



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

Minutes

5th Annual Meeting of SSED (32nd overall)

held in conjunction with the

12th International Symposium on Solubility Phenomena

at TU Bergakademie Freiberg, Freiberg, Germany

22-23 July 2006

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

Saturday, 22 July 2006

Morning Session 1: 9:00 - 12:00

- Welcome of the participants (Full List of Participants is in Appendix 1)** H. Gamsjäger
Heinz Gamsjäger, Chairman of the SSED welcomed the participants.
All of the participants introduced themselves and their affiliation.
- Approval of the Minutes of the 4th Annual Meeting of SSED (31st overall) held in conjunction with the 29th International Conference on Solution Chemistry, Portoroz, Slovenia, 26 August 2005** D. Knox
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 after correction of two typographical errors.
- Other Items for Agenda** H. Gamsjäger
No additional items were suggested for the agenda at this time. However, some time was later added at the end of both the Saturday morning session and the Sunday afternoon session to discuss additional items.
- Franzosini Award (CV in Appendix 2)** H. Gamsjäger
Heinz Gamsjäger announced that this year's recipient of the Franzosini Award was Dr. Dewen Zeng, and noted his background and the importance of Dewen Zeng to the Subcommittee on Solubility and Equilibrium Data. Dewen Zeng, in accepting the award, thanked Heinz Gamsjäger and the SSED for their support. Jitka Eyseltova discussed the importance of relations among groups. Jack Lorimer discussed the background of the Franzosini Award.

5. **Chairman's Report for 2005 - 2006 (Full Report is in Appendix 3)** H. Gamsjäger
- a) Visibility of SSED within IUPAC
 Heinz Gamsjäger pointed out that there were items either from or about members of the SSED or its activities in several issues of Chemistry International, including volume 27 (number 5), volume 27 (number 6), volume 28 (number 1) - which had several items, and volume 28 (number 2).
- b) Books
 Wiley has recently published "Biomineralization - Medical Aspects of Solubility" by Erich and LanChi Königsberger. Although due out in September, Peter Fogg indicated that he received a copy the previous week.
- c) Completed Volumes
 Volume 81, parts 5 through 12 in the Solubility Data Series have now been published in the Journal of Chemical and Physical Reference Data.
- c) Completed SDS Projects
 Heinz Gamsjäger briefly noted recently completed projects by Jiri Hala, Hiroshi Miyamoto, Valerii Sazonov, and Andrzej Maczynski.
- d) Current SDS Projects
 Heinz Gamsjäger briefly updated the status of 8 ongoing projects
- e) New SDS Projects
 Heinz Gamsjäger briefly introduced 3 new projects and discussed their current status.
- f) 12th ISSP
 Heinz Gamsjäger briefly noted that the 12th International Symposium on Solubility Phenomena would take place starting the next day.
- Wolfgang Voigt commented that he thought the project list may be incomplete. Further discussion was postponed until after the reports of the subcommittees.
6. **Editor-in-Chief's Report for 2005 - 2006 (also included agenda items 7 and 8)** M. Salomon
- Mark Salomon reported that all manuscripts submitted in 2005 have been published. At present, the Journal of Chemical and Physical Reference Data has eight manuscripts. Publication of manuscripts is very fast if they are in the format that the journal prefers especially as regards the table formats. The submission by Hiroshi Miyamoto was in LATEX format, the status as regards publication in the Journal of Chemical and Physical Reference Data is unclear. Andrzej Maczynski has 5 manuscripts submitted.
7. **Volumes for Next Year's SDS Proposals** M. Salomon
- This subject was deferred until after the subcommittee meetings.
8. **New Formatting Guidelines for JPCRD** M. Salomon
- Mark Salomon reported that currently the Journal of Chemical and Physical Reference Data is publishing in landscape orientation, but will be switching to portrait orientation, and commented that this was acceptable and should have little effect on us as contributors. Mark Salomon also reported that Mal Chase will be retiring in a year, and that his

replacement will most likely come from within NIST.

