INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
Analytical Chemistry Division
Subcommittee on Solubility and Equilibrium Data (SSED)

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

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

1. Welcome of participants

Heinz Gamsjäger, Chairman of SSED welcomed the participants.

Introduction of participants

Attendees were asked to identify themselves and their affiliation. The Chairman welcomed in particular Dana Knox, who received the "Franzosini Award 2002" for his continuous activity within the Solubility Data Group.
The Chairman also read out the greetings from P. Fogg, A. Goto and E. Königsberger, who by various reasons could not attend the meeting.

2. Approval of Minutes of the 27th Annual Meeting (21th of SDC) held at Queensland University of Technology, Brisbane, Australia, 29-30th June 2001

The Brisbane Minutes were approved.

3. Other Items for Agenda

J. Lorimer suggested to discuss how to publish the history of subcommission V.8..
Item 12.A

4. Nomination of a Secretary for SSED

Since the former secretary Heinz Gamsjäger chairs the subcommittee nomination of a new secretary became necessary. The chairman proposed Wolfgang Voigt for this task, which was confirmed by the members of the committee. The secretary took over responsibility.

5. Chairman's Report for 2001-2002 – H. Gamsjäger, D. Shaw

The new IUPAC Organisation has been completed. The activities of SSED have to adapt the SDS projects into the new system of IUPAC.

The SSED consists now of 7 members :
Heinz Gamsjäger (Chair of SSED, Associate member of Analytical Div.)
Wolfgang Voigt (Secretary of SSED)
Mark Salomon (Editor-in-Chief)
David Shaw (Associate member of Analytical Div.)
Pirketta Scharlin
Staffan Sjöberg
Peter May

The Analytical Division is represented now by
10 Titular members of IUPAC
6 Associate members
6 National Representatives

The new guidelines of operation within the Analytical Division are published in "Chemistry International" and the secretary of SSED will send copies to participants of the meeting.

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. Referees have been : J. Rumble, K. Marsh, T. Becker, St. Baskin, H. Wanner.
One referee report is attached as A1 in the appendix.

The phantom proposal formulates 5 topics :

I. **Solubility Data of Compounds Relevant to Mobility of Metals in the Environment**
II. **Solubility Data Related to Oceanic Salt Systems**
III. **Solubility Data of Compounds Relevant to Human Health**
IV. **Solubility Data Related to Industrial Processes**
V. **Solubility Data Related to Global Climate Change**

A copy of the phantom proposal is attached to the minutes.
The actual work will proceed through individual solubility data task groups, which apply for support on the basis of the phantom proposal. Members of SSED (D. Shaw, M. Salomon, H. Gamsjäger, W. Voigt, P. Scharlin, K. Marsh) discussed the procedure for individual proposals. Guidelines for task group leaders will be distributed.
Although volumes listed in the phantom proposal will be given priority, other volumes which are nearing completion are welcome.

The work of SSED will be published in JPCRD, which is known for one of the highest impact factors among the physical and chemical journals. This ensures broad dissemination within the worlds scientific community and high scientific standard.

6. Editor-in-Chief's Report for 2001-2002 – M. Salomon

Volumes published 2001-2002

Volume 73
Chr. Balarew and T.P. Dirkse, *Metal Formates,* JPCRD, **30(1)**, 1 (2001).

Volume 74
J. Hála, *Actinide Carbonates and Carbon-Containing Compounds,* JPCRD, **30(2)**, 531 (2001).

Volume 75
H.U. Borgstedt and C. Guminski, *Non-Metals in Liquid Alkali Metals*. JPCRD, **30(4)**, 835 (2001).

Volume 76
P.G.T. Fogg, *Ethynes*, JPCRD, **30(6)**, 1693 (2001).

Volume 77
V. Sazonov and D.G. Shaw, *C2+ Nitroalkanes with Water or Organic Solvents: Binary and Multicomponent Systems*, JPCRD, **31(1)**, 1 (2002).

Volumes Submitted.

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

Volumes Ready For Submission

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

New Proposed Volumes

Solubilities of Inorganic Actinide Compounds, J. Hála. Synopsis: Except for actinide nitrates and carbonates, which have been covered earlier in separate volumes of the SDS (Volumes 55 and 74, respectively), the proposed volume would include solubilities of hydroxides, halides, sulfates, phosphates, arsenates, and other inorganic actinide compounds. Together with the two mentioned volumes, of which volume 74 included also the solubilities of actinide organic compounds, the proposed volume would represent an exhaustive collection of solubilities of all actinide compounds. The volume can be expected to be of interest for the radiochemical community, particularly for those who are engaged in the field of management and disposal of radioactive wastes, because the solubility of uranium, thorium, neptunium, plutonium, and americium compounds is one of the important factors affecting the stability of actinides in the wastes, and their behavior in the environment.

General Procedures For Submission of Reviewed Volumes

The Editor-in-Chief receives reviewed volumes from the gas/liq, liq/liq and solid/liq

chairs and carries out a final check on formats.

Supplemental information is prepared: Editorial Board and special instructions for the publisher.

