INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Analytical Chemistry Division

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA (SSED)

Minutes

3rd Annual Meeting of SSED (30th overall)

held in conjunction with the

11th International Symposium on Solubility Phenomena

at Aveiro, Portugal

24 – 25 July 2004

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

Saturday, 24 July 2004

Morning Session: 9:00 - 12:00

1. **Welcome of the participants (Appendix 1)** — H. Gamsjäger

Heinz Gamsjäger, Chairman of the SSED welcomed the participants.

All of the participants introduced themselves and their affiliation.

1a. **Organizational Announcements** — C. Magalhães

Clara Magalhães made announcements regarding meals, the tour of the salt works planned for 25 July, and the welcoming reception for the symposium

2. **Approval of the Minutes of the 2nd Annual Meeting of SSED (29th overall) held in conjunction with the 42nd IUPAC General Assembly, Ottawa, Canada, 11-12 August 2003** — H. Gamsjäger, W. Voigt

The minutes had been distributed by e-mail prior to the meeting, and also distributed as hard copies at the meeting.
Jack Lorimer indicated that his e-mail address as indicated in the attachment A1 should be amended to delete "julian". Cezary Guminski (not present) sent word that he should be added to the Transition Metals volume nearing completion on page 3 of the minutes.
The minutes were approved as amended above.

3. **Other Items for Agenda** — H. Gamsjäger

Jack Lorimer asked to add an update on history of SSED; Mark Salomon will include it in his Editor-in-Chief's report.
Heinz Gamsjäger asked that the executive committee meet at 9:00 AM Sunday if it will not inconvenience the meetings of the subcommittees scheduled for that time.

4. **Franzosini Award 2004** H. Gamsjäger

Marion Goral received the Franzosini award for his activities within the Solubility Data Group and his related efforts with the group at ICF-PAN. An announcement will be made in CI.

5. **Chairman's Report for 2003 – 2004 (Appendix 2)** H. Gamsjäger

a) Visibility of SSED with IUPAC
Heinz Gamsjäger pointed out that there were items either from or about members of the SSED in almost every issue of "Chemistry International", including the Brief History of the Solubility Data Project. Also, the SSED continues to publish volumes in the Solubility Data Series. Also, the plenary and invited papers from the 11th ISSP are expected to be published in "Pure and Applied Chemistry".
b) IUPAC Representation
Heinz Gamsjäger is currently Associate Member of the Analytical Chemistry Division and is also the Austrian representative on the Union Advisory Committee.
c) Current SDS Projects
There are currently about 15 ~ 20 ongoing projects
d) Plenary and Invited Lectures
Most of the lecturers have agreed to write a paper based on their lecture. The proceedings will be refereed externally; Heinz Gamsjäger has suggested referees.
e) IUPAC Prizes
IUPAC is now sponsoring prizes for the best poster presentations at IUPAC-sponsored conferences and symposia. The prizes consist of a certificate, a subscription to "Chemistry International" and the IUPAC Gold Book. Clara Magalhães announced the organizing committee of the 11th ISSP already has in place plans for an additional poster presentation prize as well.
f) Next Meeting of SSED
Heinz Gamsjäger pointed out that he must attend the IUPAC General Assembly meeting next year in Beijing. He suggested that members of the committee might wish consider the alternative of next meeting in August 2005 in Portoroz, Slovenia in conjunction with the ICSC meeting. He suggested reviewing the website prior to taking any decision (www.icsc2005.si/first.html).
g) Chemical Monthly
Heinz Gamsjäger noted that the SSED is well represented on the editorial board of "Chemical Monthly".

6. **Editor-in-Chief's Report for 2003 – 2004 (Appendix 3)** M. Salomon

Two additional volumes, one with several parts, were finished within the last year:
Volume 80
Volatile Fluorides, H.L. Clever
Volume 81
Hydrocarbons with Water and Seawater – Revised and Updated, Eds.Andrzej Maczynski and David G. Shaw, with contributions from Marian Goral, Barbara Wisniewska-Goclowska, Adam Skrzecz, Iwona Owczarek Krystyna Blazej, Marie-Claire Haulait-Pirson, Glenn T. Hefter, F. Kapuku, Zofia Maczynska, and Andrzej Szafranski.
Parts 1-8 done
Part 9 received
Parts 10-12 expected shortly
Short History of the Solubility Data Project
Published in *Chemistry International*
Full history of the Solubility Data Project

Formatting
Mark Salomon asked everyone currently working on volumes to please follow the formatting guidelines that are included in the editor-in-chief's report (see Appendix)

7. **Database Agreement** — D. Shaw

David Shaw reported that a web accessible database is now available in a searchable form. This includes approximately 12 to 14 volumes. New volumes are automatically included as they are submitted.
David Shaw indicated there is need to continue discussions with NIST to get data from earlier volumes entered electronically.
Heinz Gamsjäger added that volume 77 and 78 are now available.
Jack Lorimer asked if much had been put in place to correct errors in the data, David Shaw responded that yes, NIST has been good at finding and correcting typographical errors in the data, but has not updated compilations or revised evaluations.
Jack Lorimer asked if there had been any publicity to make potential users aware of the NIST database? David Shaw replied that there is an announcement in "Chemistry International" and that search engines would locate it. There was agreement that a short announcement in "Pure and Applied Chemistry" or similar publications would be helpful.
Heinz Gamsjäger asked if there were not other ways in which earlier volumes could be made electronically available. Response was that they could be scanned, but that that procedure would introduce many errors if the scan were converted to text.

7a. **Interdivisional Project** 2003-011-3-600 — D. Shaw

David Shaw reported that the project has received funding from both the Analytical Chemistry and Environmental Chemistry division. The project is compiling data for commercial pesticides. Data include solubility, Kow, pKa and vapour pressure. He asked that the participants in the project to be please be patient for a few more months as the project is "moving slowly, but it is moving".

8. **Volumes for Next Year's SDS Proposals** — M. Salomon

(This topic was included in the Editor-in Chief's Report in Item 6.)

9. **New Procedures for Data Evaluation (Appendix 4)**

Andrzej Maczynski presented a summary of TDC (Thermodynamics Data Centre) activities. — A. Maczynski,
Marion Goral presented an overview of Volume 81. — M. Goral, A. Skrzecz
Marion Goral discussed recommended methods for the evaluation of VLE/LLE data.
Adam Skrzecz discussed Floppy Book of recommended VLE/LLE data (method used in Volume 81).

