



INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Analytical Chemistry Division

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA (SSED)

Minutes

2nd Annual Meeting of SSED

held in conjunction with the 42nd IUPAC General Assembly at Ottawa, Canada

11 - 12 August 2003

The "List of Attendees" with complete addresses, telephone and fax numbers together with e-mail addresses is attached to these minutes (A1)

Monday, August 11, 2003

Morning Session: 9:00 - 12:00

1. **Welcome of the participants** H. Gamsjäger
Heinz Gamsjäger, Chairman of the SSED welcomed the participants.
Then the participants were asked to identify themselves and their affiliation.
2. **Franzosini Award 2003** H. Gamsjäger
Pirketta Scharlin received the Franzosini award for her continuous activities within the Solubility Data Group and her efforts to recruit young scientists for the work on Solubility Data Projects. An announcement will be made in CI.
3. **Approval of Minutes of the 1st Annual Meeting of SSED held in conjunction with the 10th ISSP at St. St. Constantine and Helen Resort, Varna, Bulgaria, July, 2002** H. Gamsjäger
W. Voigt
The Minutes had been distributed by e-mail before the meeting and handed out as hard copies at the meeting. The Varna Minutes were approved.
3. **Other Items for Agenda**
 - J. Lorimer asked for a discussion of the "History of the Solubility Data Project"
A brief history is on disk now and should be refereed by M. Salomon, J. Lorimer, W. Voigt.
 - Venue of the meeting in 2005
According to the decision in Varna, the odd numbered years meeting should be held in connection with the GA. The GA 2005 will be in Peking, which causes difficulties in travelling for a number of SSED members. It was proposed to

decide the venue 2005 at the meeting in Aveiro

4. **Chairman's Report for 2002 - 2003**

H. Gamsjäger

Heinz Gamsjäger pointed out a number of publications and contributions of SSED members and himself in "Chemistry International", "Pure and Applied Chem." and "Chemical Monthly", which enhanced the visibility of the subcommittee's activity. Once more Heinz Gamsjäger reminded and appreciated the successful 10th ISSP last year in Varna complemented by a social "Message from Bulgaria", which shall be translated into the languages of the SSED members (see attachment A2).

A new guideline for Publication of Volumes in the IUPAC-NIST Solubility Data Series (SDS) in Journal of Physical and Chemical Reference Data (JPCRD) was prepared (see attachment A3)

In the discussion it was suggested to put the project of St. Sjöberg (Speciation) on the SSED list.

5. **Report about the Meeting of the Division of Analytical Chemistry**

H. Gamsjäger,

D. Shaw

The subcommittee was informed about activities and initiatives in ACD as

- the directory of expertise, where the SSED is asked for completion and corrections
- ongoing discussion on project ideas (K_{OW} project, mass spectroscopy, traceability in Analytical Chem.)
- the revision of the orange book

The chairman of SSED reported at the ACD Meeting about the activities of the SSED, its visibility inside and outside IUPA (see attachment A4, A5) and argued against too formal handling of preconditions for successful passing of project proposals like "stake-holders" or end-users. Results from long-standing collaborations in SSED (or former SSD) like the books "**The Experimental Determination of Solubilities**" and "Chemicals in the Atmosphere - Solubility, Sources and Reactivity" or the book proposal (meanwhile accepted by Wiley & Sons) "**Medical Applications of Solubility**", E. Königsberger and LanChi Königsberger (eds.) (see attachment A5) would never have been reached with short-termed and non-flexible project proposals.

Further information from the division meeting concerned

- availability of financial support for conferences in developing countries and for new topics
- refereeing plenary and invited lecturers

For the revision of the section of solution equilibria in the orange book participation of a small task group (D. Shaw, H. Gamsjäger, M. Salomon, P. Fogg, P. Scharlin) was recommended.

6. **Editor-in-Chief's Report for 2002 - 2003**

M. Salomon

Three volumes were finished within the last year:

Volume 77

V. Sazonov and D.G. Shaw, *C2+ Nitroalkanes with Water or Organic Solvents: Binary and Multicomponent Systems*, JPCRD, **31(1)**, 1 (2002)

Volume 78

Acetonitrile, Binary Systems, Eds. Valerii P. Sazonov and David G. Shaw

Volume 79

Azides, Cyanides, Cyanates, and Thiocyanates of Alkali Metals, Alkaline Earth Metals and Ammonium, J. Hála.