Heinz Gamsjäger asked, regarding the submission in LATEX, whether a chemistry student with computer know-how should not be asked to assist in converting the submission to Word? Jack Lorimer commented that the conversion was possible but difficult and laborious.

Heinz Gamsjäger, in reference to new SDS proposals, discussed and showed the "Project Submission Guidelines" including the forms and methods. The protocol is to submit proposals first to him, and then he will then submit them to IUPAC as chair of the subcommittee.

Alex de Visscher noted that one project generated a series of papers, and asked if this was now the norm? Mark Salomon replied that this was not generally true, but that it made sense in that particular case (referring to the project dealing with the mutual solubility of alcohols and water)..

9. **Status of NIST Funding** H. Gamsjäger

Heinz Gamsjäger reported that this was still under negotiation.

9a. **News Items** J. Lorimer

Jack Lorimer reported several news items related to IUPAC:

- a) Red Book was published in Fall 2005. There are some nomenclature changes, especially hydrates.
- b) 8th edition of ST was just published, and can be ordered from International Bureau of Weights and Measures
- c) Green Book is essentially done, but many comments were received. It is hoped that it will be finished in 2006.
- d) It was noted that many societies are involved in nomenclature besides IUPAC

9b. **Educational Project** C. Magalhães

Clara Magalhães noted that the project was still ongoing and that she would give a full report next year.

9c. **Logistics for Subsequent Meetings** W. Voigt

Wolfgang Voigt indicated where each of the subcommittees should meet.

9. **Morning Session was adjourned at 10:25.** H. Gamsjäger

Afternoon Session: 14:00 - 17:00

10. **Meeting of Subcommittees**
Subcommittee: Gas Solubilities D. Knox
Subcommittee: Liquid Solubilities D. Shaw
Subcommittee: Solid Solubilities W. Voigt

Sunday, 23 July 2006

Morning Session: 9:00 - 12:00 (2 concurrent activities)

11a. **Meeting of Subcommittees (if necessary)**
Subcommittee: Gas Solubilities D. Knox

- 11b. Subcommittee: Liquid Solubilities
Subcommittee: Solid Solubilities
Meeting of Glossary Task Group
- D. Shaw
W. Voigt
D. Shaw

Afternoon Session: 14:00 - 17:00

- 12a. **Report of Gas/Liquid Subcommittee** D. Knox

Dana Knox reported that the subcommittee met during the afternoon session of the previous day. Members present were Pirketta Scharlin, Peter Fogg, Justin Salminen and Dana Knox.

Alan Mather's project is probably postponed indefinitely. If there is no further response within one month, it should be dropped from the list.

Pirketta Scharlin's project (carbon dioxide in aqueous non-electrolyte solutions) is progressing well. Alan Mather is helping with the evaluations. If those are completed, it may be possible that it will be ready for review by early 2007.

Dana Knox's project (solids and liquids in supercritical carbon dioxide) is stalled due to the size of project. It will be reconstructed into smaller projects and additional co-workers sought.

Peter Fogg has proposed a new project involving alkynes. Currently it is a gas/liquid project but by adding higher alkynes its scope would also fall within the liquid/liquid and solid/liquid areas. Mark Salomon commented that were some examples of this having been done in the past. David Shaw noted that there were some pentynes in water included in volume 81.

- 12b. **Report of Liquid/Liquid Subcommittee** D. Shaw

David Shaw reported that the subcommittee met during the afternoon of the previous day. Members present were Marian Góral, Valerii Sazonov, David Shaw and Andrzej Maczynski.

David Shaw reported that completed projects include Hydrocarbons with Water and Seawater by Andrzej Maczynski. This has already been published as volume 81 of the SDS in the Journal of Chemical and Physical Reference Data.

Also completed is Acetonitrile: Ternary and Other Multicomponent Systems by Valerii Sazonov. This was sent to the Journal of Chemical and Physical Reference Data in February.

Another completed project is Mutual Solubility of Alcohols and Water (an update of SDS Vol 15) by Andrzej Maczynski. This was sent to the Journal of Chemical and Physical Reference Data in May.