The volume is then sent to the editor of JPCRD (Mal Chase) who then carries out another check on formats before sending the manuscript to the American Institute of Physics (AIP). The AIP sends page proofs to M. Chase and M. Salomon for final check.

Upon final approval, Claim Forms for all contributors, subcommittee chairs and the E-I-C are submitted to IUPAC for payments.

The E-I-C receives 25 reprints from the AIP which are forwarded to Dr. Fabienne Meyers at the IUPAC Secretariat for distribution to each contributor and others upon recommendation of the Chair and E-I-C.

General Notes on Previously Published Volumes.

A number of volumes published by Pergamon Press* and Oxford University Press* quickly sold out and the publishers decided not to reprint these volumes. Several inquiries were made to republish volumes 37, 38 and 62 in the JPCRD, but no decisions have been made. This possibility will be pursued in the coming year.

Volume 37
D.G. Shaw, *Hydrocarbons with Water and Seawater. Part I: Hydrocarbons C5 to C7*

Volume 38
D.G. Shaw, *Hydrocarbons with Water and Seawater. Part II: Hydrocarbons C8 to C36*

Volume 62
P. Scharlin, *Carbon Dioxide in Water and Aqueous Electrolyte Solutions*

For volumes 1-65, unsold volumes are available for sale at the IUPAC Secretariat for USD 80 per volume at the following URL:
<http://www.iupac.org/publications/sds/index.html>.

Title	Quantity
Volume 9: W. Hayduk, *Ethane* (1982)	9
Volume 16/17: E. Tomlinson and A. Regosch, Antibiotics: *1,-Lactam Antibiotics* (1985)	9
Volume 19: C.L. Young, *Cumulative Index: Volumes 1-18* (1985)	9
Volume 22: T. Mioduski and M. Salomon, *Scandium, Yttrium, Lanthanum and Lanthanide Halides*	9
Volume 25: C. Hirayama, Z. Galus and C. Guminski, *Metals in Mercury* (1986)	9
Volume 30: H. Miyamoto and M. Salomon, *Alkali Metal Halates, Ammonium Iodate and Iodic Acid*	9
Volume 31: J. Eysseltova and T.P. Dirkse, *Alkali Metal Orthophosphates* (1988)	9
Volume 35: A.N. Paruta and R. Piekos, *4-Aminobenzenesulfonamides. Part II: 5-membered Hete*	9
Volume 36: A.N. Paruta and R. Piekos, *4-Aminobenzenesulfonamides. Part III: 6-membered Hete*	9
Volume 39: C.L. Young, *Cumulative Index: Volumes 20-38* (1989)	9
Volume 40: J. Hala, *Halides, Oxyhalides and Salts of Halogen Complexes of Titanium, Zirconium,*	9
Volume 42: P.G.T. Fogg and W. Gerrard, *Hydrogen Halides in Non-aqueous Solvents* (1990)	9
Volume 44: H. Miyamoto, E.M. Woolley and M. Salomon, *Copper and Silver Halates* (1990)	9
Volume 45/46: R.P.T. Tomkins and N.P. Bansal, *Gases in Molten Salts* (1991)	9
Volume 47: R. Cohen-Adad and J.W. Lorimer, *Alkali Metal and Ammonium Halides in Water and*	9
Volume 49: F. Getzen, G. Hefter and A. Maczynski, *Esters with Water. Part II: Esters 7-C to 32-C*	9
Volume 50: P.G.T. Fogg, *Carbon Dioxide in Non-aqueous Solvents at Pressures Less Than 200 I*	9
Volume 52: I. Lambert and H.L. Clever, *Alkaline Earth Hydroxides in Water and Aqueous Solution*	9
Volume 54: W.E. Acree, Jr., *Polycyclic Aromatic Hydrocarbons in Pure and Binary Solvents* (199	42
Volume 55: S. Siekierski and S.L. Phillips, *Actinide Nitrates* (1994)	43
Volume 56: D. Shaw, A. Skrzecz, J.W. Lorimer and A. Maczynski, *Alcohols with Hydrocarbons* (1	41
Volume 57: W. Hayduk, *Ethene* (1994)	42
Volume 58: W.E. Acree, Jr., *Polycyclic Aromatic Hydrocarbons: Binary Non-aqueous Systems, Pa*	43
Volume 59: W.E. Acree, Jr., *Polycyclic Aromatic Hydrocarbons: Binary Non-aqueous Systems, Pa*	42
Volume 60: A.L. Horvath and F.W. Getzen, *Halogenated Methanes with Water* (1995)	40
Volume 61: C.-Y. Chan, K.H. Khoo, E.S. Gryzlova and M.-T. Saugier-Cohen Adad, *Alkali Metal ar*	43
Volume 63: H.U. Borgstedt and C. Guminski, *Metals in Liquid Alkali Metals, Part I: Be to Os* (199	16
Volume 64: H.U. Borgstedt and C. Guminski, *Metals in Liquid Alkali Metals, Part II: Co to Bi* (199	16
Volume 65: J.J. Fritz and E. Koenigsberger, *Copper(I) Halides and Pseudohalides* (1996)	27

Starting with volume N°. 66, individual SDS volumes (issues) of JPCRD are available both as special subscriptions to The Series and as reprints of selected issues. For more information, visit the JPCRD web site at <http://ojps.aip.org/jpcrd/>, or email NIST at <jpcrd@nist.gov>.

