiler)
20	1.03 - 1.04	6.86 - 6.92	0.0176 - 0.0177
Solubility of water in diethyl ether			
t (°C)	cm <sup>3</sup> (2) / 10cm <sup>3</sup> (1)	g (2) / 100 g sln (compiler)	x <sub>2</sub> (compiler)
20	0.08	1.10	0.0441

The assumptions  $1 \text{ cm}^3 (1) = 0.71352 \text{ g}(1)$  and  $1 \text{ cm}^3 (2) = 0.9982323 \text{ g}(2)$  at 20 °C by the International Critical Tables [International Critical Tables vol. 3, New York 1928] were adopted in the calculations.

### Auxiliary Information

#### Method/Apparatus/Procedure:

The titration method was used. 10 cm<sup>3</sup> of solvent in a test tube was titrated with the other component till the solution clouded.

#### Source and Purity of Materials:

- (1) Source not specified; distilled over Na, change of boiling point 1 °C.  
 (2) Not specified.

#### Estimated Error:

Solubility:  $\pm 0.01 \text{ cm}^3$ .

## Attachment A.6

### New Formatting Guidelines for JPCRD A Review from the EIC's Freiberg Report

[1] The American Institute of Physics (AIP) has switched to a portrait style publication for the future solubility data series articles.

[2] Changes in handling of references which will permit AIP to allow the reader to access the early references (assuming that they are available on line). For this purpose, a section has been added to each volume entitles "Cumulative Set of References" which contains all the references from the introductory material and the critical evaluations - this cumulative set is in alphabetical order by lead author and chronologically within the same author. Note that there are two issues of which to be aware.

One is that with each critical evaluation, the references numbers will not be continuous, but they will be sequential.

Second is that with each 'experimental data' the references which occur in the "Auxiliary Data" section must be handled differently. These references have now been buried within the text. These latter references are not used in the indices created by IUPAC-NIST and will not be backward cited by AIP (see the revised compilation for the diethyl ether - water system in the EIC 2006-2007 report).

[3] Lastly, the electronic format that we have been using seems to be acceptable to AIP for quick and efficient conversion to page proofs - use of the equation editor, use of the table format options, each data table be one continuous table (no continuation heading on a succeeding page).

As an example of these format changes, please view the Attachment A.7 for selected pages from Volume 82 of the Solubility Data Series (C8-C18 Alcohols with Water).

[4] Indices; Since articles J. Phys. Chem. Reference Data are published in .pdf format, searches by chemical name, Registry Number and authors are easily accomplished using the "Search" or "Find" command in .pdf documents. Thus all indexes will no longer be required which will save consider time in preparing SDS volumes.

[5] Introductory Materials ("Front Matter"). Previous SDS volumes published in JPCRD all contained the appropriate introduction to the subject matter, i.e. Gas/Liquid, Liquid/Liquid and Solid/Liquid systems. These introductory materials will no longer be published in the SDS articles in JPCRD. However, the author's preface will be retained. Thus, reference to any of these "Introductions" should simply be given in the Author's Preface to his or her volume. The reference could be for a previous Introduction published in JPCRD or a web site. For example, one could provide the SSED web site's URL which is <http://www.unileoben.ac.at/~IUPAC/welcome.html>.

**Attachment A.7**  
**Format changes**

See ref Part 5 from [www.iupac.org/publications/sds/2007/82\\_abstract.html](http://www.iupac.org/publications/sds/2007/82_abstract.html)

Or Journal of Physical and Chemical Reference Data, Vol. 36, No. 3, pp. 685-731, 2007  
> on-line abstract DOI [10.1063/1.2391321](https://doi.org/10.1063/1.2391321)

**Attachment A.8**  
Subcommittee Report on Gas Solubilities

**IUPAC Project Progress Report**

**Date:** July 2007

**Task Group Leader:** Pirketta Scharlin

**Project number:** 2002-044-1-500

**Project Title:** Solubility data related to industrial processes.  
Carbon dioxide in aqueous non-electrolyte solutions.

**Report:**

1. Current status of project: Ongoing project.

Data up to 1988: around 300 data sheets were put into electronic form manually from the old paper versions and updated to meet the requirements of the Journal of Physical and Chemical Reference Data.