A current project is C3 and Higher Nitriles by Valerii Sazonov with David Shaw and Marian Góral. The proposal has been prepared and will be submitted. About 20/300 data sheets have been completed. Estimated completion is by the end of 2008.

Another current project is Mutual Solubility of Ethers, Ketones and Water. The proposal has been prepared and submitted, but final approval has not yet been received from IUPAC. 90 compounds have been done. They may be split for publication (one part on ethers, the other on ketones). The estimated completion date is mid-

2007.

Project No. 2005-017-1-500: *Glossary of Terms Related to Solubility*. The Orange Book has a section on solubility that is very inadequate, treating solubility of ionic salts only. The Division was highly receptive to replacing it with a modern list of terms. David Shaw, Jack Lorimer, Heinz Gamsjäger and Pirketta Scharlin have been working on this for about one year. They have compiled a list of 150 terms with draft definitions, and reached consensus on most of the definitions. A draft document will be prepared, which will then go through IUPAC review and eventually be published in *Pure and Applied Chemistry*. The Analytical Chemistry Division will no longer print the Orange Book, it will only be available online. Entries from the Orange Book will go into the Gold Book.

Project No. 2003-011-3-600 has been deleted. The joint project between the Analytical Division and the Environmental Division is inactive and unlikely to be revived.

A new project is on the solubility of furfural by Valerii Sazonov.

Another possible new project is on the solubility of esters and phenols in water by Andrzej Maczynski and Marian Góral.

At this point the report was opened up for questions.

Wolfgang Voigt asked why the Orange Book will be available on the web only; there is a danger that the definitions may change too often. Jack Lorimer discussed the Gold Book update and indicated that in the past errors were also corrected once per year. David Shaw mentioned that the Orange Book has always been a collection of IUPAC reports; the new scheme removes only the lag time. He also commented that as regards online vs print, the online version will be accessible to a much more general audience, not just the chemistry community.

12c. **Report of Solid/Liquid Subcommittee (Report distributed is in Appendix 4)**

W. Voigt

Wolfgang Voigt reported that the subcommittee had met over the course of the past day and that Christo Balarew, Jack Lorimer, Mark Salomon, Jitka Eysseltova, Wolfgang Voigt, Dewen Zeng, Heinz Gamsjäger, Clara Magalhães, Alex de Visscher, Masakazu Makino and Cezary Guminski were present. Wolfgang Voigt distributed a handout that represented the report of the subcommittee; it is attached to these minutes as Appendix 4. He then reviewed the items within the report.

Jack Lorimer commented that he should not be listed on the project Alkaline Earth Metal Carbonates; he also suggested that Erich Königsberger should not be either. Wolfgang Voigt replied that we should hold off deleting them as they may still contribute. Alex de Visscher commented that there has been a very limited amount to this point. Clara Magalhães noted that Erich Königsberger should be added to the project Metal Carbonates.

Cezary Guminski expressed his thanks to Dewen Zeng, and also to Wolfgang Voigt for catalyzing the meeting with Dewen Zeng.

13. **Report on the 12th ISSP – Freiberg, Germany, 2006**

W. Voigt

Wolfgang Voigt deferred to Daniela Freyer, Daniela Freyer reported that there are

128 registrations from 30 countries, including 10 registrations that were for the workshop only. There are 103 contributions, including 64 poster presentations, 31 short oral presentations, and 8 plenary or invited lectures. In addition, there 24 supporting attendees. Wolfgang Voigt pointed out that there are many cultural events as well.

Wolfgang Voigt indicated that the workshop is intended to produce a state-of-the-art paper on thermodynamic databases. The number of participants was kept low to try to maximize the likelihood of accomplishing this result.

Jack Lorimer asked if there is a contribution from NIST to the workshop? Wolfgang Voigt replied that Ken Marsh is coming at the suggestion of NIST.

Heinz Gamsjäger asked about the paper? Wolfgang Voigt replied that, as suggested by Earle Waghorne, he is contacting James Bull, scientific editor of *Pure and Applied Chemistry*, to include it in the ISSP issue.

