



INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Analytical Chemistry Division

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA (SSED)

Minutes

4th Annual Meeting of SSED (31st overall)

held in conjunction with the

29th International Conference on Solution Chemistry

at Portoroz, Slovenia

26 August 2005

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

Friday, 26 August 2005

Morning Session 1: 9:00 - 10:30

Moments of Remembrance

H. Gamsjäger

A moment of remembrance was held for our two colleagues, Roger Cohen-Adad and Adam Skrecz, both of whom passed away since our last meeting. A short obituary for Adam written by colleagues in Poland will appear in *Chemistry International*.
On a happier note, Heinz Gamsjäger announced the wedding of colleague Justin Salminen.

1. **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.

2. **Approval of the Minutes of the 3rd Annual Meeting of SSED (30th overall) held in conjunction with the 11th International Symposium on Solubility Phenomena, Aveiro, Portugal, 24-25 July 2004**

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.

3. **Other Items for Agenda**

H. Gamsjäger

Cezary Guminski asked to add a discussion item about Chinese literature; item will be added after agenda item 8 as item 8a. He also asked to discuss the status and effect of IUPAC restructuring; this item will be added after agenda item 5 as item 5a.

4. **Franzosini Award** H. Gamsjäger

Heinz Gamsjäger announced that there was no recipient this year, and that the proceeds will be reinvested to next year. He called for nominations for the Franzosini Award to be given next year in Freiberg, and noted that giving two awards may be possible. He will make a final call for nominations at a later date.

5. **Chairman's Report for 2004 - 2005 (Full Report is in Appendix 2)** H. Gamsjäger

a) Visibility of SSED within IUPAC

Heinz Gamsjäger pointed out that there were items either from or about members of the SSED in several issues of *Chemistry International*, including a remembrance of Roger Cohen-Adad. Also, volume 77 of Pure and Applied Chemistry contained papers based on the plenary and invited lectures from the 11th ISSP held in Aveiro, Portugal.

b) Completed Volumes

Volumes 79, 80 and 81 in the Solubility Data Series were published in the *Journal of Chemical and Physical Reference Data*.

c) Current SDS Projects

Heinz Gamsjäger briefly updated the status of 10 ongoing projects

d) Postponed SDS Projects

Heinz Gamsjäger briefly discussed problems that 6 other ongoing projects have encountered that have led to their postponement. Projects should be "de-listed" if they are inactive. One of the projects in this category is that of Alan Mather; Heinz Gamsjäger pointed out that Pirketta Scharlin is for input from Alan, and that she should be informed of any problems as she may want a different critical evaluator. Another project in this category is that of Valerii Sazonov, who received funds for Aveiro last year. Vladimir Valyashko and Heinz Gamsjäger discussed this project and decided to leave as is for now (a subsequent update appears in the full report in the appendix).

e) New SDS Projects

Heinz Gamsjäger briefly introduced 6 new projects and discussed their current status.

f) Book Proposal

Heinz Gamsjäger discussed the new book proposed by Trevor Letcher to be entitled "Developments and Applications in Solubility". He pointed out that several SDS contributors, and speakers from the 11th ISSP, have been invited to contribute to it. Earle Waghorne reported that Trevor Letcher regards it as a joint project between Division 1 (Physical) and Division 5 (Analytical).

Heinz Gamsjäger indicated that the SSED group get a "plug" in the book since so many members of SSED are contributing.

Discussion ensued (primarily Vladimir Valyashko and Heinz Gamsjäger) on how SSED may be "misplaced" in the Analytical Division, but that there are no plans to change this.

Heinz Gamsjäger reported that he had suggested at the Analytical Chemistry Division (ACD) meeting at the IUPAC General Assembly in Beijing held 13-14 August 2005 that the ACD "Critical Evaluation" Task Group should review appropriate chapters of the book. This idea was approved.