10. **Teaching of Undergraduate Students** — C. Magalhães

Clara Magalhães reported that due to preparations for the 11th ISSP not as much progress was made as desired this past year. A book has been developed (in Portuguese) for primary school students and indicated it would be on view during the meeting and during the 11th ISSP.
Reginald Tomkins made some suggestions about possible funding sources.
Several others made helpful suggestions and offered encouragement.
Heinz Gamsjäger commented that this represents important work and an emerging need.

11. **Equilibrium Data Report** — H. Wanner

Glenn Hefter commented that a report on Equilibrium Data activities would be in

order. All present agreed.
Hans Wanner reported on work on the speciation of heavy metals (Hg, Cu, Zn, Cd, Pb), each review resulting in a publication.
Hans Wanner indicated that project underway include
Performance assessment of waste management. Radioactive waste
Need for data on actinides
Development of procedures on how to treat data: ionic solutions? Uncertainties in experimental data?
Goal is to provide data that user can use more or less directly, therefore extrapolating to zero ionic strength; thus providing recommended data at zero ionic strength and 25 C.
Heinz Gamsjäger thanked Hans Wanner for the report and commented that Kip Powell mentioned that the speciation work should be included / mentioned in "Chemistry International" under the activities of SSED. Hans Wanner agreed.
Jack Lorimer noted that there are equilibrium projects as well.
David Shaw suggested that Kip Powell be asked to assign project number that indicate that the various equilibrium projects be part of SSED.

Recess — Heinz Gamsjäger asked that all of the working groups should try to complete their meetings during the remainder of the day. This would allow the SSED to resume its meeting the next morning and would thus accommodate the excursion to the salt works planned for Sunday afternoon. The morning session concluded at approximately 12:45. — H. Gamsjäger

Afternoon Session: 14:00 – 18:00

The afternoon session was devoted to meetings of the gas-liquid, liquid-liquid and solid-liquid working groups.

Sunday, 25 July 2004

Morning Session: 10:00 - 12:00

(All subcommittees had managed to complete their meetings on Saturday.)

12. **Reports of Subcommittees and Projects (Appendix 5)** — P. Scharlin, D. Shaw, W. Voigt

Pirketta Scharlin (Chair, Gas-Liquid working group) reported that *Solubility of Carbon Dioxide in Aqueous Non-Electrolyte Solutions* (P. Scharlin, J. Salminen) was on track for completion in 2005. *Solids and Liquids in Supercritical Carbon Dioxide* (D. Knox) needs reorganization to limit scope of the volume somewhat, then it should be completed in 2006. *Mutual Solubility of Carbon Dioxide and Lower Alkanes at Pressures above 2 bar* (A. Mather) is overdue and has not been reported on and thus must be postponed indefinitely. The project by L. Clever needs a proposal.
David Shaw (Chair, Liquid-Liquid working group) reported that the volume on *Acetonitrile* (V. Sazonov, D. Shaw, A. Skrzecz) was nearly complete. The *Hydrocarbon/Water Update* (in 12 parts) was nearly done (see agenda item 6 above). Proposals were forthcoming for the projects on *C-3 and Higher*

Nitriles (V. Sazonov, A. Skrzecz, D. Shaw) and for the project by A. Maczynski, A. Skrzecz and M. Goral. The interdivisional project on *Critical Compilation of Pesticide Data* is still in the early stages.
Wolfgang Voigt (Chair, Solid-Liquid working group) reported that the two-part volume *Solubility Data related to Oceanic Salt Systems: Part I. Binary systems containing sodium, potassium, and ammonium sulfate* (C. Balarew, R. Bouaziz, R. Cohen-Adad, J. Lorimer, N. Ariguib) and *Part II. Magnesium chloride-water and calcium chlorides-water and their mixtures* (W. Voigt) had encountered problems due to the unavailability of several contributors. As a result, it is being reorganized and will not finish by 2006.
Wolfgang Voigt reported that the two volumes involving *Solubility Data of Compounds Relevant to Mobility of Metals in the Environment* are proceeding. *Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb)* (C.Magalhães, H. Gamsjäger and K. Sawada) has completed the compilation sheets and half of the required evaluations and is considering including modelling and end-user advice. *Alkaline earth metal carbonates.* (E. Königsberger, J. Vanderdeelen and J. Lorimer) has complete compileations and evaluations and needs only to incorporate some modelling. *Inorganic actinide compounds.* (J. Hala , M. Salomon) is proceeding on schedule.
Wolfgang Voigt reported that the three volumes involving *Solubility Data fo Compounds Relevant to Human Health* were also proceeding. *Solubility of substances related to urolithiasis* (E. Königsberger and L.-C. Königsberger) is proceeding on schedule. *Solubility of hydroxybenzoic acids and hydroxybenzoates* (A. Goto, H. Miyamoto) has completed nearly all the compilation sheets and many of the evaluations; completion is expected by late 2005. *Solubility of halogenated aromatic hydrocarbons* (A. Goto, R. Goto, M. Makino, and H. Miyamoto) has completed the compilation sheets and needs limited evaluation due to small size of volume. A proposal of how to do an evaluation will be made by the end of 2004.
Wolfgang Voigt reports that there is a single volume in the category *Solubility Data Related to Industrial Processes*: *Lead Sulfate* (J. Lorimer) will not be completed within the next two years.
Wolfgang Voigt also reported on the following other, or new, projects. *Solubility of Sugars in Aqueous and Nonaqueous Solutions* (João AP Coutinho) has compilation sheets ready and is determining evaluation strategies. It is proposed to get a project number under the "human health" category. *Transition and 12 to 14 Main Group Metals, Lanthanides, Actinides and Ammonium Halates* (H. Miyamoto, R. Miyamoto, C. Guminski, M. Salomon) is an update volume and is essentially ready. It is proposed to substitute it for the lead sulfate volume in the category "industrial processes". J. Eysseltova has started compilation work on solubility of alkaline metal nitrates in water and is willing to propose an appropriate project in 2005.
Heinz Gamsjäger asked that P. Scharlin, D. Shaw, W. Voigt and M. Salomon provide appropriate revisions to the current website list of proposals anticipated to finish within the next two years.

13. **Report on the 11th ISSP, Aveiro, Portugal in 2004** — C. Magalhães

Clara Magalhães reported that all was in readiness and that the welcoming reception would be that evening in the exhibition hall. The symposium will feature more than 40 contributed papers as well as 53 posters, with most of the contributions from outside Portugal. The plenary talks will be 50 minutes plus 10 for questions and answers; invited papers 25 plus 5; oral contributions 15 plus 5. There will also be a roundtable on modelling and computing Monday afternoon. There will be prizes for best posters; the winners will be announced

at the closing ceremony on Thursday afternoon.