14. **Future International Symposia on Solubility Phenomena**

H. Gamsjäger

Heinz Gamsjäger reported that Marcelle Gaune-Escard will be at the ISSP later in the week and that she will discuss plans for the 13th ISSP with the SSED membership then. Earle Waghorne commented that, based on his last communication with her, she is still planning to hold the 13th ISSP in Marseille in 2008, and that he is planning the 14th ISSP in Dublin in 2010.

Subsequently, during the 12th ISSP, Marcelle Gaune-Escard announced that she in fact would not be able to host the 13th ISSP in Marseille after all. Earle Waghorne subsequently agreed to host the 13th ISSP in Dublin in 2008, and Dana Knox tentatively agreed to host the 14th ISSP in 2010.

Heinz Gamsjäger then raised the issue of where and when the 6th Annual Meeting of the SSED (33rd overall) would be held next year. Suggested sites were in Torino in conjunction with the IUPAC General Assembly taking place 4-12 August 2007, or in Perth, Australia in conjunction with the 30th International Conference on Solution Chemistry taking place 16-20 July 2007. After some discussion, there was general consensus to meet in Torino at the "front end" of the General Assembly.

14a. **Additional Agenda Items**

H. Gamsjäger

Jack Lorimer commented that only Hans Wanner was here from the equilibrium "side" of SSED. Hans Wanner has the only equilibrium-related project, Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands. For this project, mercury has already been published, copper has been for publication/review, and lead is ongoing. Discussion ensued as to why there is so little interest / participation of the "equilibrium" side of SSED. James Sangster asked "What was in it for them? Probably they perceive nothing."

David Shaw pointed out that we had thought to develop / promote projects related to both solubility and equilibrium. The Analytical Chemistry Division has not channelled people interested in equilibrium projects through SSED. An example is the stability constant project. Instead, ACD receives reports directly, not SSED. For the stability constant project, L.D. Pettit is bowing out, and Erich and LanChi Königsberger are getting it; as a result, it will probably then be through SSED. David Shaw concluded his comment by noting the Analytical Chemistry Division needs to be impressed with the importance of having them linked to SSED, even if only intellectually.

Heinz Gamsjäger pointed out that many invitations had been made over several years, but mostly all had been declined.

Hans Wanner indicated willingness to try to bring people in in the future, for instance those involved in Heavy Metals in the Environment project. He also noted that all current projects are aqueous.

David Shaw stated that Heinz Gamsjäger should ask the Analytical Chemistry Division to put SSED members on equilibrium projects so that reports can pass through the SSED, and that we should also try to have all contributors listed in the Book.

Heinz Gamsjäger pointed out that Kip Powell has stated that we can not have all members listed on the website.

David Shaw observed that the new President of the Analytical Chemistry Division may be different - so we should try again!

Jack Lorimer pointed out that the Physical Chemistry Division lists 2 pages!

Heinz Gamsjäger stated the Analytical Chemistry Division does not want so many listed.

Alex de Visscher commented that such attitudes should be in past. Clara Magalhães noted the problem with the invites was of long standing. Hans Wanner observed that all was said.

Wolfgang Voigt asked that regarding the Franzosini Award, should we also give a certificate? The consensus seemed to be in agreement.

15. **Adjournment**

H. Gamsjäger

The 5th Annual Meeting (32nd overall) of the Subcommittee on Solubility and Equilibrium Data was adjourned at 15:30.

Attachments

A1

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A2

Item 4 on the Agenda: Franzosini Award

Award Winner's CV

Curriculum Vitae



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Personal information:

Name: Dewen Zeng
Sex: male
Date of Birth: 21. Sept. 1967
Place of Birth: Hunan, P. R. China
Nationality: Chinese

Education

Dr.rer.nat., Institute of inorganic chemistry, [TU Bergakademie Freiberg](#), Germany, 2003.

M. Eng., Department of non-ferrous metallurgy, [Central South University](#), P.R.China, 1992.

B.Eng., Department of non-ferrous metallurgy, [Central South University](#), P.R.China, 1989.

Experience

Professor, 2004-2006

[College of chemistry and chemical engineering, Hunan Univesity](#), P.R.China.