*Note that Pergamon printed 500 copies each of volumes 1-53, and Oxford University Press printed 200 copies each of volumes 54-65.

7. Database agreement

The NIST pilot project on data conversion of SDS volumes to the on-line Webbook is finished. Response of potential users has been positive. Additional volumes will be converted in the next 1 – 2 years. Requested volumes, which are out of print will be preferred, that is "Hydrocarbons in Water" (Vol. 37, 38) and " Carbon Dioxide in Water and Aqueous Electrolyte Solutions" (Vol. 62).

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SSED achieved an outstanding scheme in on-line publication through the NIST contract. We are working to implement 3 active ways of transferring the IUPAC-NIST SDS volumes into the internet, which will make the results of the projects available for the scientific and engineering community:

- conversion of previous volumes into the Webbook
- automatic transfer of evaluated data in current volumes into the Webbook
- on-line publication of JPCRD

The Webbook is free of charge for the user.

8. Volumes for the next years

Topic is treated by the reports of liquid-gas, liquid-liquid and solid-liquid group (13.1., 13.2., 13.3)

9. Status Report on the Textbook " The Experimental Determination of Solubilities" by R.P.T. Tomkins

The complete manuscript was submitted to John Wiley & Sons, Ltd. (Chichester, U. K.) in March 2002 as a CD.

R. Tomkins met with Jenny Cossham (Publishing Editor in March 2002 to discuss details of various phases in the publication process. The text will be typeset.

The following represent the people at John Wiley who are responsible for producing the text.

Jenny Cossham	(Publishing Editor)
Sarah Corney	(Production Manager)
Irene Cooper	(Copy Editor)

As of July 1, Ms. Cooper is copy-editing each chapter prior to its being sent to the typesetter.

Ms. Cooper is submitting all queries to the individual authors by e-mail with copies to R. Tomkins. Replies will be sent to Ms. Cooper with copies to R.P.T.T.

TIMETABLE FOR COMPLETION OF TEXT

1. copyediting – completed by mid-August, 2002
2. Page Proofs should be available by the end of September, 2002.
3. Page Proofs will be sent to the individual authors with instructions to send them to R. Tomkins who will collate all changes in a Master Copy. 5 weeks will be allowed for this part.
4. Estimated date for publication in January 2003.

NOTES

1. In order to meet the Wiley deadlines, it is very important for all the authors to respond to the copy-editor queries and to make corrections to the page proofs as soon as possible.
2. All authors are requested to check EQUATIONS and Reference citations very

carefully.

Costs are still unknown. The logo of the ISSP will be introduced in the book.

10. Project: Solubilities of Salts in Seawater – Ch. Balarev

There was no activity within this project in the last period.

11. Teaching of undergraduate students: Experimental and theoretical aspects – C. Magalhães

Clara Magalhães elucidated her efforts in organizing support for an appropriate task group. Under the new structure CCE is responsible to support teaching projects and C. Magalhães will turn to Atkins as the chairman.

12. History of Commission on Solubility Data (V.8.)

It was pointed out that with the reorganization of IUPAC the work of commission V.8. should be summarized and appreciated in a suitable form. As publishing media were proposed:
"Chemistry International" (H. Ohtaki)
"Chem. Heritage Magazine" (J. Lorimer)
"J. Chem. Eng. Data"(K. Marsh)
The present version of the history of SDC comprises about 8 pages text and 10 pages appendix.

13. Reports on Projects

13.1. Gas/Liquid Systems – P. Scharlin

Within the time period to 2004 it is planned to finish four volumes:

1. Project # 2001-052-1-500
   Solubility of volatile fluorides in all solvents
   (H.L. Clever) year of completion: 2003
   approved as non-funded Project
2. **Solubility of Carbon dioxide in aqueous Non-electrolyte Solutions**
   (P. Scharlin, J. Salminen) year of completion: 2003
   listed in Phantom proposal as IV.14
3. **Mutual Solubility of Carbon dioxide and lower alkanes at pressures above 2 bar**
   (A.E. Mather) year of completion: 2003
   listed in Phantom proposal as IV.13
4. **Solubility of Solids and Liquids in Supercritical Carbon dioxide**
   (D.E. Knox) year of completion: 2004
   listed in Phantom proposal as IV.15

13.2. Liquid/Liquid Systems – D. Shaw

Present:

Andrzej Maczynski
Kenneth Marsh
Valerii Sazonov
David Shaw
Adam Skrzecz

Volumes in Preparation and Other Projects

1. **"Acetonitrile: Ternary and Other Multicomponent Systems"** Sazonov, Shaw and Skrzecz, Estimated Completion: 2003, Sazonov will prepare a justification of the volume including relevance of the systems to industrial processes; based on this Shaw will prepare a project proposal; Sazonov will begin compilation and evaluation, completing one system at a time and email drafts to Shaw and Skrzecz for comment.