- 5a. **Status of IUPAC Restructuring** C. Guminski
- Heinz Gamsjäger indicated that the President, Vice President and Past President all say that the new structure is better. Glenn Hefter asked if anyone outside the hierarchy felt the same way? Several people (James Sangster, Glenn Hefter, Earle Waghorne, Vladimir Valyashko, Alex DeVisscher) all discussed the difficulty of getting funds to attend meetings. Glenn Hefter mentioned the activities of Physical Chemistry and the International Association of Chemical Thermodynamics that runs the Chemical Thermodynamics symposia, and does so outside of IUPAC with separate accounts. Glenn Hefter further noted that no one from the Equilibrium side of SSED was present in Portoroz; Heinz Gamsjäger replied that nonetheless activity related to the Equilibrium side was in fact proceeding, and that he would forward information on this activity. Cezary Guminski raised the question of getting additional younger members involved in IUPAC.
6. **Editor-in-Chief's Report for 2004 - 2005 (Full Report is in Appendix 3)** (M. Salomon)
- Heinz Gamsjäger discussed the Editor-in-Chief's report in the absence of Mark Salomon. Copies of the report as submitted by Mark Salomon were distributed, and is included here in Appendix 3.
Cezary Guminski reported some problems with indexing regarding item 5 under Volumes in Preparation.
7. **Database Agreement** (D. Shaw)
- There was a feeling that this item did not require discussion, especially since David Shaw was not present. Glenn Hefter asked an update on its status. Heinz Gamsjäger reviewed the pertinent parts of the minutes from last year's minutes.
8. **Volumes for Next Year's SDS Proposals** (M. Salomon)
- This topic was included in the Editor-in Chief's Report (see Appendix 3). James Sangster expressed great interest in the suggestion of a possible volume on ionic liquids. A discussion ensued as to whether they should be considered as molten salts? James Sangster will contact Mark Salomon to pursue his interest in this area.
- 8a. **Problems with Chinese Literature** C. Guminski
- Cezary Guminski reviewed the difficulties in using Chinese literature, including no translations and difficulties of access. Heinz Gamsjäger commented that Wenchuan Wang (former national representative for China) may be able to help; he is also the national representative for ACD. However, he would probably want monetary support if substantive help is required. Glenn Hefter suggested that SSED should ask, not individual workers. Wolfgang Voigt suggested establishing a new project to fund translations for other projects. It was noted that if we make someone a co-author, they will receive some money. Heinz Gamsjäger indicated that he would make inquiries to identify any potential collaborators / translators from China.
- 8b. **SSED Membership** H. Gamsjäger
- Heinz Gamsjäger brought up the issue of SSED membership. A great deal of intense discussion ensued about whether the membership list should be: a short list (officers only) or a list that also includes all those leading projects or a long list that includes all of those actively participating in SSED meetings and/or activities. No resolution was reached during the morning session.
9. Morning Session 2 (agenda item 9) was cancelled; subcommittee members were asked to meet over lunch and/or before afternoon session. **Morning Session 1 was adjourned at 12:10.** H. Gamsjäger

Afternoon Session: 14:00 - 18:00

10. **Reports of Subcommittees and Projects**

W. Voigt

Only the Solid/Liquid Systems chairperson was present, thus projects in this area were discussed first.

Solid/Liquid

Wolfgang Voigt first discussed the projects related Oceanic Salts, noting that contributors are missing / no longer available and that the work must therefore be reorganized. He proposed that as a first step to proceed with only the $MgCl_2 / H_2O$, and to work with Vladimir Valyashko and his Russian colleagues about how to proceed in the future, with a decision to be reached at Freiberg. Heinz Gamsjäger commented that the contract with the Journal of Chemical and Physical Reference Data is paid by the volume and that splitting the work is costly. Wolfgang will discuss with Mark Salomon to resolve the issue. Heinz will also discuss the issue with Mark, as Mark should account for this in the new contract (current contract expires this year).

Wolfgang Voigt next discussed the projects related to Mobility of Metals in the Environment. Regarding the project about alkaline earth metal carbonates headed by by Jan Vanderdeelen, he stated that Alex De Visscher should be co-author. They will review the evaluations, which have some serious errors. Alex discussed this topic in some detail; additional discussion involved Glenn Hefter, Vladimir Valyashko and Wolfgang Voigt. This project is expected to be complete by the end of 2006. The metal carbonate project headed by Heinz Gamsjäger is proceeding satisfactorily.

Wolfgang Voigt next discussed the projects related to the solubility of compounds relevant to human health. In particular he discussed the projects about hydroxybenzoic acids and hydroxybenzoates headed by Ayako Goto and Hiroshi Miyamoto, and about halogenated aromatic hydrocarbons headed by Ayako Goto with co-workers Rensuke Goto, Masakazu Makino and Hiroshi Miyamoto.

Wolfgang Voigt mentioned that he had no new information about the sugar project.

Jitka Eysseltova proposed a new project for solubility in aqueous systems of $LiNO_3$ and $NaNO_3$. She already has perhaps 100 or more sheets for $LiNO_3 / H_2O$.