Scientific associate, 1999-2003

Institute of inorganic chemistry, [TU Bergakademie Freiberg](#), Germany

Teaching assistant, 1992-1998

Department of Non-ferrous Metallurgy, [Central South University](#), P.R.China

Research Interest

- Critical evaluation of solubility equilibrium data based on reliable thermodynamic models
- Correlation of structures and properties of complex salt-water mixtures
- Development and modification of various thermodynamic models

- Prediction of new phase change materials in thermodynamic models
- Prediction of solubility phase diagrams of salt lake brine.

Publication

Book:

- 1 Zeng, D.; “Thermodynamische Modellierung von Salz-Wasser-Systemen von der Lösung bis zur Salzsammelze”, Shaker Verlag, ISBN: 3-8322-1844-0, (in German), 2003.

Patent:

- 2 Neuschuetz, M.; Glausch, R.; Zeng, D.; Voigt, W., Heat-storage medium, used as latent heat storage medium or in building, air-conditioning or thermal insulation, contains ternary mixture of water and 2 of lithium, sodium, magnesium, potassium, calcium and zinc nitrates, Patent number: WO2004007635-A1, DE10231844-A1, AU2003242718-A1, EP1521814-A1, KR2005016961-A, US2005247906-A1, JP2005533142-W, CN1668718_A.

Periodical:

- 3 Zeng, D.; Zhou, H.; Voigt, W. “Thermodynamic consistency of the solubility and vapor pressure of a binary saturated salt + water system. II. $\text{CaCl}_2 + \text{H}_2\text{O}$ ”, will be presented in the 12th ISSP.
- 4 Zeng, D.; Zhou, J., “Thermodynamic consistency of the solubility and vapor pressure of a binary saturated salt + water system. I. $\text{LiCl} + \text{H}_2\text{O}$ ”, *J. Chem. Eng. Data*, 51 (2006) 315-321.
- 5 Zeng, D.; Born, M.; Wambach, K., “Pyrolysis of EVA and its application in recycling of photovoltaic modules”, *Journal of Environment Science*, 16 (2004) 889-893.
- 6 Zeng, D.; Fang, C.; Chen, S., “Phase diagram prediction of the heat storage systems $\text{Mn}(\text{NO}_3)_2\text{-M}(\text{NO}_3)_n\text{-H}_2\text{O}$ (M=Ca, Mg and Li) with modified BET-Model”, *Trans. Nonferrous Met. Soc. China*, 14 (2004) 1192-1198.
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- 11 Liu, H.; Zhang, C.; Zeng, D., “A new look at f -pH diagram (?)—All equilibrium f -pH diagram for M-H₂O system”, *Trans. Nonferrous Met. Soc. China*, 10 (2000) 808-812.
- 12 Zhang, C.; Liu, H.; Zeng, D.; Li, C., “A new method of computing multi-component E-pH diagrams”, *Journal of Central South University of Technology*, 6 (1999) 23-27.
- 13 Zhang, C.; Liu, H.; Zhong, D.; Zeng, D. “Thermodynamic analysis of smelting process of nickel sulfides concentrates”, *Zhongguo Yuese Jinshu Xuebao* (in Chinese), 9 (1999) 805-810.
- 14 Zhang, C.; Wang, Z.; Zeng, D.; Tan, P. “Study on viscosity of FeO-MgO-SiO_2 ”, *Kuangye Gongcheng* (in Chinese), 18(3) (1998) 41-43.
- 15 Zhang, C.; Li, C.; Zeng, D. “Fuel cells and their functional materials”, *Yuese Jinshu, Yelian Bufen* (in Chinese) (1998), 45-48.