Literature survey was carried out for years 1989-2004. These data have been tabulated into electronic form.

Literature survey was carried out for year 2005. Tabulation of these data into electronic form is in progress.

About 380 data pages altogether are now in the required electronic format. The compiled data consist of 60 different solvent systems, including aqueous solutions of alcohols, ethers, ketones, carboxylic acids, sugars, and nitrogen containing organic compounds.

Evaluation of aqueous alkanolamine systems is now in progress. Two evaluations ( $CO_2$  in aqueous monoethanolamine and  $CO_2$  in aqueous triethanolamine) are in draft form and two more ( $CO_2$  in aqueous diethanolamine and  $CO_2$  in aqueous methyl-diethanolamine) have been initiated.

Update for years 2006-2007 is being carried out.

2. Progress relative to 'milestones': Relative to 'milestones' given in the original project submission form, the project is late. (See # 3.)

3. Difficulties encountered (or concerns): Evaluations and some data collections have been delayed. However, we are making slow progress now. Lack of time continues to be the biggest obstacle to a more rapid progress.

4. Projected completion date (documents ready for external review): It is really very difficult to foretell completion date. (See # 3.)

5. Please list all of the intended outputs and the dissemination plan for this project (viz. articles, CD, conference presentations; etc.). These may have been expanded since project approval:

Intended outputs: Journal of Physical and Chemical Reference Data and IUPAC-NIST Solubility Database.

Dissemination plan: Access to the information of the Solubility Data Series is provided to chemists through the specialist abstracting journals, principally Chemical Abstracts and to potential non-chemist users via the IUPAC and SSED web sites which are catalogued by various commercial search engines. Furthermore, the abstract of the respective JPCRD article will be published in CI, as recommended by the ACD officers.

6. If your project is within 6 months of completion, how do you plan to utilize any remaining budget for this project? -

7. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them: -

## **IUPAC Project Progress Report**

**Date:** July 2007

**Task Group Leader:** H. Lawrence Clever

**Project number:** 2006-034-1-500

**Project Title:** The solubility of oxygen in all solvents (update of SDS vol 7. 1981)

### **Report:**

1. Current status of project:
2. Progress relative to 'milestones':
3. Difficulties encountered (or concerns):
4. Projected completion date (documents ready for external review): **December 31, 2007 at earliest**
5. Please list all of the intended outputs and the dissemination plan for this project (viz. articles, CD, conference presentations; etc.). These may have been expanded since project approval:
6. If your project is within 6 months of completion, how do you plan to utilize any remaining budget for this project?
7. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them:



## **IUPAC Project Progress Report**

**Date:** July 2007

**Task Group Leader:** D.E. Knox

**Project number:** 2002-045-1-500

**Project Title:** Solubilities in Supercritical Carbon Dioxide

### **Report:**

1. Current status of project:

Slow progress is being made, at present only being worked on by myself and one part/time undergraduate student who has just started. Previous student discontinued work on project in late 2006.

2. Progress relative to 'milestones':

No significant progress since late 2006, other than rearrangement of project into smaller, more manageable parts

3. Difficulties encountered (or concerns):

Main concern is lack of personnel and students, would greatly benefit from collaborative effort. Also, it is a very large project which has necessitated subdividing into smaller pieces to allow for completion of at least the smaller pieces

4. Projected completion date (documents ready for external review):

At present, earliest would be early 2008

5. Please list all of the intended outputs and the dissemination plan for this project (viz. articles, CD, conference presentations; etc.). These may have been expanded since project approval:

When finished, results will be part of the Solubility Data Series

6. If your project is within 6 months of completion, how do you plan to utilize any remaining budget for this project?

N/A, there is no budget for this project

7. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them:

N/A

**Attachment A.9**  
Subcommittee Report on Liquid Solubilities

Chairman's Report: August 2007

Completed Projects

Project 2002-050-1-500 (Valerii Sazonov, Task Group Chair) Solubility of acetonitrile: ternary and quaternary systems. Status: complete; published as:

Sazonov, V.P., D.G. Shaw, A. Skrzecz, N.I. Lisov, and N.V. Sazonov, 2007, IUPAC-NIST Solubility Data Series. 83. Acetonitrile: Ternary and Quaternary Systems, Journal of Physical and Chemical Reference Data, **36**, 733-1131.