14. **Report on future ISSP's** — H. Gamsjäger, W.Voigt

Wolfgang Voigt reported that plans for the 12th ISSP in Freiburg, Germany are proceeding. The preferred dates will be the week of 24-29 July 2006. There are shuttles from both Dresden and Leipzig (~ 40 km), and hotel prices are in the range of 20 ~ 150 euros. There are several touring possiblities in the area as well.

Heinz Gamsjäger asked if there were any proposals for the 13th ISSP to be held in 2008. There were none, but several persons suggested that perhaps a meeting in France, perhaps Marseille, could be organized and that M. Gaune-Escard should be consulted.

15. **Address by Hiroshi Miyamoto (Appendix 6)** — H. Miyamoto

Hiroshi Miyamoto made a very emotional speech thanking all of his "IUPAC friends and colleagues" for many years of interaction through the activities of the Solubility Data project.

Heinz Gamsjäger in turn thanked Prof. Miyamoto for his many contributions to the group.

16 **Adjournment** — H. Gamsjäger

The 3rd annual meeting (30th overall) of SSED was adjourned at approximately 12:30.

Attachments

A1

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A2

Item 5 on the Agenda: Chairman's Report 2003-2004

1. Visibility of SSED within IUPAC:

One of the chairman's major concerns is to improve the visibility of the SSED within IUPAC. Below entries are listed in *Chemistry International* and *Pure and Applied Chemistry* which report on SSED activities that occurred between August 2003 and July 2004.

***CI*, 25,** No. 5, September-October 2003
Letters from Readers
p. 18: David Shaw "Regarding H.L. Senti's review of the Sceptical Environmentalist"

***CI*, 25,** No. 6, November-December 2003
IUPAC Wire
p. 15: Pirketta Scharlin received the 2003 Franzosini Award.

***CI*, 25,** No. 6, November-December 2003
Bookworm
p. 25: Solubility Equilibria – Heinz Gamsjäger

***CI*, 26,** No. 2, March-April 2004
Internet Connection
p. 24: IUPAC Solubility Data on the Internet

***CI*, 26,** No. 3, May-June 2004
Solubility Data
pp. 12-15: "The Solubility Data Project: A Brief History", by Larry Clever

***CI*, 26,** No. 3, May-June 2004.
Bookworm
p. 31: IUPAC-NIST SDS, **79,** "Alkali and Alkaline Earth Metal Pseudohalides", *JPCRD*, **33**, pp. 1-176, 2004, Jiri Hála and Hideo.Akaiwa

Future publications in *CI*:

***CI*, 26,** No. 6 November-December 2004
IUPAC Wire
Marian Góral received the 2004 Franzosini Award.
Reports from Conferences
11th International Symposium on Solubility.Phenomena – Including Related Equilibrium Processes (Heinz Gamsjäger, report of 11th ISSP)
Bookworm
IUPAC-NIST SDS, **80,** "Volatile Fluorides", *JPCRD*, **34**, 2005, H.L. Clever, editor
IUPAC-NIST SDS, **81,** "Hydrocarbons with Water and Seawater – Revised and Updated", *JPCRD*, **34**, 2005, A. Maczynski and David G. Shaw, editors

Future publications in *PAC*:

***PAC*, 77**, (2005) pp. 513-655
Lectures from Symposia
Papers based on presentations at the 11th International Symposium on Solubility

Phenomena – Including Related Equilibrium Processes, Aveiro, Portugal, 25-29 July 2004 (H. Gamsjäger, G.T. Hefter, M.C.F. Magalhães, conference editors)

2. Current SDS Projects (February 2004):
As listed in http://www.iupac.org/divisions/V/502/index.html and new ones. The individual projects are discussed in the reports of the chairs for gas, liquid and solid solubilities.

Project number: 2001-052-1-500 (previous 581/15/89)
Project Title: Solubility of volatile and gaseous fluorides in all solvents
Task Group Leader: **H. L. Clever**

Project number: 2002-025-1-500
Project Title: Solubilities of Inorganic Compounds of Actinides (except carbonates)
Task Group Leader: **J. Hála**

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** (co-leader: **E. Königsberger**)

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**

Project number: 2002-034-1-500
Project Title: Solubility data related to oceanic salt systems. Part II. Magnesium chloride-water and calcium chlorides-water and their mixtures
Task Group Leader: **Wolfgang Voigt**

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**

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**

Project number: 2002-037-1-500
Project Title: Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons
Task Group Leader : **Masakazu Makino and Ayako Goto**

Project number: 2002-042-1-500

Project Title: Solubility Data Related to Industrial Processes: Lead Sulfate
Task Group Leader: **J.W. Lorimer**

Project number: 2002-043-1-500
Project Title: Solubility Data Related to Industrial Processes: Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane
Task Group Leader: **A.E. Mather**

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**

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**

Project number: 2002-050-1-500
Project Title: Solubility data related to industrial processes; Acetonitrile: ternary and other multicomponent systems.
Task Group Leader: **Valerii Sazonov**

Project number: 2003-011-3-600
Project Title: A critical compendium of pesticide physical data
Task Group Co-Leaders: **Don Wauchope and David Shaw**

Project number: 2003-018-1-500
Project Title: Mutual solubility of hydrocarbons with water (update of volumes 37 and 38)
Task Group Leader: **Andrzej Maczynski**

3. Analytical Chemistry Division Committee (Vienna. February 16 and 17, 2004**).**
The chairman participated in this ACDC meeting and reported there on the following SSED activities:
(i) Two volumes completed , namely "Solubility of volatile and gaseous fluorides in all solvents" by Larry Clever and "Azides, Cyanides, Cyanates, and Thiocyanates of Alkali Metals, Alkaline Earth Metals and Ammonium", by Jiri Hála. The SSED aims to place all new evaluated data in the NIST-IUPAC solubility data base http://srdata.nist.gov/solubility/.
(ii) SSED provides frequent news reports to the Secretariat for *CI* and has improved publicity in recent years. The March/April issue of *CI* has an article on the NIST-IUPAC Solubility Database: (*CI* 2004, *26*, 24)
(http://www.iupac.org/publications/ci/2004/2602/ic_solubility.html)
(iii) As a result of the long-standing collaboration on Solubility Data Projects with Wiley & Sons, a proposal had been accepted for a book "**Medical Applications of Solubility**", E. Königsberger and LanChi Königsberger (eds.)