Further volumes are near to completion:

Project # 2001-052-1-500

Solubility of volatile fluorides in all solvents

(H.L. Clever) , approved as non-funded project

Transition Metal, Lanthanide and Ammonium Halates: Vol. 4

(H. Miyamoto, R. Miyamoto), submission form has to be prepared

Other volumes are in an advanced state:

Alkaline Earth Metal Carbonates in Aqueous Solutions

(J. Vanderdeelen, E. Königsberger)

Solubility of Hydroxybenzoic Acids and Hydroxybenzoates

(A. Goto and H. Miyamoto)

On occasion of his visit to Aveiro M. Salomon met João AP Coutinho, who would be willing to work on the volume of solubilities of sugars, which was started by Raul Herrera earlier.

R.P.T. Tomkins reported that the Textbook " The Experimental Determination of Solubilities" has been printed now and presented a copy of the volume.

7. **New SDS Project: Octanol-water Partition Coefficients** D. Shaw
This new project will be an interdivisional project (ACD and Environmental Div.). Besides D. Shaw, J. Sangster and A. Skrzec will contribute from SSED side.

Afternoon Session: 14:00 – 18:00

8. **Individual Meetings of Task Group Leaders and volume contributors in the working parties gas-liquid, liquid-liquid and solid-liquid**
9. **Joint Meeting ACD/SSED 16:00 – 18.00**
Participants: Gamsjäger, May, Moore, Powell, Salomon, Scharlin, Shaw, Voigt
results see topic 11.

Tuesday, August 12, 2003

Morning Session: 9:00 - 12:00

10. **Discussion of problems with preparation of volumes** all participants
At present the volumes in JPCRD are printed in landscape format, a portrait format would be preferable though. Conversion seems to be not easy.
11. **Discussion of working principles of the SSED in the future** SSED, J. Lorimer
Report on the Joint Meeting ACD/SSED:
- the phantom proposals are generic in nature
 - specific proposals referring to the phantom proposal cannot be considered as accepted automatically; they have to fulfil the specific requirements of every proposal
 - Planning of financial allocations within a given proposal needs more

- flexibility
- the end-user can be implemented in the last stage of a project; he must not be an active compiler or evaluator
- the question was raised how to secure IUPAC compatible symbols in volumes printed in JPCRD; it was suggested that J. Lorimer should check example pages in an official way
- the two proposals of SSED in question had been accepted several months before by D. Moore; there was a problem of communication flow from secretary to the subcommittee
- the new K_{ow} as an interdivisional project was discussed as mentioned under topic 7.

12. **Report on status of volume projects**

Task Group Leaders

Solubility of Carbon dioxide in aqueous Non-electrolyte Solutions

(P. Scharlin, J. Salminen) year of completion: 2004/05

listed in Phantom proposal as IV.14

Mutual Solubility of Carbon dioxide and lower alkanes at pressures above 2 bar

(A.E. Mather) listed in Phantom proposal as IV.14

year of completion was planned to 2003, however, no new information from A.E. Mather; P. Scharlin will ask for the present status

Solubility of Solids and Liquids in Supercritical Carbon dioxide

(D.E. Knox) completion at best end of 2004

listed in Phantom proposal as IV.15

Acetonitrile: Ternary and Other Multicomponent Systems"

Sazonov, Shaw and Skrzecz, Estimated Completion was 2003, Sazonov will prepare a justification of the volume including relevance of the systems to industrial processes;

C-3 and Higher Nitriles: Binary and Multicomponent Systems

Sazonov, Shaw and Skrzecz, Estimated Completion Date: 2004, Work will commence when 1. above is complete.

Hydrocarbons with Water (Update)

Maczynski, Shaw and Skrzecz, Estimated Completion Date: update to be produced in sections over the next 2 years

Alkaline Earth Metal Carbonates in Aqueous Solutions

(J. Vanderdeelen, E. Königsberger)

listed in Phantom proposal as I.1.

The volume is nearly being completed, the critical evaluation has been performed, however, some problems occurred with the content of the preface in relation to the volume's content. The problem was pointed out by J. Lorimer and discussed with H. Gamsjäger and W. Voigt. Also it was suggested to compare some of the evaluated solubility data with model calculations by E. Königsberger.