Project 2005-006-1-500 (Andrzej Maczynski, Task Group Chair) Mutual solubility of alcohols and water. Status: complete; published as:

Maczynski, A. and D.G. Shaw, 2007, IUPAC-NIST Solubility Data Series. 82. Alcohols with Water-Revised and Updated: Part 1. C<sub>4</sub> Alcohols with Water, Journal of Physical and Chemical Reference Data, **36**, 59-132.

Maczynski, A. and D.G. Shaw, 2007, IUPAC-NIST Solubility Data Series. 82. Alcohols with Water-Revised and Updated: Part 2. C<sub>5</sub> Alcohols with Water, Journal of Physical and Chemical Reference Data, **36**, 133-190.

Maczynski, A., D.G. Shaw, M. Góral and B. Wisniewska, 2007, IUPAC-NIST Solubility Data Series. 82. Alcohols with Water-Revised and Updated: Part 3. C<sub>6</sub> Alcohols with Water, Journal of Physical and Chemical Reference Data, **36**, 399-444.

Maczynski, A., D.G. Shaw, M. Góral and B. Wisniewska, 2007, IUPAC-NIST Solubility Data Series. 82. Alcohols with Water-Revised and Updated: Part 4. C<sub>7</sub> Alcohols with Water, Journal of Physical and Chemical Reference Data, **36**, 445-484.

Maczynski, A., D.G. Shaw, M. Góral and B. Wisniewska, 2007, IUPAC-NIST Solubility Data Series. 82. Alcohols with Water-Revised and Updated: Part 5. C<sub>8</sub>-C<sub>17</sub> Alcohols with Water, Journal of Physical and Chemical Reference Data, **36**, 685-731.

Current Project

Project 2006-032-1-500 (Marian Góral, Task Group Leader) Solubility data related to industrial processes. Mutual solubility of ethers and ketones. Compilation is nearly complete and evaluation is in progress; estimated completion 2008; according to an email from Allan Harvey the work will be published as two volumes of three parts each. One volume covers ethers and the other ketones.

New Project

Valerii Sazonov, Task Group Leader D. Shaw, M. Góral, and M. Salomon, Higher nitriles ( $C_{3+}$ ): binary and multicomponent systems.

Proposal submitted

**Valerii Sazonov, Task Group Leader: Nitriles C+3: Binary and Multicomponent Systems**

**Task Group Members: David Shaw, Marian Góral, Mark Salomon**

## Attachment A.10 Subcommittee Report on Solid Solubilities

**Torino, August 2007**

### **Seawater system components**

According to the agreement achieved last year at the meeting in Freiberg work is concentrated on binary systems  $MgCl_2-H_2O$ ,  $CaCl_2-H_2O$  and  $K_2SO_4-H_2O$ .

Compilation work for  $MgCl_2-H_2O$  is ready, evaluation will be ready end of this year as promised in the meeting 2006. W. Voigt will submit a project application form for a  $MgCl_2-H_2O$  volume and  $CaCl_2-H_2O$  volume. The latter project will be performed together with Prof. Dewen Zeng. For  $CaCl_2-H_2O$  compiling had been started and a first attempt to develop a new evaluation strategy was made and published (D. Zeng, H. Zhou, W. Voigt Thermodynamic Consistency of Solubility and Vapor Pressure of a Binary Saturated Salt + Water System: II.  $CaCl_2 + H_2O$  Fluid Phase Equilibria, (2007)

I. Eyseltova accepted to take over the responsibility for the volume of  $K_2SO_4-H_2O$  and will send in a submission form after having received the material from R. Bouaziz through Ch. Balarew. Ch. Balarew confirmed that he was in contact with R. Bouaziz and has got the compilation sheets of this system. (subsequently noted as done)

### **Solubility data of compounds relevant to mobility of metals in the environment**

**Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb) C. Magalhães, H. Gamsjäger and K. Sawada ( 2002-032-1-500)**

Clara Magalhaes informed about difficulties in the data evaluation and attempts to achieve progress by using the FACTSAGE program, to solve this problem she contacted E. Königsberger and G. Erikson at the occasion of the 30<sup>th</sup> ISCS in Perth. Further detailed plans will be given in September from her side.