(iv) Pirketta Scharlin had been awarded The Franzosini Award 2003 (see *CI*, 2003, 25(6), 15.
(v) Wolfgang Voigt (Freiberg, Saxonia, Germany) – to be added to subcommittee membership

Associate Member of the Analytical Chemistry Division
In the Minutes of the ACDC meeting in Vienna the duties of the Analytical Chemistry Division **Associate Members** and **National Representatives** are summarized, see below. It is essential that the SSED is represented in the ACDC. At present Heinz Gamsjäger is Associate Member and Christo Balarew is National Representative of Bulgaria.

Duties of Associate Members:

General

1. Represent their specific interest groups, subcommittees, or working parties, i.e.:
    - WPHQA (liaise with BIPM CCQM and ISO REMCO)
    - Solubility and Equilibrium Data (liaise with NIST)
    - ICTNS
    - CCE
    - CPEP
    - Others as might arise

External to the ACD

1. Promote the activities and aims of the ACD and the IUPAC project system.
2. Monitor current trends and emerging needs in analytical chemistry
3. Represent ACD, as appropriate, or requested, at IUPAC-sponsored conferences.
4. Interact with user groups, identify new ones

Internal to the ACD

At the ACD committee level

1. Assist in the development of ACD strategy
2. Contribute to the work of an ACD Team responsible for a 'Core Activity' or an 'Emerging Need'.
3. Assist the Nominations' Committee in identification of new ACD members

Projects:

1. Contribute to solicitation of new project proposals and identification of Task Groups.
2. Review new project proposals and vote on contestable funding of projects.
3. Contribute to review of outputs from funded projects
4. Actively promote project dissemination and implementation of dissemination plans.

Duties of the National Representatives

External to the ACD

1. Promote the activities and aims of the ACD and the IUPAC project system.
2. Interact with regional groups; identify and communicate regional needs in analytical chemistry
3. Seek NAO funding to attend ACD meetings.

Internal to the ACD

At the ACD committee level

1. Contribute to the work of an ACD Team responsible for a 'Core Activity' or an 'Emerging Need'.
2. Assist the Nominations' Committee in identification of new ACD members

Projects:

1. Contribute to solicitation of new project proposals and identification of Task Groups.
2. Review new project proposals and vote on contestable funding of projects.
3. Contribute to review of outputs from funded projects

4. Guidelines for IUPAC Poster Prizes

IUPAC sponsor a prize for the best poster at IUPAC sponsored conferences and national chemical society meetings. The Executive Committee approved the following Guidelines:

(1) Prizes will be awarded at all IUPAC Congresses and Division-sponsored meetings where poster sessions are held.

(2) Prizes will be awarded at national meetings if requested. Not more than one meeting per country a year will apply, and that meeting should be selected by the relevant NAO.

(3) In all cases except IUPAC Congresses, there will be normally two, but a maximum of three prizes per conference.

(4) Selection of prize-winners is in the control of the conference organizers.

(5) Each prize will consist of (i) a certificate signed by the President (ii) a copy of the *Gold Book* (iii) two years' subscription to *Chemistry International*. National Adhering Organizations are asked to inform their national chemical societies of this program and to inform the Secretariat of any plans to award IUPAC Poster Prizes at a national meeting. Likewise, Division Committees are asked to inform the organizers of meetings sponsored by their Divisions of this opportunity.

5. *Monatshefte für Chemie - Chemical Monthly*

The SSED is well represented in the Editorial Board of this International Journal of Chemistry

Editorial Board	**Regional Editors**
H. Falk (Managing Editor)	**P. Braunstein**

Johannes-Kepler-Universität Linz Natural Products Chemistry, Physical and Theoretical Organic Chemistry	Universite Louis Pasteur Strasbourg, France
H. Gamsjäger (SSED) Montanuniversität Leoben Physical Chemistry	**E. Königsberger (SSED)** Murdoch University Murdoch, AUSTRALIA
B. Kräutler Universität Innsbruck Organic Chemistry	**R. Neier** Institut de Chimie, Neuchatel Switzerland
F. Pittner Universität Wien Biochemistry	**A. Pfitzner** Universität Regensburg Regensburg, Deutschland
U. Schubert Technische Universität Wien Inorganic Chemistry	**K. Sawada (SSED)** Niigata University Niigata, Japan
P. Schuster Universität Wien Theoretical Chemistry	**O. Vogl** University of Massachusetts Amherst, MA, USA

6. 4th Annual Meeting of SSED

The next Annual Meeting of SSED (August 26, 2005) will be held in conjunction with the 29th International Conference on Solution Chemistry (August 21 - 25, 2005 http://www.icsc2005.si) on the Adriatic coast of Slovenia (Portoroz).

7. Union Advisory Committee

H. Gamsjaeger is, for the term 2004/2005, member of this *ad hoc* committee.

A3

Item 6 on the Agenda: Editor-in-Chief's Report

Volumes submitted and/or published in 2003

1. Volume 80, *Volatile Fluorides*, H.L. Clever, ed.

2. Volume 81, *Hydrocarbons with Water and Seawater–Revised and Updated*, Andrzej Maczynski and David G. Shaw, eds. With contributions by Marian Goral,Barbara Wisniewska-Goclowska, Adam Skrzecz, Iwona Owczarek, Krystyna Blazej, Marie-Claire Haulait-Pirson, Glenn T. Hefter, F. Kapuku, Zofia Maczynska, and Andrzej Szafranski.

- Part I: C_5 Hydrocarbons with water.
- Part II: Benzene with water and heavy water.
- Part III: C_6H_8 - C_6H_{12} Hydrocarbons with Water and Heavy Water.
- Part IV: C_6H_{14} Hydrocarbons with Water.
- Part V: C_7 Hydrocarbons with Water and Heavy Water.
- Part VI: C_8H_8 - C_8H_{10} Hydrocarbons with Water.
- Part VII: C_8H_{12} - C_8H_{18} Hydrocarbons with Water.
- Part VIII: C_9 Hydrocarbons with Water.

Other Publications

- "History of The IUPAC Solubility Data Project," H.L. Clever, abridged version published in *Chem. Intern*., 2004.
- Full paper accepted by *J. Chem. Eng. Data*.

Other Issues on Formatting

1. Page formatting. Various types of formatting compilation and critical evaluations as long as there is consistency throughout the volume. Samples are attached in the appendix.

2. Layouts. For introductory materials such as the Preface, Table of Contents, and List of Figures, the *Journal of Physical and Chemical Reference Data* publishes articles in a 2-column layout with 9 point font size (Times New Roman). Most manuscripts received by the Editor-in-Chief are prepared in a 1-column, 12 point format which is perfectly acceptable as the publisher (the American Institute of Physics (AIP)) easily converts the introductory materials to the 2-column format and 9 point font size.