- 16 Zhang, C.; Liu, H.; Zeng, D.; Zhong, D. "Program system for computer plotting of predominance area diagrams", *Zhongnan Gongye Daxue Xuebao (in Chinese)*, 29 (1998) 241-244.
- 17 Zeng, D.; Li, Z.; Liu, H.; Zhang, C., "Determination of viscosity of high Mg content slag of FeO-SiO₂-CaO-MgO system", *Zhongnan Gongye Daxue Xuebao (in Chinese)*, 28 (1997) 343-346.
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- 19 Li, Z.; Zhang, C.; Zeng, D.; Xu, S.; Tan, P. "Non-pollution metallurgical process of zinc sulfide concentrate - Hot-press briquetting and its mechanism", *Zhongnan Gongye Daxue Xuebao (in Chinese)*, 27 (1996) 680-684.
- 20 Tan, P.; Zhang, C.; Li, Z.; Zeng, D. "Copper loss in slag during Noranda matte-making process - computer simulation", *Youse Jinshu, Yelian (in Chinese)* (1996) 7-9.
- 21 Zeng, D.; Li, Z.; Xu, S.; Tan, P.; Zhang, C. "The technical reform of spent electrolyte treatment system of Jinchuan copper refinery", *Youse Jinshu, Yelian (in Chinese)*, (1996) 5-8.
- 22 Zeng, D.; Li, Z.; Tan, P.; Xu, S.; Zhang, C. "Thermodynamic study on nickel sulfidizing precipitation conditions", *Zhongguo Youse Jinshu Xuebao (in Chinese)*, 6(3) (1996) 35-38.
- 23 Tan, P.; Zhang, C.; Li, Z.; Zeng, D. "Computer model of distribution of the VA elements in copper smelting", *Zhongnan Gongye Daxue Xuebao (in Chinese)*, 26(4) (1995) 479-83.
- 24 Zhang, C.; Tan, P.; Li, Z.; Zeng, D.; Wu, C. "Mathematical model of distribution behaviors of the VA-group elements in copper smelting", *Zhongnan Gongye Daxue Xuebao (in Chinese)*, 26 (1995) 343-8.
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International Meeting:

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- 27 Tan, P.; Zhang, C.; Zeng, D.; Li, Z. "Viscosity of high magnesium content FeO-Fe₃O₄-SiO₂-CaO-MgO slag at nickel flash smelting conditions", Editor(s): Mishra, Brajendra. *EPD Congress 1999, Proceedings of Sessions and Symposia held at the TMS Annual Meeting, San Diego, Feb. 28-Mar. 4, 1999* (1999), 333-340. Publisher: Minerals, Metals & Materials Society.
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- 30 Zeng, D.; Zhang, C.; Li, Z., "Thermodynamic study on the sulphadizing precipitation of nickel", *Proceedings of the International Conference on Mining and Metallurgy of Complex Nickel Ores, Jingchang, China, International Academic Publishers, ISBN 7-80003-273-X/TF.9, 263-266.*
- 31 Zeng, D.; Zhang, C.; Li, Z. "Hydrometallurgical process for the treatment of waste Ni-Cu-Zn alloy", *Resources Recycling Technology, Proceedings of the 2nd International Symposium on East*

Asian, 14-16, Oct. 1993, Seoul, Korea, 380-385.

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A3

Item 6 on the Agenda: Chairman's Report 2005-2006

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

Activity Report 2005 – 2006

1. Visibility of SSED within IUPAC 2005/2006

CI, 27, No. 5, September-October 2005

Bookworm

p. 29: H. Lawrence Clever (editor), IUPAC-NIST Solubility Data Series 80.
Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon and Silicon and Xenon
Fluorides in All Solvents

CI, 27, No. 6, November-December 2005

Mark your Calendar

p. 38: First announcement 12th ISSP, Freiberg, Germany, 24-29 July, 2006

CI, 28, No. 1, January-February 2006

The Project Place

p. 22 Trevor M. Letcher, (Task Group Chairman, Interdivisional (I and V) project),
Developments and applications in solubility. Many contributors from members of
Solubility Data Group

p. 22 David Shaw (Task Group Chairman), Glossary of Terms Related to Solubility

p. 23 Hiroshi Miyamoto (Task Group Chairman), Solubility Data Series: Transition
and 12 to 14 Main Group Metals, Lanthanide, Actinide, and Ammonium Halates

Making an imPACt

p. 30 Solubility Data Series—Recent Reports

H. Lawrence Clever, et al. “Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon,
and Silicon and Xenon Fluorides in all solvents” (IUPAC-NIST Solubility Data
Series Vol. 80)