**Alkaline earth metal carbonates. Alex de Visscher, J. Vanderdeelen, J. Lorimer E. Königsberger ( 2002-031-1-500)**

A. de Visscher successfully applied for Killam resident fellowship at Schulich School of Engineering to work on **Solubility of alkaline earth carbonates in water and electrolyte systems. A volume in the IUPAC-NIST Solubility Data Series**. The application was supported by the commission (see Attachment A.12). According to the working plan and intention of Alex de Visscher the volume should be ready (in the old format) at the end of 2008.

### **Solubility data of compounds relevant to human health.**

**Solubility of hydroxybenzoic acids and hydroxybenzoates A. Goto, H. Miyamoto (2002-036-1-500)**

Ayako Goto delivered a written report and sample data sheets from re-formatting. If JPCRD can accept the re-formatted sheets (not in the new format demanded recently), the volume is ready to send for print. Due to an eye operation and many duties at the university no further progress could

be made. However, the volume is very attractive for a variety of users and should be finished as fast as possible. In this respect A. Goto expressed the necessity for financial support.

**Solubility of halogenated aromatic hydrocarbons A. Goto, R. Goto, M. Makino, and H. Miyamoto (2002-037-1-500)**

According to the proposal of J. Lorimer last year Masakazu Makino prepared a draft including correlation plots solubility - melting point and enthalpies (poster at IUPAC conference). A draft report of the compilation sheets was prepared, however, an expert review on the data situation as suggested in the last year meeting was not attempted. Since these data are highly requested the commission is searching for a way of publishing in a suited form.

**Solubility of substances related to urolithiasis. E. Königsberger and L.-C. Königsberger (2002-035-1-500)**

No new information.

**Other systems and proposals**

**Aqueous lanthanide chloride systems. C. Guminski and T. Mioduski**

The work about the chlorides will be finished this year and the volume will be ready next year.

**Solubility in systems aqueous containing  $\text{LiNO}_3$  and/or  $\text{NaNO}_3$**

I. Eysseltova will prepare a submission form for these systems. The member of the sub-commission already earlier confirmed that these systems are of basic interest in science and technology.

W. Voigt

## Attachment A.11

ISSP - 2010

### English version of the proposal

#### Preliminary information on the Symposium in St. Petersburg:

The technical part of Symposium will be organized by Monomax Meetings & Incentives – this company specializes in conference management, destination management and event management.

The Conference site chosen to be the Baltiets Hotel, a modern recreational complex situated in a picturesque suburb of St-Petersburg called Repino, by the Gulf of Finland. It is a seaside resort in the refreshing Karelian pine groves at a distance of 40 km from the center of Saint-Petersburg. It is know not only for its scenic sights, charming pines and sandy beaches, but also for historical mansions in Repino.

**Address:** St. Petersburg, Repino, Primorskoje shosse, 427

The hotel has a number of conference halls to accommodate up to 240 persons. All of them equipped for all sorts of meetings activities, including computers, screens, microphones and power supplies for personal uses.

#### **Capacities:**

	Area (sq. m)	Theater (persons)	Classroom (persons)
Concert Hall	350	240	
Dining Room	270	220	
Big Conference Hall	328		100
Medium-sized Conference Hall	102		60
Small Conference Hall	50		20
Classroom	74		30
Child Room	70		40

**Registration fee –350 Euros.**

**Registration fee covers:** conference kit (book of Abstracts, etc.), participation in all the scientific sessions, coffee, welcome reception and, probably, banquet and excursion.

Shuttle service would be organized additionally.

#### **Accommodations:**

Baltiets Hotel

**Today prices:** Single accommodation **3000 RUR** Double accommodation **3650 RUR**

(In July 2007: 1 EURO = 35 RUR) Prices include breakfast, lunch and dinner, all served in Buffet style.