Cezary Guminski proposed a new project for lanthanum halides (chlorides to start) in water (Cezary would be taking over from T. Miodoski). Heinz Gamsjäger asked that Cezary include a reference to industrial systems in proposals for both of these so that they may be included under the phantom proposal.

Liquid/Liquid

Glenn Hefter reported (in the absence of David Shaw) that Marian Góral states that the volume on alcohol / water will be finished soon.

Marian Góral stated that he or Andrzej Maczynski will be producing a proposal in about October entitled "Mutual solubility of ethers and ketones with water".

It was noted that there was no information about Valerii Sazonov's project.

11. **Report on the 12th ISSP - Freiberg, Germany, 2006**

W. Voigt

Wolfgang Voigt reported that the various committees have been formed. The preferred topics (some tailored to the local industry) have been listed. There will be a parallel workshop entitled "Quality Assurance in Thermodynamic Databases for Performance Assessment Studies in Waste Disposal". Preliminary registration will be due by 15 November 2005. Earle Waghorne will be the symposium editor. Preliminary choices for plenary lecturers include: Gerd Maurer, Hans Wanner, John O'Connell, Joan Brennecke and William Acree, among others, as well as someone in gas hydrates and someone in geochemistry. Wolfgang further mentioned that both the social program and the post-conference tour are in the planning stages, and that the prices for very good hotels are the range of 50 - 70 USD.

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

H. Gamsjäger

Heinz Gamsjäger reported that Marcelle Gaune-Escard had stated (when they met in Beijing) that she would be in Portoroz (*she arrived after the meeting had concluded*) and could host the 13th symposium in 2008. Earle Waghorne has agreed to host the 14th symposium in 2010 and could host the 13th symposium instead if a problem arises with holding it in France. Dana Knox will consider hosting the subsequent symposium in the USA.

13. **Additional Agenda Items**

H. Gamsjäger

The issue of the Subcommittee member listings was again brought up for discussion. Heinz Gamsjäger indicated that IUPAC will not support listing all participants on the IUPAC website. Several people pointed out most of the participants are volunteering their time and that their only hope of receiving support to participate in SSED activities is if they are listed as active members. After much discussion it was decided to list the officers on the IUPAC website, but to include a link to the SSED homepage where everyone could be listed. The current officers were decided to be:

Chair: Heinz Gamsjäger

Secretary: Dana Knox

Gas/Liquid: Dana Knox

Liquid/Liquid: David Shaw

Solid/Liquid: Wolfgang Voigt

Editor-in-Chief: Mark Salomon

Homogeneous Equilibria: Hans Wanner

Other Equilibria: Wolfgang Hummel

Stability: Erich Königsberger

14. **Adjournment**

H. Gamsjäger

The 4th Annual Meeting (31st overall) of the Subcommittee on Solubility and Equilibrium Data was adjourned at 16:10.

Attachments

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Attendees at the Meeting

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Item 5 on the Agenda: Chairman's Report 2004-2005

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

Activity Report 2004 – 2005

1. Visibility of SSED within IUPAC 2004/2005

CI, **26**, No. 6, November-December 2004

IUPAC Wire

p. 17: Marian Góral received the 2004 Franzosini Award.

CI, **27**, No. 1, January-February 2005

Conference Call

p. 30: "Solubility Phenomena", by Heinz Gamsjäger

PAC, **77**, March 2005

p. iii: In memoriam. Professor Roger Cohen-Adad: Scientist, teacher, and gentleman

Lectures from Symposia

Papers based on presentations at the 11th International Symposium on Solubility Phenomena (11th ISSP), Aveiro, Portugal, 26-29 July 2000 pp. 513-665

(H. Gamsjäger, G.T. Hefter, M.C.F. Magalhães, eds.)

CI, **27**, No. 3, May-June 2005

IUPAC Wire

IUPAC Poster Prizes

2004 IUPAC Poster Prize Recipients

Solubility Phenomena-ISSP 2004-Aveiro, Portugal

Ada Villafáfila García (Department of Chemical Engineering, Technical University of Denmark, Lyngby) "Solid-liquid-vapour equilibrium for sparingly soluble salts found in natural waters"

Mara G. Freire (Department of Chemistry University of Aveiro) "Oxygen solubility in perfluorocarbon emulsions and Water solubility in perfluorocarbons"

Remembering Two Prominent IUPAC Members

Roger Cohen-Adad and **H. Steffen Peiser**

2. Completed SDS Volumes

Volume 79: J. Hala and H. Akaiwa,

"Alkali and Alkaline Earth Metal Pseudohalides,"