Andrzej Maczynski (volume editor), “Hydrocarbons with Water and Seawater –
Revised and Updated” (IUPAC-NIST Solubility Data Series Vol. 81; part I to VIII)

CI, 28, No. 1, March-April 2006

Features

p.4 Maria Clara F. Magalhães, Rosa Maria Oliveira, “Art and Science: Looking in
the same direction” (Exhibition at 11th ISSP)

2. *New Wiley Book*

Biom mineralization – Medical Aspects of Solubility

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 biom mineralization
processes”

Erich Königsberger and LanChi Königsberger

Chapter 3 “Calcium and magnesium phosphates: normal and pathological mineralization”

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

3. Completed SDS Volumes

Volume 81: Andrzej Maczynski *et al.*,

"Hydrocarbons with Water and Seawater – Revised and Updated,"

J. Phys. Chem. Ref. Data, **2005**, 34, No. 3, parts 5 and 6 (pp. 1399-1553).

J. Phys. Chem. Ref. Data, **2005**, 34, No. 4, parts 7 and 8 (pp. 2261-2342).

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

J. Phys. Chem. Ref. Data, **2006**, 35, parts 11 to 12, in press.

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, manuscript sent to Dr. Mark Salomon for publication in JPCRD, probably SDS vol. 82

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, manuscript sent to Dr. Mark Salomon for publication in JPCRD, probably SDS vol. 84

Project number: 2002-050-1-500

Project Title: **Acetonitrile: Ternary and Other Multicomponent Systems**

Task Group Leader: Valerii P. Sazonov

Starting date: January 2003

Report: Project has been completed in January 2006, manuscript sent to Dr. Mark Salomon for publication in JPCRD, probably SDS vol. 83

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: 1. Projected completion date (documents ready for external review): Parts 1 to 5 have been submitted to the Journal of Physical and Chemical Reference Data, or are under external review.

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:

Report: Projected completion date (documents ready for external review):
December 2006

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): *Postponed to the end of 2007*

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 to end 2006

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

Report: Projected completion data(documents ready for external review):?

Project Number: 2002-037-1-500

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

Task Group Leader: Masakazu Makino and Ayako Goto

Starting Date: 2002

Report: Project completion date(documents ready for external review): 2007(expected date).

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

Project number: 2002-045-1-500

Project Title: **Solids and liquids in supercritical carbon dioxide**

Task Group Leader: D.E. Knox

Starting date: 2002, Report: Projected completion date:Uncertain, perhaps end 2006

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: Projected completion date (documents ready for external review):**2007**

6. New SDS Projects

H.L. Clever, editor: **Oxygen and Ozone** (update of Volume 7 of the *IUPAC Solubility Data Series*),

Marian Goral, Andrzej Maczynski, editors: **Mutual Solubility of Ethers and Ketones with Water**,

Cezary Guminski, editor: **Rare Earth Metal Chlorides (Sc, Y, Lanthanoids) in Water and Aqueous Systems**

A4

**Item 12c on the Agenda: Report of the Solid/Liquid
Subcommittee**

Report of the Subcommittee on Solid Solubilities

W. Voigt

Freiberg, July 2006

Solubility data related to oceanic salt systems

Part I. Binary systems containing sodium, potassium, and ammonium sulfate (2002-033-1-500) C. Balarew, R. Bouaziz, R. Cohen-Adad, J.W. Lorimer, N. Ariguib. Part II. Magnesium chloride-water and calcium chloride-water and their mixtures (2002-034-1-500) W. Voigt