Solubility of Hydroxybenzoic Acids and Hydroxybenzoates

(A. Goto and H. Miyamoto)

listed in Phantom proposal as III.6

Volume is in a very advanced state and can be completed in year 2004

Lead Sulfate

(J.W. Lorimer)

listed in Phantom proposal as IV.12

Project will be completed in 2004

Transition Metal, Lanthanide and Ammonium Halates: Vol. 4

(H. Miyamoto, R. Miyamoto)

Compilation and evaluation sheets have been revised and checked,
The project is related to the Phantom proposals topic IV and will be completed in 2004

Solubility of Halogenated Aromatic Hydrocarbons

(A. Goto, M. Makino, R. Goto and H. Miyamoto)

listed in Phantom proposal as III.7.

there problems arose with the critical evaluation procedure due to the small number of data for individual substances as well as with the experimental techniques used by the authors.

The project is ongoing but a finishing date cannot be given

Solubility data related to oceanic salt systems.

Part I. Binary systems containing sodium, potassium, and ammonium sulfate (2002-033-1-500)

Part II. Magnesium chloride-water and calcium chlorides-water and their mixtures (2002-034-1-500)

For part I. the actual situation is uncertain and Ch. Balarew will make suggestions in the near future how to proceed.

For part II. the system $MgCl_2-H_2O$ is compiled, $CaCl_2-H_2O$ under work. It is considered to include the $SrCl_2-$ and $BaCl_2-H_2O$ systems

Molybdates and Tungstates of Alkaline and Alkaline Earth Metals

(V. Valyashko, J. Sangster)

Compilation is nearly completed, however, a suited evaluation strategy has to be developed. Completion not before 2004. It is a non-funded project.

C. Guminski is ready to complete the work of Mioduski on **Lanthanoide halides**. The material in typed and hand-written form from Mioduski is at present in Freiberg and will be sent to C. Guminski together with an up-dated CA search.

In the discusson it was emphasized that projects listed in the phantom proposal should be given first priority !!

Future International Symposia on Solubility Phenomena

13. **2004: 11th ISSP - Aveiro, Portugal**

C. Magalhães
M. Salomon

M. Salomon reported from his visit in Aveiro that the organizing committee has all under control except funding, where several different ways have to be tried out (US Army, UNESCO)

A list of invited speakers exists (see attachment A6)

The conference will be located at the university campus 15-20 min. away from the hotels

2006: 12th ISSP - Freiberg, Germany

W. Voigt

W. Voigt is ready for organizing the conference with low fees for participants.

14. **Nomination of a new secretary for SSED**

H. Gamsjäger

The nomination of a new secretary was found necessary because the former secretary became vice-rector of his home unversity. Dana Knox was elected as the new secretary by acclamation. D. Knox agreed to take over this responsibility.

15. **Adjournment**

Attachments

A1

Attendees at the Meeting

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A2

10th ISSP, Social Aspect:

Message from Bulgaria

To the future generations

May you, who will come after us, never forget your roots.

They are not only the source of our national pride and identity, they are also our only real link with the whole world. They are the reason for the past, present and future dignity of our nation.

Olga Markova, The role of Bulgarian culture in world civilization ? Hristo Botev ?
Sofia 2002, p. 49.

German Translation

An unsere Nachkommen

Möget ihr, die ihr nach uns kommt, niemals die Wurzeln eurer Herkunft vergessen. Diese sind nicht nur der Ursprung unseres nationalen Selbstbewußtseins und unserer Eigenart, sie verbinden uns auch in einzigartiger Weise mit allen Kulturen dieser Welt. Sie sind die Grundlage für die Würde unseres Volkes. So war es in der Vergangenheit, so ist es in der Gegenwart und so wird es auch in aller Zukunft sein.

More Translations expected



A3

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Guidelines For Publication of Volumes in the IUPAC-NIST Solubility Data Series (SDS) in the Journal of Physical and Chemical Reference Data (JPCRD)

The guidelines established under the auspices of the former IUPAC Commission V.8 have undergone changes as a result of the 2000 IUPAC General Assembly in Brisbane. The revised guidelines are discussed in detail below.

In brief, the following 7 steps summarize the procedures for publication of a volume in the SDS. Details are given following this summary.

1. Proposal for a „volume“ to SSED.
2. Acceptance of the proposal by the SSED.
3. Review of the volume during preparation paying attention to JPCRD and IUPAC guidelines and formats.
4. Preparation of a brief written proposal for review and inclusion as part of a phantom proposal (if applicable) or as a new project on the standard IUPAC form).
5. Submission of the Project Submission Form to the ACD.
6. Completion of the draft volume and final review by the SSED.
7. Submission of the volume to JPCRD.