*Some pictures (main building, rooms, map):*



Repino



## **Attachment A.12**

A. de Visscher: Killam resident fellowship

Killam resident fellowship

Letter of Application

### **Solubility of alkaline earth carbonates in water and electrolyte systems. A volume in the IUPAC-NIST Solubility Data Series**

Alex De Visscher  
Schulich School of Engineering  
Department of Chemical and Petroleum Engineering

#### Introduction

The Solubility Data Series is one of the flagship projects of the International Union of Pure and Applied Chemistry (IUPAC). It is the development of a series of monographs for the dissemination of reference data on the solubility of substances of industrial, environmental and/or medical importance. The process is guided by an extensive internal as well as external review process. In 1979-1996, IUPAC published 65 volumes in the series as books. Since volume 66, the monographs are published jointly by IUPAC and the National Institute for Standards and Technology (NIST) as papers in the Journal of Physical and Chemical Reference Data. The data are also entered in the NIST property data base and is accessible through the Chemistry Webbook (<http://webbook.nist.gov/chemistry/>). The most recent volume is number 81, on the solubility of C<sub>5</sub>-C<sub>36</sub> hydrocarbons in water. The total series contains more than 25,000 pages. More information on the Solubility Data Series can be found on the IUPAC web site (<http://www.iupac.org/publications/sds/index.html>) or in J.W. Lorimer, *Chem. Int.* **18**, no. 2 (1996) 47-50.

One of the next volumes that are slated for publication is a volume on the solubility of alkaline earth carbonates in water and in aqueous electrolytes. As the volume editor it is my responsibility to bring this publication to fruition. The bulk of the work is done, but an estimated 400 hours of work is still required to extract reference thermodynamic data and reference solubilities from the compiled data. The purpose of this Killam Resident Fellowship application is to make time available to finish this volume.

#### Rationale for the Killam Resident Fellowship

The Solubility Data Series is an important program because it generates a large amount of data in an accessible form. The solubility of substances is a property that is required in many fields in science and engineering. It is used as auxiliary information in many fields of research including physics, chemistry, environmental sciences, and medical sciences. The solubility of substances is also useful data in the validation of thermodynamic models. The volume on the alkaline earth



carbonates that I am completing is a particularly important one, because it involves a ubiquitous group of minerals that are receiving an increased attention in the context of global change and carbon dioxide storage. It is also important in an industrial context (scale formation) and in construction (concrete).

The patronage of both IUPAC and NIST for this program underscores its importance and prestige. Being editor of a volume is a boost of the international visibility of a scientist and the research institution that employs them.

Most of the work for this volume has already been accomplished. The work was initiated in 1996 by Dr. Jan Vanderdeelen of Ghent University, Belgium, a fellow of IUPAC. I followed this work as his research and teaching associate from 2001 on, and contributed to the work in the form of two papers (De Visscher and Vanderdeelen, 2003, 2005). Upon his retirement in 2004, Dr. Vanderdeelen handed over the project to me. I quickly realized that I would not be able to finish the project before my move to Canada in May 2005, so I brought it over. Ever since, I made very little progress to the project because doing otherwise would interfere with my research and teaching activities as a Canada Research Chair in Air Quality and Pollution Control Engineering. A Killam Resident Fellowship would allow me to complete the project, and accrue the international recognition that is associated with a volume of the Solubility Data Series, without interfering with my career as a Chair. In short, this fellowship would generate a great added value for a comparatively minor effort.

### Project Description

The project is subdivided into two phases: a compilation phase and an evaluation phase. The two phases are separate: data that is shown to be flawed in the evaluation is not eliminated from the compilation, for reasons of accountability.

The compilation phase is the retrieval of all the published literature that reports measurements of the solubility of alkaline earth carbonates (beryllium carbonate, magnesium carbonate, calcium carbonate, strontium carbonate, barium carbonate and radium carbonate) back from the first measurements in 1846 up to the present. The measurement data are compiled on standard data sheets that contain essential information like reference citation, conditions (temperature, pressure, starting material, etc.), and the measurement method. Data are converted to molalities for consistency and thermodynamic rigor. To date, more than 150 data sheets, covering the period 1846-1996 have been compiled.

The evaluation phase is a critical check of the reliability of the data. This is based on several criteria:

- Papers reporting detailed information on purity, origin, and crystallographic structure of the materials are considered to be more reliable than papers that do not provide this information.