J. Phys. Chem. Ref. Data, **2004**, *33*, No. 1, 1-176.

Volume 80: H. Lawrence Clever *et al.*,

"Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon, and Silicon and Solid Xenon Fluorides in all Solvents,"

J. Phys. Chem. Ref. Data, **2005**, *34*, No. 1, 201-438.

Volume 81: Andrzej Maczynski *et al.*,

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

J. Phys. Chem. Ref. Data, **2005**, *34*, No. 2, parts 1. and 2. (pp. 441-552) parts 3. and 4. (pp. 657-753).

3. Current Projects

IUPAC Project Progress Report

August 2005

Project number: 2002-025-1-500

Project Title: Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds

Task Group Leader: *J. Hala*

Report:

1. Current status of project: *The volume "Inorganic Actinide Compounds" will comprise some 370 compilation data sheets (of these 355 already prepared) and 10-15 critical evaluations (2 already prepared). Literature is covered till the end of 2004. Also, most of the work on indexes has been done.*

2. Progress relative to 'milestones': *6 to 9 months late.*

3. Difficulties encountered (or concerns): *In spite of all efforts, about 60 documents could not have been compiled. An Appendix will be added listing these documents.*

4. Projected completion date (documents ready for external review): *Summer or early fall 2005*

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: *The results of this project will be published in JPCRD and will eventually be included in the web-accessible solubility database maintained by the US National Institute of Standards and Technology.*

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *No IUPAC budget.*

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: -----

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: *J. Vanderdeelen / A. De Visscher*

Report:

1. Current status of project: *Modeling of the data as suggested at the Ottawa SSED annual meeting was initiated.*
2. Progress relative to 'milestones': *Substantial delay due to retirement of J. Vanderdeelen and relocation from Belgium to Canada of A. De Visscher.*
3. Difficulties encountered (or concerns): *See 'milestones'. The modeling project as proposed in Ottawa will be kept to a minimum. This means, for example, that CO₂-H₂O-MCO₃ data will be used to derive solubility constants between 0-100°C with a simple Pitzer model. The redefined scope and objective of this project will officially be agreed upon on the next SSED annual meeting. Budget will not cover entire travel and subsistence cost to SSED annual meeting in Portoroz.*
4. Projected completion date (documents ready for external review): *Late in 2006.*
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: *Publication in J Phys Chem Ref Data as a Solubility Data Series volume.*
6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *Travel and subsistence for SSED annual meeting in Portoroz.*
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:

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*

Report:

1. Current status of project: *Ongoing project. The various metals are in different stages. Ni: compilation and critical evaluation completed. Cd: critical evaluation completed, Zn, Cu, Fe: compilation and evaluation essentially completed. Mn: compilation advanced, evaluation started. Pb, compilation advanced, evaluation started. Co, Hg, Ag compilation advanced, evaluation not yet started.*
2. Progress relative to 'milestones': *Relative to 'milestones' given in the original project submission form, the project is about one year late.*
3. Difficulties encountered (or concerns): *Activities connected with the 43rd General Assembly and the 40th IUPAC Congress 13 – 21 August 2005, though very stimulating with respect to this project, meant time consuming commitments for HG.*
4. Projected completion date (documents ready for external review): *The draft of this SDS volume is expected to be ready for external review by the end of 2006.*

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: *The results of this project will be published in JPCRD and will eventually be included in the web-accessible solubility database maintained by the US National Institute of Standards and Technology. A poster with the title "Thermodynamic Analysis and Application of Metal Carbonate Solubilities" is being contributed and presented at the 40th IUPAC Congress 2005 in Beijing, China.*

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *Not applicable*

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: *A (book) project: # 2005-016-1- Developments and applications in solubility by Trevor Letcher has come up and appropriate references to the SDS volume "solubilities of metal carbonates" should be provided for in this book.*

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*

Report:

1. Current status of project: *ongoing*

2. Progress relative to 'milestones': *evaluations essentially completed, typing of compilation sheets continued*

3. Difficulties encountered (or concerns): –

4. Projected completion date (documents ready for external review): *mid 2006*

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: *Volume for Solubility Data Series*

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *N/A*

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:

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:

1. Current status of project:

All of the solubility data of hydroxyl benzoic acids and hydroxybenzoates have been compiled. A total of 440 original studies treating ternary systems published from 1898 to 2001 has been carried out. The solubilities of hydroxyl benzoic acids and alkyl p-hydroxybenzoates in water and in various alcohols at various temperatures were statistically evaluated. A manuscript to be submitted to the Journal of Physical and Chemical Reference Data is in preparation. The title is as follows; IUPAC-NIST Solubility Data Series. Hydroxybenzoic Acids and Hydroxybenzoates with Water or Organic Solvents: Binary and Multicomponent Systems.