3. Equations. To ease their task in reformatting manuscripts, the AIP and *JPCRD* editor (Mal Chase) asks all authors to use an Equation Editor when entering equations. Many manuscripts simply insert equations in the body of text which is apparently an inconvenience for the AIP.

4. Tables and Data Entry. The use of tabs to create and align data in tables is not acceptable. All data tables should be created using the "insert table" feature of the word processor program.

Appendix: Samples of Data Page Formatting from Published Volumes

From Volume 81, A. Maczynski and D. Shaw, *Hydrocarbons with Water and Seawater–Revised and Updated*, Part VIII (note use of entering equations in the body of the text which the AIP has requested that in future we use an equation editor for this purpose).

Components:	**Evaluators:**
(1) Isopropylbenzene (cumene); C_9H_{12}; [98-82-8] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral. B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, February, 2004.

Critical evaluation of the solubility of isopropylbenzene (1) in water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	Price[6]	298
Glew and Robertson[3]	298 - 353	Sanemasa *et al.*[7]	288 - 318
McAuliffe[4]	298	Stearns *et al.*[8]	298
McAuliffe[5]	298	Sutton and Calder[9]	298

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + D\,[(T_{\min}/T)\ln(T_{\min}/T) + 1 - [(T_{\min}/T)], \quad (1)$$

where: $\ln x_{\min,1} = -11.53$; $D = 45.78$; $T_{\min} = 290$.

Eq. 1 is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 1.
All the experimental and reference data are listed in Table 2 and shown in Figure 1.

Critical evaluation of the solubility of water (2) in isopropylbenzene (1)

The experimental solubility data for (2) in (1) have been investigated by Englin *et al.*[2] at 273 - 323 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2\,(1/T_r - 1) + d_3\,(1 - T_r)^{1/3} + d_4\,(1 - T_r), \quad (2)$$

where: $d_1 = -0.329$; $d_2 = -2.962$; $d_3 = 0.152$; $d_4 = -6.247$; $T_r = T / 574.0$.

Eq. 2 was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of isopropylbenzene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 3 and shown in Figure 2. Since only one experimental data point is available at each temperature, no data can be Recommended. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

Rejected Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[10] are independent data. Therefore these data are Rejected.

References:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[3]D. N. Glew and R. E. Robertson, J. Phys. Chem. **60**, 332 (1956).
[4]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[5]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[6]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[7]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[8]R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).
[9]C. Sutton and J. A. Calder, J. Chem. Eng. Data, **20**, 320 (1975).
[10]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Table 1. The data categories for solubility of isopropylbenzene (1) in water (2)			
T / *K*	*Recommended* ***(data in good agreement (±30%) with each other and with the reference data)***	**Tentative** (data in good agreement (±30%) with the reference data)	*Doubtful* (data in poor agreement (>30%) with the reference data)
288.2		Sanemasa *et al.*[7]	
298.1		Glew and Robertson[3]	
298.2	Andrews and Keefer[1], Sutton and Calder[9], Sanemasa *et al.*[7]	McAuliffe[4], McAuliffe[5], Price[6]	Stearns *et al.*[8]
303.1		Glew and Robertson[3]	
308.1		Glew and Robertson[3]	
308.2		Sanemasa *et al.*[7]	
313.1		Glew and Robertson[3]	
318.1		Glew and Robertson[3]	
318.2		Sanemasa *et al.*[7]	
323.1		Glew and Robertson[3]	
328.1		Glew and Robertson[3]	
333.1		Glew and Robertson[3]	
338.3		Glew and Robertson[3]	
343.5		Glew and Robertson[3]	
348.3		Glew and Robertson[3]	
353.4		Glew and Robertson[3]	

Table 2. Experimental values for solubility of isopropylbenzene (1) in water (2)		
T / *K*	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values x_1 ±30%
288.2	$8.92 \cdot 10^{-6}$ (T; Ref. 7)	$9.9 \cdot 10^{-6}$
298.1	$1.20 \cdot 10^{-5}$ (T; Ref. 3)	$1.0 \cdot 10^{-5}$
298.2	$1.09 \cdot 10^{-5}$ (R; Ref. 1), $7.90 \cdot 10^{-6}$ (T; Ref. 4), $7.50 \cdot 10^{-6}$ (T; Ref. 5), $7.23 \cdot 10^{-6}$ (T; Ref. 6), $9.22 \cdot 10^{-6}$ (R; Ref. 7), $2.50 \cdot 10^{-5}$ (D; Ref. 8), $9.78 \cdot 10^{-6}$ (R; Ref. 9)	$1.0 \cdot 10^{-5}$
303.1	$1.24 \cdot 10^{-5}$ (T; Ref. 3)	$1.0 \cdot 10^{-5}$
308.1	$1.28 \cdot 10^{-5}$ (T; Ref. 3)	$1.1 \cdot 10^{-5}$
308.2	$1.03 \cdot 10^{-5}$ (T; Ref. 7)	$1.1 \cdot 10^{-5}$
313.1	$1.34 \cdot 10^{-5}$ (T; Ref. 3)	$1.1 \cdot 10^{-5}$
318.1	$1.42 \cdot 10^{-5}$ (T; Ref. 3)	$1.2 \cdot 10^{-5}$
318.2	$1.16 \cdot 10^{-5}$ (T; Ref. 7)	$1.2 \cdot 10^{-5}$
323.1	$1.50 \cdot 10^{-5}$ (T; Ref. 3)	$1.3 \cdot 10^{-5}$
328.1	$1.60 \cdot 10^{-5}$ (T; Ref. 3)	$1.4 \cdot 10^{-5}$
333.1	$1.72 \cdot 10^{-5}$ (T; Ref. 3)	$1.5 \cdot 10^{-5}$
338.3	$1.86 \cdot 10^{-5}$ (T; Ref. 3)	$1.6 \cdot 10^{-5}$
343.5	$2.03 \cdot 10^{-5}$ (T; Ref. 3)	$1.8 \cdot 10^{-5}$
348.3	$2.21 \cdot 10^{-5}$ (T; Ref. 3)	$2.0 \cdot 10^{-5}$
353.4	$2.42 \cdot 10^{-5}$ (T; Ref. 3)	$2.2 \cdot 10^{-5}$