2. **"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.

3. **"Hydrocarbons with Water (Update)"** Maczynski, Shaw and Skrzecz, Estimated Completion Date: update to be produced in sections over the next 2 years, Shaw will contact Gerry Dalton (NIST) to develop detailed plan; Skrzecz will be responsible for updating literature search and Maczynski will be responsible for re-evaluation of systems using methods developed at the Thermodynamics Data Center, Warsaw.

4. **"Ethers with Water"** Maczynski, Skrzecz, and Shaw; schedule not yet firm.

13.3. Solid/Liquid Systems – W. Voigt

Within the period to end of 2004 the following volumes shall be prepared for publication:

1. **Alkaline Earth Metal Carbonates in Aqueous Solutions**
   (J. Vanderdeelen, E. Königsberger)
   listed in Phantom proposal as I.1.
   The volume is nearly completed, critical evaluation performed, some minor changes will be made until end of year 2002, will be submitted for publication in 2003

2. **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 will be completed in year 2003

3. **Lead Sulfate**
   (J.W. Lorimer)

listed in Phantom proposal as IV.12
Project will be completed in 2004

4. **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 2003

5. **Alkali Metal and Ammonium Perchlorates**
   (C.E. Chan, K.H. Khoo, E. Gryzlova, M.-Th. Cohen-Adad)
   Volume is ready and presently reviewed by M.-T. Cohen-Adad and ready for submitting to JPCRD in 2004

6. **Solubilities of Inorganic Actinide Compounds**
   (J. Hála)
   This represents a new project proposal (see EiC report) and is related to Phantoms proposal **I. Solubility Data of Compounds Relevant to Mobility of Metals in the Environment**

7. **Solubility of Haloganated Aromatic Hydrocarbons**
   (A. Goto, M. Makino, R. Goto and H. Miyamoto)
   listed in Phantom proposal as III.7.
   Work on this project is ongoing and can be finished in 2004

8. **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.

14.1. Venue of the 2003 Meeting of SSED (GA in Canada)

After discussing other possibilities for the odd-year meetings (for example in combination with participation in international conferences related to the topics of solubility and equilibria) it was decided to meet within the framework of the General Assembly in Canada as envisaged before. For the members of the committee participation at the meeting is compelling.

It was emphasized that for further progress in the project task groups work according to the phantom proposal (see also remarks of H. Wanner in App. A1) participation of former members of Commission on Equilibrium Data (V.6) seems to be necessary. K. Marsh and H. Gamsjäger will discuss the issue of a combined meeting with K. Powell and P. May / St. Sjöberg, respectively.

14.2. Future International Symposia on Solubility Phenomena

2004: 11th ISSP – University of Aveiro, (Aveiro,Portugal)

tentative date will be second half of July

Conference titel : **International Symposium on Solubility Phenomena**

including related Equilibrium Processes

Members of the former Commission V.6 ("Equilibrium Data") will be involved in the preparation of the conference (scientific committee, invited lectures)

2006: 12th ISSP – University of Freiberg/Saxonia, (Freiberg,Germany) was proposed

W. Voigt confirmed to be ready for hosting the symposium.

15. 10th ISSP and Workshop "Solubility Phenomena – Application for Environmental Improvement"

The **10th International Symposium on Solubility Phenomena** has been held on 21st - 26th July. **Workshop** "Solubility Phenomena - Application for Environmental Improvement" has been held in conjunction with the Symposium.
About 170 scientists from 39 countries have participated in the Symposium and Workshop. 19 plenary lectures, 50 oral presentations and 72 poster presentations have been given at the two scientific events.

The **main thematic topics of the Symposium** included:

- Quantitative Structure - Solubility Relationships;
- Solubility Diagrams, Phase Relationships and their Application;
- Application of Solubility Data for Environmental Improvement of Polluted Waters and Soils;
- Application of Solubility Data in Marine-Type Solutions and Industrial Wastes Treatment.

The **main problem discussed at the Workshop** was the ecological status of Black Sea as well as of the rivers flowing into the Black Sea. The presentations were directed into:

- Pollution Level and Pollution Sources of Danube, Dnieper, Dniester, Bug and other Rivers Flowing into the Black Sea
- Black Sea Fluxes. Monitoring of the Black Sea

Two round tables "Pollution of Rivers" and " Black Sea Fluxes" have been organized.
A round table for reinforcement of the regional participation in integrative European programs for solving of ecological problems has been also organized. A new research project "Clean Black Sea" for regional cooperation and submission to the European Commission, 6th FP, has been considered and approved.
It is planned to publish the plenary and invited lectures in "Pure and Applied Chemistry" under the editorship of D. Shaw (USA).
The complete scientific program including the abstracts of oral and poster presentations were delivered to the participants in form of a printed volume and a well structured CD-ROM.