1. Proposal for a Volume. Brief summaries of a proposed volume are submitted by author(s) either by letter or orally to the chair of the working party (the three working parties are gas/liquid, liquid/liquid and solid/liquid). Normally, authors present these

summaries at one of the yearly meetings of SSED. Authors summarize the nature (topic) of their proposed volume, estimates of size of the volume and time required to complete the volume, and the names of colleagues (co-editors and/or compilers) who have agreed to contribute to the volume. The working party either accepts or declines these proposals.

2. Acceptance of the proposal by the SSED. Volume proposals are evaluated both on the basis of the proposed topic (relevance to areas emphasized in phantom proposal¹⁾, appropriate scope, and relationship to other volumes previously published and in preparation) and the qualifications of the proposed task group (in terms of scientific expertise in the systems to be covered, familiarity and prior experience with procedures and standards of the Solubility Data Series, and facility with the English language). If the proposed volume is accepted by the working party, the chair presents details to the full subcommittee. The proposal is discussed and either accepted, declined or modifications are suggested.

3. Review of the volume during the preparation stage. Authors initially submit sample compilations and critical evaluations to the working party chair and to the Editor-in-Chief. The working party chair and the Editor-in-Chief send selected critical evaluations and compilations to SSED members for review (e.g., the Task Group members). At this stage, all reviewers are known to the authors. If additional expertise is needed, scientists outside of the SSED are sought for additional review. These initial submissions are reviewed for scientific content and for the formats required by the JPCRD. This is a continuing process throughout the course of the project. ***It is a strict rule that these volumes do not serve as a vehicle to publish any data which has not been published in a peer-reviewed journal.*** Throughout the course of preparation of the volume, additional detailed discussions on scientific content and formatting are carried out at the yearly meetings of SSED and by extensive email correspondence.

4. Preparation IUPAC Project Submission Form. In the initial stages of a project, the SSED prepares a Project Submission Form identifying the project as one included in the Phantom Proposal¹⁾ or as a new project. The Project Submission Form is based on input from the authors, working party chair, task group members and the SSED chair.

5. Submission of the Project Submission Form to the ACD. With approval of the SSED, the Project Submission Form is submitted to the ACD by the SSED chair. While the scientific responsibility for the Solubility Data Projects in general rests entirely with SSED, the estimation of the impact of a particular volume in the field is also the responsibility of ACD.

6. Completion of the draft volume and final SSED review. Throughout the course of the project, i.e. steps 3-5 above, the working party chair and the Editor-in-Chief receive various sections of the volume for final comments and discussion, and upon completion of the manuscript, the complete draft volume is submitted to the Editor-In-Chief. The Editor-In-Chief reviews the prior reviews related to the volume and may request further internal or external review as he judges appropriate.

¹⁾ The efforts to find a compromise between the new short-time project-driven system of IUPAC and the requirements of data evaluations for long-term work resulted in a "Phantom Proposal" with a four years' period. The Proposal was approved at 2nd of July 2002. Consequently volumes within its range receive higher priority.

7. Submission of the volume to JPCRD. When accepted by the Editor-in-Chief as "final" electronic copy, the volume is submitted to the editor of JPCRD for review by the journal. If there are comments by JPCRD reviewers, these are responded to by the authors and, when possible, by the Editor-in-Chief if these are simple comments. Both the editor of JPCRD and the Editor-in-Chief review the proofs before publication.



A4

Visibility of SSED within IUPAC

CI, 24, No. 4, July 2002

New Books and Publications

p. 21: IUPAC-NIST SDS, **76**, "Solubility of Ethyne in Liquids", *JPCRD*, **30**, pp. 1693-1875, 2001, P.G.T. Fogg *et al.*

CI, 24, No. 5, September 2002

New Books and Publications

p. 28: IUPAC-NIST SDS, **77**, "C₂₊ Nitroalkanes with Water or Organic Solvents: Binary and Multicomponent Systems",
JPCRD, **31**, pp. 1-121, 2002, V.P. Sazonov *et al.*

PAC, 64, No. 10, October 2002

Lectures from Symposia

p. 1785-1920: 13 Plenary and invited lectures presented at the 10th International Symposium on Solubility Phenomena, Varna, Bulgaria, 22-26 July 2002 (David Shaw, ed.)