- Papers that do not report temperature are not considered for evaluation. Papers that do not report the pressure in systems that are pressure-dependent are considered with great suspicion.
- Papers that use a method or assumption that is known to be flawed are rejected in the evaluation.
- Papers from authors that reported flawed data elsewhere are treated with great suspicion if the same method was used.
- Solubility data from different sources are plotted together, in order to assess the spread of the data and to spot outliers. This is simple in the binary system metal carbonate – water, which depends mainly on the temperature with only a minor pressure effect. However, the ternary system metal carbonate – water – carbon dioxide is much more difficult to evaluate that way because it depends strongly on both temperature and CO<sub>2</sub> partial pressure. In the latter case, the next method is more revealing.
- By means of a thermodynamic model, the solubility data are converted to thermodynamic solubility constants, which mainly depend on the temperature, with only a minor pressure effect, and these solubility constants are plotted versus temperature for comparison like in the previous method.
- Thermodynamic properties are derived from the data, and compared with independent measurements. For instance, the Gibbs free energy and the entropy of the calcite – aragonite transition in calcium carbonate can be calculated from the data, and compared with independent determinations of Königsberger et al. (1989).

Critical evaluations have been completed for beryllium carbonate, magnesium carbonate, strontium carbonate, and barium carbonate, and a partial evaluation of the data of calcium carbonate has been made. However, the methodology of the previous evaluator was severely criticized upon internal review by the Subcommittee of Solubility and Equilibrium Data, so the data needs to be re-evaluated. I proposed a new approach, which was accepted by the Subcommittee.

### Current Status

The current version of the manuscript is about 300 pages (single interline, font size 10 pt.), of which about 225 pages are compilations and 75 pages are evaluations. It is estimated that the manuscript will be close to 350 pages in its final form, and 200 pages in published form (plus or minus 50, depending on the journal lay-out, which is currently under review).

As indicated above, the compilation is nearly completed. Remaining issues are:

- Papers published after 1996 have not been included yet.
- The conversion of concentrations to molalities was based on electrolyte solution densities from an unreliable reference. This is especially important in the case of solubilities in electrolyte solutions. These conversions need to be adjusted.
- The current compilations assume atmospheric pressure (101.325 kPa) when the pressure was not explicitly stated. However, some measurements were made at sufficiently high altitudes to affect the solubility significantly in the case of the system metal carbonate –

water – carbon dioxide. Corrections are required here. If the location of the measurements is unknown, then the data must be rejected.

- Likewise, there is no correction for water vapor pressure in the compilations unless the authors of the original papers explicitly accounted for it. This means that the reporting of the data in the compilations is inconsistent. This must be rectified.

The resolution of the above issues will require approximately 100 hours of work.

As indicated above, the data need to be re-evaluated. A preliminary re-evaluation of the data for the metal carbonate – water – carbon dioxide was conducted with the approach accepted by the Subcommittee on Solubility and Equilibrium Data. The following issues remain:

- The modifications in the compilations indicated above need to be introduced into the evaluations, both in the manuscript and in the Excel files used for the evaluations. An estimated 500 data points need to be re-entered.
- Auxiliary information used in the evaluation (equation of state and solubility of CO<sub>2</sub>, for instance) needs to be evaluated, as an evaluation should rely on evaluated auxiliary information only.
- The preliminary evaluation of the metal carbonate – water – carbon dioxide data needs to be updated.
- The metal carbonate – water data need to be evaluated, and consistency with the metal carbonate – water – carbon dioxide data should be checked.
- The data for solubility in aqueous electrolytes should be evaluated.
- The derivation of thermodynamic properties like the Gibbs free energy and the entropy of dissolution need to be determined, and evaluated against independent data.

The resolution of these issues will require approximately 100 hours of work.

The final write-up and publication of the monograph requires the following work items not included above:

- The introduction (20 pages) needs to be rewritten to reflect the new evaluation methodology, with a detailed description of the thermodynamic model used.
- The evaluations (currently 55 pages, probably around 80 pages in final form) need to be rewritten for about 80%.
- Manuscript needs to be submitted for publication, and revised according to the comments of the reviewers.

The final write-up will require an estimated 200 hours.

### Timing

The grant is requested for Winter 2008.

As indicated above, the completion of the project will require about 400 hours of time.