The organizers are to be congratulated on providing a well-organized meeting and conference that provided valuable new information on many aspects of solubility phenomena and was enriched with interesting excursions in the Black Sea Region and the country side as well as with traditional Bulgarian ceremonies

16. Adjournment

The meeting was adjourned at 17:00, July 21, 2002.

APPENDIX

A1

#2002-004-1 ‚Solubility Data Series'

Project Title: „Phantom Proposal"
Series Title: Solubility Data Series
Task Group Chairman: Heinz Gamsjaeger

Rev. 1

Overall Rating: VERY SUITABLE

The proposed plan for priority projects in the Solubility Data Series contains 16 projects in five areas of application. The compilation and critical assessment of solubility data by an internationally acknowledged board of experts is of great value for the international scientific community. The IUPAC is an appropriate body to carry out the proposed projects. All 16 projects seem to have a valid justification to be carried out. However, my qualification may be insufficient to adequately judge the value of Projects 8-9 and 13-16.

Detailed proposals have not yet been submitted for any of the 16 projects, and dissemination plans or project budgets have not been specified yet.

Nevertheless, I would like to draw attention to the following two points:

In Commission V.5, a critical assessment of equilibrium data for environmentally significant heavy metals (Cd, Cu, Hg, Pb, Zn) and inorganic ligands is currently being carried out (Task Group Chairman: Staffan Sjöberg). It seems important to me that the data evaluation in Projects 1 and 2 (alkaline earth carbonates and metal carbonates) is carried out in a way consistent with that of the mentioned V.5 project. Otherwise the recommended values from the two projects would probably be incompatible, thus preventing their common use. This essentially means to extrapolate the equilibrium constants to ionic strength zero and to provide the user with the extrapolation details. This procedure increases the general applicability of the recommended data. Experience with the ionic strength extrapolation procedure is available to some extent in Commission V.5, and especially in the Chemical Thermodynamic Data Base (TDB) Project of the OECD Nuclear Energy Agency [1-4].
Only few of the 16 project descriptions indicate the performance of critical assessments of the compiled data. This should be done in all 16 projects. As a result of the critical assessments, reliable data should be selected. The rationale and criteria for

the selection of recommended data should be described in a sufficiently transparent way.

References:
[1] Grenthe, I., Fuger, J., Konings, R.J.M., Lemire, R.J., Muller, A.B., Nguyen-Trung, C., Wanner, H., Chemical Thermodynamics of Uranium, Amsterdam: North-Holland, 1992, 715p.
[2] Silva, R.J., Bidoglio, G., Rand, M.H., Robouch, P.B., Wanner, H., Puigdomenech, I., Chemical Thermodynamics of Americium, Amsterdam: North-Holland, 1995, 374p.
[3] Rard, J.A., Rand, M.H., Anderegg, G., Wanner, H., Chemical Thermodynamics of Technetium, Amsterdam: North-Holland, 1999, 544p.
[4] Lemire, R.J., Fuger, J., Nitsche, H., Rand, M.H., Rydberg, J., Spahiu, K., Sullivan, J.C., Ullman, W.J., Vitorge, P., Wanner, H., Chemical Thermodynamics of Neptunium and Plutonium, Amsterdam: North-Holland, 2001, 836p.

A2 Attendance List

28th Annual Meeting (1st of Subcommittee on Solubility and Equilibrium Data)
St. St. Constantine and Helen Resort, Varna,Bulgaria.
20th – 21st July 2002

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A3 Phantom Proposal

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PROJECT SUBMISSION FORM

v. 12/2000

Any individual or group can submit a project, with or without current affiliation with an IUPAC body. Projects can be submitted at any time. For detailed information, see the additional ***Guidelines for Completion of the Project Submission Form***. Frequently Asked Questions on ***Project Submission and Approval Process*** are also available on the Union's web site at <http://www.iupac.org/projects>.

The form should be completed with a word processor and returned to the IUPAC Secretariat, preferably as an e-mail attachment at <secretariat@iupac.org>. Please do not remove section headers and answer all questions; indicate NA when a question does not apply to the proposal.

for administrative use only	*Submitted_____;#*
Date	
Project Title	"Phantom Proposal"
Series Title *(if applicable)*	Solubility Data Series
Task Group Chairman	(including address and e-mail) Heinz Gamsjaeger
Task Group Members	(including address and e-mail)
Name of the person submitting this form ***if not*** *the proposed Task Group Chairman*	(including address and e-mail)

Objective

As agreed during the 41st General Assembly, the Solubility Data Project is submitting this "phantom proposal" in order to provide an opportunity for the Union to evaluate our plans for priority subjects to be treated over the next three year period. This proposal summarizes and justifies 16 high priority volumes for the IUPAC-NIST Solubility Data Series which we expect to actively pursue. Subsequent proposals which include detailed workplans and budgets for volumes which are endorsed as a result of this proposal may be submitted subsequently.

Description
PROJECTS FOR PHANTOM PROPOSAL

The following paragraphs describe 16 volumes (1 to 16) in the Solubility Data Series grouped around five broad themes (I. to V.)