2. Progress relative to milestones:

The compiled data and the evaluated data will be submitted to the JPCRD.

3. Difficulties encountered (or concerns):

We have no problems because Professor Wolfgang Voigt and Dr. Mark Salomon gave appropriate suggestions to the Task Group at the 3rd Annual Meeting of SSED, University of Aveiro, Portugal. Due to the many commitments of the Task Group Chair the completion of this project has been somewhat delayed, but after this summer the situation will improve.

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

We would like to finish this project in about half a year.

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:

An article (JPCRD) is in preparation. Every compiled sheet has been checked and arranged to submit.

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

We have not got any budget for our project in advance, although we asked for some budget last year. We would like to get some budget for our project hereafter. If possible, we hope to get refunded for some of the traveling expenses of our group.

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:

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, Ayako Goto, and Rensuke Goto*

Report:

1. Current status of project:

First, we have started to study the aqueous solubility of polychlorinated biphenyls (PCBs) among the halogenated aromatic hydrocarbons, because much attention has been paid to these chemicals as environmental contaminants. For two years, we have compiled the aqueous solubility data of PCBs since 1949 and have started to evaluate them.

2. Progress relative to milestones:

It is well known that the number of PCB congeners is 209. We have compiled about 40 – 50 % of the solubility data including biphenyl. We have paid special attention to the solubility of chlorinated biphenyl isomers.

3. Difficulties encountered (or concerns):

The number of data investigated until today was too small to evaluate them on the basis of statistical methods. In addition to this, the values tended to depend largely upon respective experimental systems.

On the other hand, it was found that the aqueous solubility data should be separated into two categories, liquid-liquid and solid-liquid system, because the melting point of some PCBs is near room temperature.

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

We would like to finish this project by 2007.

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?

We have not got any budget for our project, though we asked some budget last year. We would like to get some budget for our project hereafter. If possible, we hope to get a few traveling expense for our group,

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:

We have pointed out that the aqueous solubility data of PCBs extend over two categories, liquid-liquid and liquid-solid system. Now we are preceding this project in liquid-liquid sub-committee, but the above issue persists among us.

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*

Report:

1. Current status of project:

Ongoing project. Search for the very present literature (2003-2005) is continuously under way.

Altogether about 370 data pages have now been compiled and updated to the format required for the Journal of Physical and Chemical Reference Data. At the moment, the compiled data consist of 60 different solvent systems, including aqueous solutions of alcohols, ethers, ketones, carboxylic acids, sugars, and nitrogen containing organic compounds. Compilation of new data is in progress along with the search for the most recent literature.

Among the solvent systems consisting of aqueous solutions nitrogen containing organic compounds, the aqueous alkanolamine systems form an important section. Compiled data on the CO₂ + aqueous alkanolamine systems (107 compilations on 36 different solvent systems, about 250 pages altogether) have been sent to Professor Alan E. Mather (in November 2003) for preparation of critical evaluation of these systems. Professor Mather has now promised to complete his part by the end of 2005.

2. Progress relative to 'milestones':

Relative to 'milestones' given in the original project submission form, the project is late. (For the reasons, see # 3).

3. Difficulties encountered (or concerns):

Lack of time continues to be a problem and the biggest obstacle to a more rapid progress: The work within this project cannot be done during the office hours because people working for the project are still active in their normal working life and their responsibilities for their university must take the priority.

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

Completion date depends on the progress in the critical evaluation of the CO₂ + aqueous alkanolamine systems. Supposing the evaluation will be completed by the end of 2005, the documents could be ready for external review in September 2006.