As stated in the report from the meeting in Portoroz 2005 the oceanic salt project volumes were postponed and the whole project has to be re-organized after the death of R. Cohen-Adad and the lost contact to R. Bouaziz. Thus during the Freiberg meeting Ch. Balarew, J. Lorimer, M. Salomon, I. Eysseltova and W. Voigt have discussed this issue. The sub-committee members agree that continuation of the oceanic salt system project is important. In order to obtain definite results in near future changes in the compiling and evaluation strategy were proposed. In the original procedure it was tried to coordinate compiling and evaluation work for the binary and higher-component systems in such a way that complete papers were elucidated only once. However, it was necessary to treat at the same time binary, ternary and higher-component systems, which requires a too high degree of organization and is time-consuming. Now compiling work for the binary systems will concentrate only on the binary data points even in papers with systems containing more components. The new strategy is supported by new publication format in JPCRD. In this manner the work on $\text{MgCl}_2\text{-H}_2\text{O}$, $\text{CaCl}_2\text{-H}_2\text{O}$, $\text{Na}_2\text{SO}_4\text{-H}_2\text{O}$ and $\text{K}_2\text{SO}_4\text{-H}_2\text{O}$ will be continued and accelerated.

- The part of $\text{MgCl}_2\text{-H}_2\text{O}$ will be definitely ready in 2007.
- For the part $\text{CaCl}_2\text{-H}_2\text{O}$ Prof. Dewen Zeng agreed to contribute. He has particular experience with this system from work on thermodynamic modeling.
- I. Eysseltova accepted to take over the responsibility for the volume of $\text{K}_2\text{SO}_4\text{-H}_2\text{O}$. Ch. Balarew came recently again into contact with R. Bouaziz, who is living now in Israel. Ch. Balarew will establish contact to R. Bouaziz again for transfer of previous work to Jitka Eysseltova. Then updating of references and compilation sheets will follow.
- The group proposed Christo Balarew should visit Marie-Therese Cohen-Adad in spring next year in order to go through all the material already collected and evaluated by Roger Cohen-Adad with the main focus on the system $\text{Na}_2\text{SO}_4\text{-H}_2\text{O}$. Appropriate support for this task seems to be necessary.

Furthermore the following principles were fixed.

- Despite the fact that modern system evaluations try to involve all thermodynamic properties of the system including properties of dilute solutions data evaluation in this task group will focus only on equilibria of saturated solutions.
- For the systems $\text{MgCl}_2\text{-H}_2\text{O}$ and $\text{CaCl}_2\text{-H}_2\text{O}$ application of the standard Pitzer equation is not appropriate. The Cohen-Adad - Lorimer approach (used for the alkaline metal halides earlier) will be applied for data evaluation.

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 Magalhães reported that work with Cd and Ni carbonates is done. With lead carbonates certain difficulties have to be overcome. Work will come to end in 2007.

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

The volume is ready in respect to compilation sheets. After the 11th ISSP in Aveiro Alex de Visscher took over responsibility for data evaluation. During this work it became clear that detailed re-evaluation is necessary. According to Alex de Visscher estimates the work can be finished in 2007. Help from outside in this stage of work is not really worthwhile.

Solubility data of compounds relevant to human health.

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

Progress is made in accordance with the schedule. No new information. Originally participation of E. and L.-C Königsberger at the meeting had to be cancelled by personal reasons.

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, the volume is ready to send for print.

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

Masakazu Makino explained that only data of about 45 compounds exist. Data evaluation in the traditional manner is not possible. Since solubility data of this class of compounds are highly needed from the public it is proposed to prepare a status report on the solubility data available with a preface of an expert view on these data and an elucidation of the methods used for solubility or phase equilibria determinations for these compounds. J. Lorimer proposed to consider estimations of maximum solubilities on the basis of melting points and enthalpies.

It was agreed to finish this small part in 2007.

Other systems and proposals

Aqueous lanthanide systems. C. Guminski and T. Mioduski

Project submission form was sent to IUPAC this year. C. Guminski reported on the status of his work. There appeared a number of relatively new Russian and Chinese (about 50) papers. Dewen Zeng was asked to help in translation.

Solubility in system aqueous containing LiNO_3 and/or 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.

Solubility of arsenic compounds

Clara Magalhães has long-standing experience with compounds of arsenic. Despite the importance for protection of human health little is done in respect to a systematic collection and evaluation of the thermodynamic properties including solubilities. She informed the committee about an on-going IUPAC activity on arsenic compounds. Members of SSED point out that independent from other activities it would be appropriate to propose a solubility project. After finishing the carbonate project, an arsenic proposal will be prepared by C. Magalhães.