Table 3. Experimental values for solubility of water (2) in isopropylbenzene (1)		
T / K	Experimental values x_2 (T=tentative)	Reference values x_2 ±30%
273.2	$1.04 \cdot 10^{-3}$ (T; Ref. 2)	$1.2 \cdot 10^{-3}$
283.2	$1.46 \cdot 10^{-3}$ (T; Ref. 2)	$1.6 \cdot 10^{-3}$
293.2	$2.02 \cdot 10^{-3}$ (T; Ref. 2)	$2.2 \cdot 10^{-3}$
303.2	$2.71 \cdot 10^{-3}$ (T; Ref. 2)	$3.0 \cdot 10^{-3}$
313.2	$3.66 \cdot 10^{-3}$ (T; Ref. 2)	$4.0 \cdot 10^{-3}$
323.2	$4.72 \cdot 10^{-3}$ (T; Ref. 2)	$5.3 \cdot 10^{-3}$

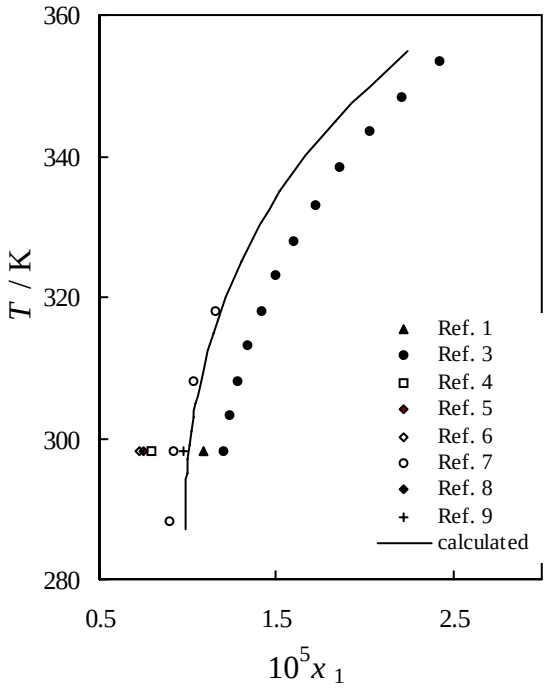

Fig. 1. All the solubility data for isopropylbenzene (1) in water (2)

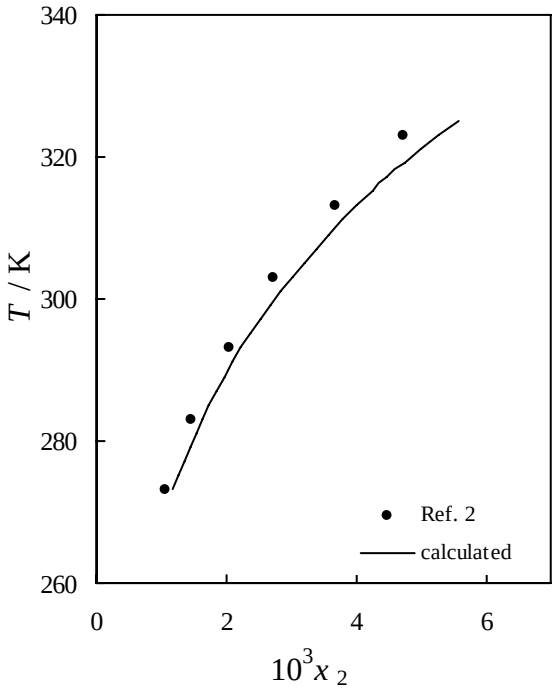

Fig. 2. All the solubility data for water (2) in isopropylbenzene (1)

Components:	**Original Measurements:**
(1) Isopropylbenzene; C_9H_{12}; [98-82-8] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
Variables: One temperature: 25 °C	**Prepared by:** A. Maczynski and Z. Maczynska

Experimental values:

The solubility of isopropylbenzene in water at 25 °C was reported to be 0.0073 g (1) / 100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $1.09 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for twenty h in a constant temperature bath at 25 °C. A sample (5 - 20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10 - 50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:
(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 151.5 - 152.0 °C
(2) not specified.

Estimated Error:
not specified.

From Volume 78, V. Sazonov and D.G. Shaw, *Acetonitrile Binary Systems*, JPCRD, **31(4)**, 989 (2002).

4. Acetonitrile + Inorganic compounds

Components:	**Evaluator:**
(1) Acetonitrile; C_2H_3N; [75-05-8] (2) Carbon disulfide; CS_2; [75-15-0]	Valerii P. Sazonov, Technical University, Samara, Russia, August, 2001

Critical Evaluation:

Solubilities in the system comprising acetonitrile and carbon disulfide have been reported in four publications.

Poppe[1] determined the upper critical solution temperature and the effect of pressure (0.58 to 9.8 MPa) by the synthetic method. Dorby[2] determined the upper critical solution temperature. Mutual solubility of (1) and (2) was studied also by Govindaraian et al.[3] between 320 and 323 K by the visual observation method. Sivaraman et al.[4] between 319 and 324 K and between 0.1 and 4.05 MPa measured the mutual solubilities of (1) and (2) using the synthetic method and these data were reported in graphical form, numerical data were extracted from the published graphs for this evaluation.

The upper critical solution temperature has been reported as 323.36 K[3-4], 324.05 K[1] and 324.2 K[2]. The data[1-3] are in reasonable agreement and thus their average value: UCST = (323.7 ± 0.4) K is recommended. The corresponding critical solution composition has been reported in as x_{c1} = 0.408[3] and x_{c1} = 0.409[4]. These data give an average x_{c1} = (0.408 ± 0.001), which is recommended.

The value of dT_c/dP was reported to be 0.0197 K·kPa^{-1} by Poppe[1] and be 0.247 K·MPa^{-1} by Sivaraman et al.[4].

All experimental values reported in[3,4] have been approximated by an equation based on the scaling law (described in the introduction to this volume) for which the following parameters have been derived:

a_1 = 0.7194, a_2= 1.5113, b_1 = 10.9953, b_2 = -6.4110

(mean standard error of estimate was 0.0115).

For approximation x_{c1} and UCST from data[3,4] have been used. In the opinion of the evaluator, the mutual solubilities calculated by this equation may be treated as tentative. The results of calculations for the selected temperatures are presented in Table. This relationship together with experimental points reported in[3,4] are also presented in Fig. 3.