CI, 24, No. 6, November 2002

Awards and Honors

p. 17: Dana Knox receives the Franzosini Award

IUPAC Projects

p.20-21: New Solubility Data Projects, 1) Solubility data of compounds relevant to mobility of metals in the environment, 2) Solubility data related to oceanic salt systems, 3) Solubility data related to industrial processes

Reports from Conferences

p.31-32: Solubility phenomena – application for environmental improvement (John W. Lorimer, report of 10th ISSP)

CI, 25, No. 2, March – April 2003

Mark your Calendar

p.36: First announcement of “Solubility Phenomena, Including Related Equilibrium Processes” (11th ISSP, 25-29 July 2004, Aveiro, Portugal)

CI, 25, No. 3, May – June 2003

IUPAC Wire

p. 10: David Shaw appointed to *JPCRD* Editorial Board

Bookworm

p. 21: IUPAC-NIST SDS, **78**, “Acetonitrile Binary Systems”, *JPCRD*, **31**, pp. 989-1133, 2002, V.P. Sazonov *et al.*

The Project Place

Solubility data of compounds relevant to human health, 1) Solubility of substances related to urolithiasis, 2) Solubility of hydroxybenzoic acids and hydrobenzoates, 3) Solubility of halogenated aromatic hydrocarbons

CI, 25, No. 4, July – August 2003

Bookworm

p. 30: The Experimental Determination of Solubilities, G.T. Hefter and R.P.T. Tomkins, (eds.), John Wiley & Sons 2003

p. 31: Chemicals in the Atmosphere-Solubility, Sources and Reactivity, P. Fogg and J. Sangster, (eds.), John Wiley & Sons 2003

Where 2B&Y

p. 36: Second, detailed announcement of “Solubility Phenomena” 25-29 July 2004, Aveiro, Portugal

A5

NEW BOOK PROPOSAL: John Wiley & Sons

Medical Applications of Solubility, Erich Königsberger and LanChi Königsberger (eds.)

The topic is primarily concerned with the role of solubility in understanding the fundamental mechanisms and processes associated with the formation of a variety of pathological biominerals, in vivo, from various perspectives. These include fundamental thermodynamic and kinetic concepts but also unconventional approaches such as the relation to liquid-precursor processes and industrial chemical processes.

- Erich Königsberger (Franzosi Award 1994) and LanChi Königsberger (Franzosi Award 1998): “Solubility phenomena related to normal and pathological biomineralisation processes”
- Felix Grases and Antonia Costa Bauza: “Mechanisms of renal calculi formation and development”
- M. Clara F. Magalhães (hosts the 11th ISSP, 2004): “Calcium and magnesium phosphates: normal and pathological mineralisation”
- Tim St. Pierre and Wanida Chua-anusorn: “Pathological biomineralisation of iron”
- Gordon Parkinson (Editorial consultant for project 2002-031-1-500, Alkaline Earth Metal Carbonates in Aqueous Solutions): “Pathogenic biomineralisation – lessons for and from industry”
- Laurie Gower: “Relevance of a polymer-induced liquid-precursor (PILP) mineralisation process to normal and pathological biomineralisation”

A6

11th ISSP: Plenary and Invited Lectures
(still incomplete)

- S. Sjöberg**, *Sweden* - Chemical speciation and solubilities in aqueous heavy metal system
- J. P. Grolier**, *France* - Modifications of the vitreous transition of polymers through gas solubility
- M. Costa-Gomes**, *France* - Gas-liquid interactions in solution
- K. Thomsen**, *Denmark* - Modelling electrolyte solutions with Extended UNIQUAC
- U. Domanska-Zelazna**, *Poland* - Solubilities and thermophysical properties of "ionic liquids"
- G. Hefter**, *Australia* - Ion solvation in aqueous-organic mixtures
- P. Williams**, *Australia* - Solutions in the big laboratory: towards a model for metals at the Earth surface
- M. Hugerat**, *Israel* - Using solubility phenomena to teach chemistry for kids
- M. N. Ponte**, *Portugal* - Solubility in supercritical fluids
- E. Macedo**, *Portugal* - Solubility of sugar, aminoacids and proteins
- D. Knox**, *USA* - Supercritical Extraction Experiments
- J. Vanderdeelen**, *Belgium* - Consistency issues of solubility data and solution thermodynamics of electrolytes
- W. Hummel**, *Switzerland* - Solubility equilibria and geochemical modelling in the field of radioactive waste disposal
- W. Königsberger**, *Australia* – Prediction of electrolyte solubilities in multicomponent aqueous solutions