My current teaching load for the winter term is as follows:

ENGG 201: Properties of Fluids and Solids

Lectures: 3hr/week + 6hr/week of preparation

Tutorials: 1.5hr/week + 1.5hr/week of preparation (incl. making up quizzes)

Labs: 3hr/week

Student guidance, office hours: variable

Midterm grading: 20hr

Final exam grading: 20hr

Total time:  $13\text{weeks} \times 15\text{hr/week} + 40\text{hr} = 235$  hours

ENCH 531: Chemical Process Design

Tutoring of 4 groups of students: 4hr/week

Midterm report reading: 10 hours

Midterm exam: 5 hours

Final report reading: 25 hours

Final exam: 10 hours

Total time:  $13\text{weeks} \times 4\text{hr/week} + 50$  hours = 102 hours

Teaching relief of the winter term would free up an estimated 337 hours of time. This time would be devoted to the solubility project in case the Killam Resident Fellowship is granted. The remaining 63 hours of work will be done during the spring and summer terms of 2007.

Optionally, part of my teaching responsibilities of Fall 2007 can be pushed forward, which would enable me to make progress during the fall of 2007 as well.

Dissemination Plan

As indicated before, the monograph will be published in the Journal of Physical and Chemical Reference Data, which publishes the majority of data that is considered as standard data by physicists and chemists. The data will also be included in the NIST property data base, which will make it available on the NIST Chemistry Webbook. Two papers have already been published based on the work (De Visscher and Vanderdeelen, 2003, 2005), and progress on the work has been reported on two international conferences. Upon completion of the work the final conclusions will be presented on an international conference as well.



**Institut für Anorganische Chemie**

Leipziger Str. 29

09596 Freiberg

tel.: +49(0)3731-39 3194

e-mail :Wolfgang.Voigt@chemie.tu-freiberg.de

fax: +49(0)3731-39 4058

Chair, Killam Resident Fellowships Committee c/o Research Services,  
ERRB Building, Research Park University of Calgary 2500 University Drive NW Calgary, Alberta Canada  
T2N 1N4  
FAX: +1 403 289 0693

Freiberg, 9/03/2007

*Killam resident fellowship*

**Letter of support**

**for**

**Dr. Alex De Visscher**

Schulich School of Engineering

Department of Chemical and Petroleum Engineering

Dear Madam, Dear Sir,

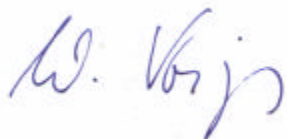
I know Dr. de Visscher from our common work within the IUPAC "Subcommittee on Solubility and Equilibrium Data". About four years ago he agreed to take the responsibility to make a final critical evaluation of a volume entitled:

**"Solubility of alkaline earth carbonates in water and electrolyte systems"**

As the chair for „Solid-liquid solubilities task group“ I had intensive discussions with Dr. De Visscher how to proceed and finish this work, which was started by Prof. Vanderdeelen long time ago. Prof. Vanderdeelen collected a huge amount of data and tried a first critical evaluation. However, this was not done on the basis of advanced electrolyte thermodynamics. Several times at committee meetings we discussed how this volume can be finished. It is the expectation of the

committee that in the light of the actual discussion on climate change in connection with CO<sub>2</sub> balances a soon publication of recommended solubility data of the most important carbonates by IUPAC-NIST, especially as function of CO<sub>2</sub> pressure, will make this volume to a standard book in environmental and chemical-technological research and applications. With Dr. Visscher we are convinced to have found one of the few persons world-wide, who are able to perform this work on the appropriate scientific level. The solubility data series is highly accepted world-wide and distribution of the “carbonate volume” will have a large impact on the visibility of your institution and the researcher working at it.

Reading the work-load estimations in the application of Dr. De Visscher I can state that his numbers of hours are low limits, that is the real work is much more as I know from the detailed study of the manuscript and discussions with Dr. De Visscher. If Dr. Visscher on the basis of the Killam fellowship can find the necessary time to complete the “carbonate volume” it will be recognized very positive by the IUPAC body, especially by division (V). From my point of view the support of this project will have a very positive impact on the status of Dr. De Visscher within the international network of scientists, on the recognition of your institution and on the quality of environmental research.



Prof. Dr. Wolfgang Voigt

Chair of solid-liquid solubilities task group