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 utilise any remaining budget for this project? *Not applicable*

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:

Project number: 2002-045-1-500

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

Task Group Leader: *D.E. Knox*

Report:

1. Current status of project: *Active project with most of data obtained and data sheets being produced*
2. Progress relative to 'milestones': *No milestones have been established*
3. Difficulties encountered (or concerns): *As noted in previous report, data continues to appear faster than it can be compiled into data sheets. Since acquiring my new position at the university last year, I have been unable to devote sufficient time to this project. Fortunately, a graduate student, Syed Abdullah, is now working on this project with me. We have established a cut-off date of December 31, 2004 to address the first concern noted above.*
4. Projected completion date (documents ready for external review): *Mid-2006*
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: *Will be published as part of the Solubility Data Series when completed.*
6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *N/A; no budget*
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: *There is such a large amount of data in this area it may have been more appropriate to plan multiple volumes each restricted to a particular type of solute.*

Project number: 2005-006-1-500

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

Task Group Leader: *Andrzej Maczynski*

Report:

1. Current status of project: *The project is in progress*
2. Progress relative to 'milestones': *all the new 175 compilations and 17 new evaluations have been already prepared and 18 new evaluation are in preparation*
3. Difficulties encountered (or concerns): *no difficulties*
4. Projected completion date (documents ready for external review): *1.1.2006*

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: *The Volume 15 will be updated in five following articles for the Journal of Physical and Chemical Reference Data:*

Part 1, C₄ Alcohols + Water

Part 2, C₅ Alcohols + Water

Part 3, C₆ Alcohols + Water

Part 4, C₇ Alcohols + Water

Part 5, C₈ – C₁₇ Alcohols + Water

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *For the Task Group Meeting at Slovenia, August 2005.*

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.

Joint Project CED and ACD number: 2003-010-3-600

Project Title: A Critical Compendium of Pesticide Physical Chemistry Data

Task Group Leader: *Wauchope/Shaw*

Report:

1. Current status of project: *Scope of work is settled (properties to be treated and pesticides to be covered). Project is in early data compilation phase.*

2. Progress relative to 'milestones': *Project has diverged from original milestones due to 1) expanded list of properties to be treated, 2) need for additional compilers, 3) need for access to industrial data.*

3. Difficulties encountered (or concerns): *Additional task group members are needed to address expanded scope of work.*

4. Projected completion date (documents ready for external review): *No realistic estimate can be made at this time.*

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: *1) compendium of evaluated data published as a monograph or extended article in scientific journal, 2) browser-based electronic database prepared in collaboration with project 2001-022-1-600.*

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project? *Not applicable*

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:

4. Projects postponed

Projects to be taken off the IUPAC website are highlighted in yellow.

Chr. Balarew project #2002-033-1-500 and **W. Voigt** project #2002-034- 1-500 encountered problems due to the unavailability of several contributors. As a result, these projects are being re-organized and will not finish by 2006.

For details see Wolfgang Voigt's (Chair of Task Groups on solubilities in s-l systems) report.

J.W. Lorimer (2 projects): **Projects #2002-038-1-500 - and #2002- 042-1-500** have to be postponed and will not be finished in the next two years, due to Jack Lorimer's many other IUPAC commitments.

A. Mather: **Project #2002-043-1-500** is overdue and has not been reported on at the 3rd and 4th Annual Meeting of SSED (24 – 25 July 2004 and 26 July 2005, respectively) and thus must probably be postponed indefinitely.

V. Sazonov project #2002-050-1-500: No progress has been made since the previous report, however, on September 5, 2005 Valerii Sazonov indicated that he will send the Preface of this project for internal review still this September. The other parts will follow subsequently.

5. New Projects

Status of Project Submission Form highlighted in light green

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

João AP Coutinho, editor: Solubility of Sugars in Aqueous and Nonaqueous Solutions, **Project Submission Form is with H. Gamsjaeger for filling in funding requests.**

H. Miyamoto, R. Miyamoto, C. Guminski, M. Salomon, editors: Transition and 12 to 14 Main Group Metals, Lanthanides, Actinides and Ammonium Halates. **Project Submission Form is with C. Guminski for filling in completion dates.**

Jitka Eysseltova, Solubility in aqueous systems containing LiNO₃ and/or NaNO₃. **Project Submission Form needed.**

T. Mioduski and C. Guminski, Aqueous lanthanide chloride systems. **Project Submission Form is with C. Guminski for filling in milestones.**

M. Goral and Andrzej Maczynski, Mutual solubility with water of ethers and ketones. **Project Submission Form needed.**

6. Book Proposal

As so many contributors to the Solubility Data Series are eager to write chapters of Trevor Letcher's book SSED fully supports this project and considers it a spin-off of its activities.