Interpolated mutual solubility of acetonitrile and carbon disulfide				
	Carbon disulfide-rich phase		Acetonitrile-rich phase	
T/K	x_1	100 w_1	x_1	100 w_1
318.2	0.189	11.2	0.656	50.7
319.2	0.204	12.1	-	-
320.2	0.222	13.3	0.601	44.8
321.2	0.245	14.9	0.569	41.6
322.2	0.278	17.2	0.532	38.0
322.7	0.302	18.9	0.507	35.7
322.8	0.308	19.4	0.501	35.1
322.9	0.315	19.9	0.495	34.6
323.0	0.323	20.5	0.487	33.9
323.1	0.332	21.1	0.479	33.1
323.2	0.345	22.1	0.468	32.2
323.3	0.363	23.5	0.451	30.7

References:
[1]G. Poppe, Bull. Soc. Chim. Belg. **44**, 640 (1935).
[2]A. Dorby, Makromol. Chem. **18/19**, 317 (1956).
[3] K. Govindaraian, S. V. Subramanyam, E. S. R. Gopal, J. Chem. Phys. **56**, 4235 (1972).
[4]A. Sivaraman, M. K. Tiwari, S. Jyothi, E. S. R. Gopal, Ber. Bunsen-Ges. Phys. Chem. **84**, 196 (1980).

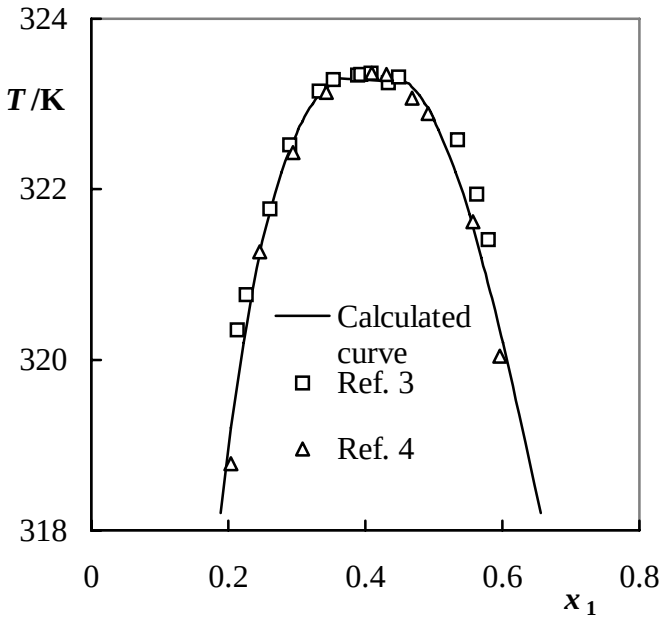

FIG. 3. Mutual solubility of acetonitrile and carbon disulfide.

Components:	**Original Measurements:**
(1) Acetonitrile; C_2H_3N; [75-05-8] (2) Carbon disulfide; CS_2; [75-15-0]	G. Poppe, Bull. Soc. Chim. Belg. **44**, 640-57 (1935).
Variables:	**Prepared By:**
T/K = 324 and *P*/kPa = 582 to 9803	Valerii P. Sazonov

Experimental Data:

The upper critical solution temperature (UCST) was reported to be 50.90 ^{o}C (324.05 K, compiler).
The value of dT_c/dP was reported to be 0.0197 K·kPa^{-1} in the pressure range 582 to 9803 kPa.

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
The synthetic method was used. Observations were carried out in sealed tubes in the presence of the vapor phase. A Cailletet tube with a Kuenen electromagnetic stirrer was used in the experiments at higher pressure. A thermostating cylinder was also used to control the temperature.	(1) Obtained from the Bureau Etalons Physico-Chimiques. (2) Obtained from the Bureau Etalons Physico-Chimiques. **Estimated Error:** Pressure: ± 100 kPa.

Components:	**Original Measurements:**
(1) Acetonitrile; C_2H_3N; [75-05-8] (2) Carbon disulfide; CS_2; [75-15-0]	A. Dorby, Makromol. Chem. **18/19**, 317-21 (1956).
Variables:	**Prepared By:**
T/K = 324	Valerii P. Sazonov

Experimental Data:

The upper critical solution temperature (UCST) was reported to be 51.0 ^{o}C (324.2 K, compiler).

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
No details were reported.	(1) Not specified. (2) Not specified. **Estimated Error:** Not reported.

From Volume 80, H.L. Clever, *Volatile Fluorides*.

COMPONENTS:	**EVALUATOR:**
(1) Xenon fluorides; XeF_2; [13709-36-9] XeF_4; [13709-61-0] XeF_6; [13693-09-9] (2) Various inorganic and organic solvents	Bruno Jaselskis Department of Chemistry Loyola University of Chicago 6525 North Sheridan Road Chicago, IL 60626 USA

CRITICAL EVALUATION

An evaluation of the solubility of the xenon fluorides, XeF_2, XeF_4, and XeF_6 in a number of inorganic solvents.

GENERAL REMARKS

The xenon fluorides are prepared and stored in copper or nickel apparatus using a vacuum line. Only xenon difluoride can be stored in dry glass. All of the xenon fluorides are powerful oxidizing and fluorinating agents and their oxidizing and fluorinating power increase with the increasing oxidation state of the xenon. Solutions are prepared by weight on a vacuum line using, either polychlorotrifluoroethane (Kel-F) or Teflon, and either copper or nickel apparatus. Because of the experimental difficulties the available solubility data are sparse, and a critical evaluation of the data is impossible. For the most part the data must be accepted as they stand.

The melting points and several vapor pressure values[4] are:

Substance	Melting point, T/K	Vapor pressure, p_1/kPa, at T/K			
		293.15	295.82	298.15	373.15
XeF_2	413.2	---	---	0.51	42.4
XeF_4	387.2	0.4	---	---	---
XeF_6	319.2	2.7	3.124	---	---

XENON FLUORIDE; XeF_2 *;* [13709-36-9]

1. XeF_2 + H_2O; [7732-18-5]

Three papers report the solubility of XeF_2 in H_2O at 273 K[1 - 3] The agreement among the three papers is satisfactory and a solubility of 0.150 mol L^{-1} is accepted as a tentative value. The evaluator judges the value to have an uncertainty of about $\pm$ 5 %.

Aqueous solutions of XeF_2 are unstable, a slightly acidic solution decomposes with a half life of about 7 hours at 273 K. In the presence of HF the decomposition is faster, and the rate constant is a function of the HF concentration.

2. XeF_2 + HF [7664-39-3]

Hyman and Quaterman[4, 5] report the solubility of XeF_2 in pure anhydrous HF at three temperatures. There are no other data to compare with these. The solutions are non-conducting and stable over the 271 to 303 K temperture interval with an enthalpy of solution of 10.5 kJ mol^{-1}.

3. XeF_2 + NOF; [7789-25-5] + HF; [7664-39-3] ($NOF{\cdot}3HF$)

Nikolaev *et al.*[6] report the solubility of XeF_2 at several temperatures in a mixed solvent of 1 mol NOF to 3 mol HF. The enthalpy of solution from the solubility values is 8.4 kJ mol^{-1}. There are no other values to compare.