I. Solubility Data of Compounds Relevant to Mobility of Metals in the Environment

Solubilities in aqueous media of sparingly-soluble metal carbonates play an important role in chemical processes whether carried out on a laboratory or an industrial scale. Solubility phenomena, i.e. dissolution and precipitation reactions, frequently control procedures for preparing, separating and purifying chemicals. Moreover, interactions of the hydrologic cycle with the cycle of rocks, as well as the naturally occurring dissolution of carbonate minerals in water and their precipitation on the ocean floor and in sediments of rivers and lakes, can often be simply described in terms of solubility equilibria, although gigantic quantities of material may be involved [1].

In addition, solubility measurements have been shown to be a powerful tool for the determination of thermodynamic properties of sparingly-soluble metal carbonates [2,3]. The thermodynamic properties of alkaline earth and transition metal carbonates play a major role for a better understanding of a wide variety of geochemical and industrial processes involving equilibria between solid carbonates and aqueous solutions. The total concentration of alkaline earth and transition metals in carbonate-bearing natural waters is predominantly determined by the solubilities of the respective hydroxides, oxides, hydroxide carbonates and neutral carbonates [4]. The thermodynamic modeling of dissolution or precipitation of sparingly-soluble metal carbonates may serve as an important tool for the prediction of the concentrations of transition metals in mine pit lakes [5]. A careful determination of thermodynamic data of metal carbonates is an essential prerequisite for the geochemical modeling of the release of trace elements from waste repositories [6]. Clearly a comprehensive compilation and evaluation of the existing solubility data is an invaluable basis for all sorts of predictive models in this field. Thus this project comprises two volumes:

1. ***Alkaline Earth Metal Carbonates*** (E. Königsberger, J. Vanderdeelen)

2. ***Metal Carbonates*** (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb) (H. Gamsjäger, C.Magalhães, H. Sawada)

It should be emphasized that contributors to the Solubility Data Series have already prepared volumes which provide (i) auxiliary data necessary for the thermodynamic analysis as Volume **62**: P. Scharlin, *Carbon Dioxide in Water and Aqueous Electrolyte Solutions* (1996) and (ii) environmentally relevant information on actinide carbonates as Volume **74:** J. Hala, *Actinide carbonates and carbon-containing compounds* (2001).

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[1] H. Gamsjäger, Solubility, *In* C.P. Marshall and R.W. Fairbridge, eds. *Encyclopedia of Geochemistry*. Kluwer Academic Publishers, 582--586 (1999).

[2] E. Königsberger, L.-C. Königsberger and H. Gamsjäger, Low-temperature thermodynamic model for the system Na_2CO_3 – $MgCO_3$ – $CaCO_3$ – H_2O. *Geochim. Cosmochim. Acta* **63**, 3105 – 3119 (1999).

[3] W. Preis and H. Gamsjäger, Thermodynamic investigation of phase equilibria in systems: Metal carbonate – water – carbon dioxide. *Chemical Monthly* **132** (2001), in press.

[4] W. Stumm and J.J. Morgan, *Aquatic Chemistry*. 3rd ed. Wiley (1996).

[5] L.E. Eary, Geochemical and equilibrium trends in mine pit lakes. *Appl. Geochem*. **14**, 963--987 (1999).

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II. Solubility Data Related to Oceanic Salt Systems

The oceanic salt system comprises the ions Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^- and SO_4^{2-}. Extended evaporitic deposits in Europe (Germany, Netherlands, Spain, France, Poland, Russia), Northern (Canada) and South America (Brasilia), Africa (Congo) as well as in Asia had been formed from these ions during evaporation – crystallization processes of sea waters in geological times. Geological surveying of these deposits, their exploitation in potash mining, rock salt mining, fertilizer production, usage of rock salt mines as repository for nuclear or chemical wastes, all this requires the exact knowledge of solubility equilibria in the multi-component oceanic salt system within a broad range of temperatures. At present also solution mining of magnesium chloride for magnesium metal production is performed or in the stage of planning in a number of places world (Netherlands, Congo, Thailand, Uzbekistan). In addition, evaporation and aerosol formation from oceans are important controlling factors for the worlds climate. Understanding of the details in coupling of evaporation and crystallization processes within the droplets transported into the upper atmosphere represents a crucial part for the formulation of material and energy exchange models. Climate changes from past time periods are manifested in the complex evaporitic deposition patterns, which are interpreted on the basis of the solid-liquid equilibria of the multi-component oceanic salt system.

In 1933, d'Ans published a comprehensive bibliography and compilation of primary data for solubilities of oceanic salts, and also made preliminary evaluations of these data. No comprehensive update to the bibliography or to the compilations has been made, despite their importance. While many partial models of seawater have been reported in the literature, these make use of only limited sets of data.