DEVELOPMENTS AND APPLICATIONS IN SOLUBILITY

Trevor Letcher, editor

Speakers at the 11th ISSP in Aveiro are printed in red

Contributors to SDS are printed in green

Information of Trevor from 2 September 2005

A. Theory, Techniques and Results

1. Thermodynamics of Nonelectrolyte Solubility by Professor Emmerich Wilhelm (Vienna)
2. Thermodynamics of Electrolyte Solubility by Professor Earle Waghorne (Dublin)
- 3.. Solubility of Solids in Bayer Liquors by Professor Glenn Hefter (Murdoch), Professor Erich Koenigsberger and Professor Peter May.
4. Solubility of Solids in Radioactive Waste Repositories by Dr. Wolfgang Hummel (Paul Scherrer Institute, Switzerland).
5. Solubility of Gases, Ionic Liquids, Solvents and Aqueous Solutions by Professor G. Maurer (Kaiserslautern).
6. Solubility Data Banks by Professor David Shaw (Harvard).
7. Solubility Phenomena in "green" Quaternary Mixtures (ionic liquid+water + alcohol + CO₂) by Professor Luis P N Rebelo and Professor M Nunes da Ponte (New University, Lisbon).
8. Solubility in Water and Seawater by Professor Rubin Battino (Wright State) and Professor Larry Clever.
9. Isotopic Effects in Solubility by Professor Alexander van Hook (Tennessee, Knoxville) and Professor Luis P N Rebelo (New University, Lisbon).
10. Solubility of Organic Solids for Industry by Professor U Domanska (Warsaw).
11. Solubility of Gases in Molten Salts by Professor Reg Tomkins (New Jersey.)
12. Solubility of Impurities in Cryogenic Liquids by Professor Dominique Richon (Ecole Des Mines, Paris) and Dr V de Stefani (Imperial College, London).
13. Solubility of BTEX and Acid Gases in Alcanolamine Solutions in relation to the Environment by Professor Dominique Richon (Ecole des Mines, Paris) and Dr C Coquelet.

B. Modeling and Simulation

14. Solubility and Molecular Modeling by Professor M Costa Gomes (Clermont Ferrand).
15. Molecular Simulation Approaches to Solubility by Professor J Ilja Siepmann and Professor Kelly E Anderson (Minnesota).
16. "Predicting Solubility with COSMO-RS" by Dr Frank Eckert (COSMOGermany)
17. Solubility and Solubility Parameters by Professor Alan Barton (Murdoch)

C. Industrial Applications

18. Solubility of Gases in Polymers by Professor Jean-Pierre Grolier and Dr S Boyer (Clermond Ferrand).
19. Solubility in the Metallurgical and Hydrometallurgical Processes by Dr J Salminen and Professor T Kashiala (Helsinki).

20. Solubility related to Reaction and Process Design by Professor **Ralf Dohrn** (Bayer, Germany).
21. Solubility in the Pharmaceutical Industry by Professor Jacques Fages (Ecole des Mines, d'Albi).
22. Solubility in Food, Pharmaceutical and Cosmetic Industries by Professor **Maria Eugenia Macedo** (Porto) and Professor Simão Pedro de Almeida Pinho (TI Bragança)
23. Solubility Data and Predictions in Industry by Professor Jurgen Gmehling (Oldenburg) and Dr W Cordes (DDBST).
24. Solubility of Gases in Industry by Professor Joan Brennecke (Notre Dame).
25. Solubility of CO₂ in Industrial Applications by Professor John Prausnitz and Dr **J Salminen** (Berkeley).
26. Solubility of the Oil Industry by Dr Tony Goodwin (Schlumberger Products) and Professor K Marsh(Canterbury)
27. Solubility in Super Critical Fluids by Professor Cor Pieters (Delft).
28. Solubility of Inorganic solids and their importance in Industry by Professor **Wolfgang Voigt** (Freiberg)
29. Liquid-liquid Solubility and Solvent Extraction in Industry by Professor Andreas Heintz (Rostock)
30. Solubility from a Nanotechnology point of view by GET

At the ACD Meeting in Beijing 13-14 August 2005 HG suggested that ACD Task Group “Critical Evaluation” (Balarew, Bonardi, Gamsjäger, Powell) should review chapter 5, highlighted in blue, prior to publication. Other chapters highlighted in lighter blue may also be reviewed by this Task Group.

A3

Items 6 & 8 on the Agenda: Editor-in-Chief's Report 2004-2005

Editor-in-Chief's Report

Item 6 on The Agenda, Volumes published in 2004-2005

1. J. Hála, Volume 79, *Alkali and alkaline earth metal pseudohalides*, JPCRD **33(1)**, 1 (2004).
2. H.L. Clever, Volume 80, *Volatile Fluorides*, JPCRD 34(1), 201 (2005).
2. A. Maczynski and D. G. Shaw, eds. with contributions by M. Goral, B. Wisniewska-Gocłowska, A. Skrzecz, I. Owczarek, K. Blazej, M-C. Haulait-Pirson, G. T. Hefter, F. Kapuku, Z. Maczynska, and A. Szafranski, Volume 81, *Hydrocarbons with Water and Seawater—Revised and Updated*, Parts 1-4, JPCRD **32(2)** (2005).
 - Part I: C₅ Hydrocarbons with water, page 441.
 - Part II: Benzene with water and heavy water, page 477.
 - Part III: C₆H₈ - C₆H₁₂ Hydrocarbons with Water and Heavy Water, page 657.
 - Part IV: C₆H₁₄ Hydrocarbons with Water, page 709.
3. A. Maczynski and D. G. Shaw, eds. Volume 81, *Hydrocarbons with Water and Seawater—Revised and Updated*, Parts 5-8: Manuscript proofs received and corrected, and publication is expected later this year or early 2006.
 - Part 5: C₇ Hydrocarbons with Water and Heavy Water.
 - Part 6: C₈H₈ - C₈H₁₀ Hydrocarbons with Water.
 - Part 7: C₈H₁₂ - C₈H₁₈ Hydrocarbons with Water.
 - Part 8: C₉ Hydrocarbons with Water.

Volumes in Preparation

1. *Hydrocarbons in Water and Seawater*. The first 8 parts have either been published or are in course of publication (see above), and the remaining parts 9-12 have been submitted and are being type set by the AIP for JPCRD. The remaining parts which will probably be published in 2006 are:
 - Part 9: C₁₀ Hydrocarbons with Water (19 systems, 10 evaluations)
 - Part 10: C₁₁ and C₁₂ Hydrocarbons with Water and Heavy Water.
 - Part 11: C₁₃ - C₃₆ Hydrocarbons with Water.
 - Part 12: C₅ - C₂₆ Hydrocarbons with Seawater.
2. Jiri Hála, *Solubilities of Inorganic Actinide Compounds*. The manuscript is essentially complete and will probably be submitted in the fall of 2005.
3. João Coutinho and his colleagues are working on a volume on sugars. Expected completion date is 2005-6 to be discussed during the SSED meeting in Portoroz.
4. H.L. Clever, *The solubility of oxygen in all solvents* (Update of SDS vol 7. 1981). . Larry Clever is working on an update to "Oxygen," and he estimates that 250 pages will be required and completion will take 18-20 months.
5. T. Mioduski and C. Guminski, Lanthanides. Cezary is revising and updating this work and will report on progress during the meeting in Portoroz.
6. V. Sazonov and D. Shaw, Acetonitrile, ternary systems. The volume is nearing completion and David Shaw will provide details during the meeting.

7. Jan Vanderdeelen, Alex De Visscher, Erich Königsberger, Jack Lorimer, *Alkaline earth metal carbonates*, in course of publication.

8. *Solubilities in supercritical CO₂* - need Dana's input here for update information.

9. Don Wauchope and David Shaw, *A Critical Compendium of Pesticide Physical Chemistry Data*; - no information available at this time.

10. Aya Goto *et al.*, *Benzoic acids and biphenyls*, - no information available at this time.

11. *Antibiotics*. No progress available at this time.

Other Publications

- "History of The IUPAC Solubility Data Project," H.L. Clever, abridged version published in *Chem. Intern.*, 2004 and full paper published in *J. Chem. Eng. Data*. I will ask Larry for specific references.

Item 8 on the Agenda: New Projects for Future Publications

The list of volumes expected to be completed in 2005-6 is difficult to predict. One volume which has been approved is Carbon dioxide in aqueous non-electrolyte solutions, by Pirketta and Justin Salminen. I believe that Justin is now at USC Berkeley, and Pirketta will not be able to attend the Portoroz meeting for personal reasons (congratulations to Pirketta by the way). Another new project submitted by Valerii and David deals with acetonitrile-water mixtures. I have no information on the status of this project at this time, but from email correspondence with David, it appears to be progressing nicely. Another new volume in progress from the group at the PAN deals with the update to the *Alcohol-water* volume: I believe this is an update to Volume 15 by Allan Barton. A progress report on this project will be presented in Portoroz by either David or Andrzej.

I assume updated information on these and other volumes will be forthcoming during the Portoroz meeting.

Other Issues

I strongly urge that SSED members be asked to prepare a list of future volumes including subject matter and suggested contributors. One topic of specific interest to me and Marcelle is ionic liquids, a very hot and important topic these days.