The goals of this part of the overall Solubility Data Series Project are:

(a) To produce up-to-date compilations of data (with bibliography), constructed in the format of the IUPAC Solubility Data Series (SDS). A partially-computerized bibliographic database with associated reprints of all relevant publications is being maintained, with over 400 relevant entries. The first of this series was published some years ago as SDS Vol. 47: Alkali Metal and Ammonium Chlorides in Water and Heavy Water: Binary Systems, R. Cohen-Adad and J.W. Lorimer, eds. (1991). A scheme for systematic extension of the series to include other binary systems, then ternary systems, etc., has been devised.

(b) To devise and document appropriate methods for critical evaluation of the data. These methods will include methods for describing paragenesis of systems, for example, compositions of solid and solution phases during the evaporite sequence in removal of water from sea water.

The following two volumes continue the treatment of binary systems and some ternary systems with saturation by one salt only:

3 ***Binary systems containing Sodium, Potassium and Ammonium Sulfate*** (C. Balarew, R. Bouaziz)

4***. Magnesium Chloride – Water and Calcium Chloride – Water and their Mixtures*** (W. Voigt)

III. Solubility Data of Compounds Relevant to Human Health

5. ***Solubility of Substances Related to Urolithiasis*** (E. Königsberger, L.-C. Königsberger)

The prevention and treatment of crystal deposition in the human body are based on the understanding of the physico-chemical properties underlying the precipitation of the substances involved. Amongst these properties, the solubilities of the crystals are very important. In the scope of urolithiasis, there are more than 20 different types of kidney stones composed of calcium oxalate hydrates (mono-, di- and trihydrate), ammonium magnesium phosphate (struvite), calcium phosphates (hydroxyapatite and brushite), uric acid and urates, cystine and xanthine. Solubilities of these substances can be incorporated

in databases of sophisticated software packages that permit solubility calculations in artificial urine solutions. The results of these simulations would lead to some understanding and/or useful suggestions regarding the cause, prevention and treatment of renal or bladder calculi. Nevertheless, proper modelling of the solubilities of these substances requires reliable solubility constants. Thus it is necessary to critically assess the literature values reported for these substances. Recently, two reviews on this subject have been published:

[1] E. Königsberger and L.-C. Tran-Ho, Solubility of substances related to urolithiasis - Experiments and computer modelling. *Current Topics in Solution Chemistry*, 2:183-202 (1997).

[2] E. Königsberger and L.-C. Königsberger, Thermodynamic modelling of crystal deposition in humans. *Pure Appl. Chem.,* 73:785-797 (2001).

6. ***Solubility of Hydroxybenzoic Acids and Hydroxybenzoates*** (A. Goto and H. Miyamoto)

Hydroxybenzoic acids and related compounds are pharmaceutically important substances. In particular, 2-hydroxybenzoic acid has been widely used as a medicine and a preservative for food products; 4-hydroxybenzoic acid alkyl esters have also been used as preservatives for food. The relation between the use of these substances and human health requires evaluation of the solubilities of 2-, 3-, and 4-monohydroxybenzoic acids and of 4-hydroxybenzoic acid alkyl esters in water, organic and mixed solvents. It is also suggested to evaluate the solubilities of: (a) 2- and 3-hydroxybenzoic acid in supercritical carbon dioxide containing organic solvents such as methanol and acetone; (b) monohydroxybenzoates, 2,3-, 2,4-, 2,5-, 2,6-, 3,4- and 3,5- dihydroxybenzoic acid salts of alkali, transition and rare earth metals in water and organic solvents**.**

7. ***Solubility of Haloganated Aromatic Hydrocarbons*** (A. Goto, M. Makino, R. Goto and H. Miyamoto)

Halogenated derivatives of aromatic and polyaromatic hydrocarbons have been widely used as heat transfer fluids, organic diluents, plasticizers, fire retardants, pesticides, waxes, etc. However, recently it has been pointed out that some of these or their related compounds, of both synthetic and natural origin, can seriously interfere with reproductive function. From the pharmaceutical and environmental viewpoints, the solubilities of these substances are useful to elucidate the movement and persistence in the environment and to estimate the hazard or risk associated with them. Therefore it is important to evaluate the solubilities of, e.g., chlorinated benzenes, biphenyl and dioxins in various media including single, binary and/or multi-component solvents, micellar solutions and polymer solutions.

8. ***Antibiotics: Peptide Antibiotics*** (Coordinator: J.W. Lorimer)

9. ***Antibiotics: Macrocyclic Lactone Antibiotics*** (Coordinator: J.W. Lorimer)

The solubilities of antibiotics are of major importance in pharmaceutical and medicinal chemistry. For example, drug delivery formulations which directly relate to anti-bacterial activities depend strongly on solubility. The search for new antibiotics resistant to continually evolving bacterial strains is a major focus of drug R&D worldwide, and here solubilities are important in helping the design processes. The compilation and critical evaluation of solubilities for these compounds can be expected to play a major role in the design and delivery of chemotherapeutic drugs now undergoing extensive R&D.

Compilations in JCPRD format are available already for many peptide and macrocyclic lactone antibiotics, with literature up to about 1985. The compilations need to be extended to cover more modern work and other antibiotics of these two classes. Task group members with this expertise are being recruited.

10. ***Noble Gases*** (H.L. Clever) (update of previous volume)

This volume will contain gas solubility data on the noble gases helium, neon, argon, krypton, xenon and radon in water, aqueous solutions and organic substances. Radon is of

environmental interest as a hazard to human health. Radon is a decay product of radium and other radioactive elements and consequently occurs naturally in the soil of many areas. It can accumulate in poorly ventilated spaces such as residential basements where it is a factor in the development of lung cancer.

11. ***Gaseous compounds of carbon, hydrogen, fluorine, chlorine, bromine and iodine*** (H.L. Clever).

This group of compounds includes numerous halogenated organics which are industrially produced in large quantities and are considered persistent organic pollutants. Many of these are of relatively low vapor pressure; the solubility data are often gas/liquid partition coefficients at or below the vapor pressure of the solute. A number of these substances can accumulate in body fatty tissues and are possible hazards to human health.

IV. Solubility Data Related to Industrial Processes

12. ***Lead Sulfate*** (J.W. Lorimer)

The solubility of lead sulfate in aqueous and non-aqueous solvents continues to present problems in the design and manufacture of the still very important lead-acid batteries, including reliable evaluated values and revision of the standard Gibbs energy of formation, which is based on rather old data. Lead sulfate is also an important health and environmental hazard, and evaluated solubilities in the presence of salts are needed to provide the basis for predictive equations for various real situations.

13. ***Carbon Dioxide and the Lower Alkanes at Pressures above 2 bar: Part 1, Methane to Butane*** (A. E. Mather)

The solubility of carbon dioxide and the lower alkanes is important as most natural gases contain CO_2 as well as these alkanes. Usually, CO_2 has to be separated from the hydrocarbons to meet the specifications on calorific value of fuels. In Enhanced Oil Recovery (EOR), carbon dioxide is used to displace the hydrocarbons from the reservoir and the solubility of CO_2 in the hydrocarbons is important to ensure that miscibility occurs, with concomitant increase in the oil recovered.

14. ***Carbon Dioxide in Aqueous Non-Electrolyte Solutions*** (P. Scharlin)

Gas solubility is one of the fundamental properties of various gas absorption processes in the chemical industry. The removal of carbon dioxide from gas mixtures is a necessary and expensive step in many processes. It is of particular importance, for example, in the purification of ammonia synthesis gas, in the synthesis of liquid fuels from coal and in the upgrading of fuel gases. Absorption with suitable solvents provides a convenient method for the removal of CO_2. The availability of accurate and reliable information on the equilibrium solubility of carbon dioxide in absorbing solvents as a function of temperature and pressure is of utmost importance in the rational design of gas-treating units. Such data will allow more economic construction and more nearly optimum operation of gas-treating plants. This volume will contain compiled and evaluated data on the solubility of CO_2 in various industrially important aqueous solvents and solvent mixtures.

15. ***Solids and Liquids in Supercritical Carbon Dioxide*** (D. E. Knox)

Carbon dioxide itself is an important industrial solvent. This volume will contain comprehensive compilations and evaluations of the existing data on the solubility of solids and liquids in supercritical CO_2.

Processing using supercritical fluids is an increasingly important area worldwide. Such processes, with their significant variation in solubility with pressure, permit the accomplishment of many processes that would be otherwise very difficult to achieve. Further, systems that employ carbon dioxide as the solvent are particularly attractive as CO_2 is environmentally friendly. There are many "green chemistry" processes employing supercritical CO_2 that are of worldwide importance. One example is found in the pharmaceutical industry, where the solutes are often thermally labile substances that would be degraded by more conventional separation processes. There are also well-established

processes in other industries, for instance, the decaffeination of coffee by extraction with supercritical CO_2. There are currently no generally recognized, critically evaluated data in this area. Furthermore, many data have been published in this area in the last decade or so. This volume is thus addressing a significant need.

V. Solubility Data Related to Global Climate Change

16. ***Fluorides of Noble Gases, Boron, Nitrogen, Sulfur, Carbon and Silicon*** (H.L. Clever)

Sulfur hexafluoride is an important greenhouse gas. Aqueous solubility data are needed to understand and model its partitioning between the oceanic and atmospheric systems.

Outcome	Compiled and critically evaluated solubility data will be published as volumes in the Solubility Data Series appearing as extended articles in the Journal of Physical and Chemical Reference Data and be made available on the world wide web through the NIST Chemistry Web Book
Dissemination Plan	
Relevant IUPAC Body (please tick box/boxes)	Physical and Biophysical ☐ Inorganic ☐ Organic and Biomolecular ☐ Macromolecular ☐ Analytical ☒ Environmental ☐ Human Health ☐ CHEMRAWN ☐ Chemistry and Industry ☐ Teaching of Chemistry ☐ Other ……

Budget (Total from all Travel Administrative Other *describe*) **Total** (in Requested from Requested from other Sources **External Funding Agency Applied to** (if	
Time Frame Planned start Duration of	
Milestones	
Anticipated Impact	
Criteria for Retrospective Evaluation	

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