4. XeF_2 + IF_5; [7783-66-6]

Nikolaev *et al.*[7] report five solubility values between 288 and 343 K with an enthalpy of solution of (17 ± 7) kJ mol^{-1}. The uncertainty of the enthalpy is a result of the scatter in the solubility values. Sladky and Bartlett[8] report XeF_2 reacts with IF_5 with gas evolution to produce aducts of $XeF_2 \cdot IF_5$. They isolated and characterized the aduct. These observations are not consistent and cannot be resolved with our present knowledge.

Nikolaev *et al.*[7] point out the decreasing solubility with solvent in the series: $NOF \cdot 3HF$ > HF > IF_5.

5. XeF_2 + CH_3CN; [75-05-8]

Meinert and Rudinger [9] report values of the solubility of XeF_2 in CH_3CN at 273 and 294 K. The enthalpy of solution is 7.2 kJ mol^{-1}. The XeF_2 in the pure dry acetonitrile (purified by the method of Coetzes *et al.*[10] is stable at 263 K. The solution can be stored for a prolonged time under this condition[11]. The solution stability depends on the temperature, the purity and the water content of the acetonitrile.

6. XeF_2 + UF_6; [7783-81-5]

Nikolaev and Sadikova[12] report one value of the solubility of XeF_2 in UF_6 at (373 ± 5) K.

7. XeF_2 + Other Solvents.

Table 1 below summarizes qualitative observations on the behavior of XeF_2 in a number of inorganic and organic solvents. No data sheets were prepared for these systems.

Table 1. Qualitative observations on the solution behavior of XeF_2 in a number of inorganic and organic solvents

Solvent	Remarks	reference
Sulfur dioxide; SO_2; [7446-09-5]	Quite soluble in the 201 to 263 temperature interval.	13
Dimethylsulfoxide; $(CH_3)_2SO$; [67-68-5]	Soluble but reacts with gas evolution; solutions are colorless.	13
Liquid ammonia; NH_3; [7664-41-7]	Sparingly soluble in the range 195 to 263 K and forms NH_4F.	13
Difluorodichloromethane; CCl_2F_2; [75-71-8]	No reaction.	13
Chlorotrifluoromethane; $CClF_3$; [75-77-9]	Sparingly soluble up to the normal boiling point.	13
1, 3-Dioxane; $C_4H_8O_2$; [505-22-6]	Dissolves and reacts.	14
1, 4-Dioxane; $C_4H_8O_2$; [123-91-1]	Dissolves and reacts.	14
Pyridine; C_5H_5N; [110-86-1]	Dissolves and reacts.	14
Dimethylformamide; C_3H_7NO; [68-12-2]	Dissolves and reacts.	14
Tetrahydrofurane; C_4H_8O; [109-99-9]	Dissolves and reacts.	14
Nitromethane; CH_3NO_2; [75-52-5]	Dissolves and reacts.	14
Tetrachloromethane; CCl_4; [56-23-5]	Sparingly soluble.	14
Trimethylphosphate; $(CH_3O)_3PO$; [512-56-1]	Dissolves at room temperature; forms quite stable solution.	14
Diphenylphophinic chloride; $(C_6H_5)_2P(O)Cl$; [1499-21-4]	Dissolves at room temperture ; forms quite stable solution.	14
Hexamethylphosphoric acid triamide; $[(CH_3)_2N]_3P(O)$; [680-31-9]	Dissolves; solutions stable up to 323 K	14
Arsenic trifluoride; AsF_3 ; [7784-35-2]	XeF_2 reacts.	15
Bromine trifluoride; BrF_3; [7787-71-	Dissolves without apparent	15

5]	decomposition.	
Iodine pentafluoride; IF_5 ; [7783-66-6]	Dissolves with gas evolution.	15
Trfluoroacetic acid; CF_3COOH; [76-05-1]	Reacts to form $FXeO_2CF_3$.	16

XENON FLUORIDE; XeF_4 ; [13709-61-0]

1. XeF_4 + HF [7664-39-3]

Hyman and Quaterman[4, 5] report the solubility of XeF_4 in pure anhydrous HF at several tempertures. The solutions are non-conducting and stable over the 271 - 303 K temperature interval. The enthalpy of solution is 28.0 kJ mol^{-1} .There are no other data to compare with these.

2. XeF_4 + NOF; [7789-25-5] + HF; [7664-39-3] (1 NOF: 3 HF)

Nikolaev *et al.*[6, 7] report the solubility of XeF_4 between 291.6 and 354.1 K in a mixed solvent of one mol NOF to 3 mol HF. The solubility is greater in the mixed solvent than in the pure HF. The estimated enthalpy of solution is > 20.1 kJ mol^{-1}.

3. XeF_4 + IF_5 ; [7783-66-6]

Nikolaev *et al*.[7] report six solubility values between 296.2 and 343 K. The solubility values are greatly scattered and the estimated enthalpy of solution from the solubility data ranges from 6 to 30 kJ mol^{-1} .

Table 2 summarizes qualitative observations on the behavior of XeF_4 in a number of inorganic and organic solvents. No data sheets were prepared for these systems.

Table 2. Qualitative observations on the solution behavior of XeF_4 in a number of inorganic and organic solvents.

Solvent	Remarks	reference
Antimony pentafluoride; SbF_5 ; [7783-70-2]	Dissolves with gas evolution.	17
Bromine trifluoride; BrF_3 ; [7787-71-5]	Forms complex species.	17, 18
Acetic anhydride; $(CH_3CO)_2O$; [108-24-7]	Decomposes.	16
Trifluoroacetic acid anhydride; $(CF_3CO)_2O$; [76-05-1]	Dissolves without reaction; no further data.	16
Diethyl ether; $(CH_3CH_2)_2O$; [60-29-7]	Sparingly soluble; decomposes.	18
Dimethylformamide; $HCON(CH_3)_2$; [68-12-2]	Dissolves without decomposition.	16
Acetonitrile; CH_3CN; [75-05-8]	Sparingly soluble	13, 16
Dimethylsuloxide; $(CH_3)_2SO$; [67-68-5]	Decomposes.	13, 16
Fluorotrichloromethane (Freon-11); CCl_3F; [75-69-4]	Insoluble.	13
Dichlorodifluoromethane(Freon-12); CCl_2F_2 ;[75-71-8]	Insoluble.	13
Tetrachloromethane; CCl_4 ; [56-23-5]	Insoluble.	19

XENON FLUORIDE; XeF_6 ; [13693-09-9]

1. XeF_6 + HF; [7664-39-3]

Hyman and Quaterman[4,5] report the solubility of XeF_6 in pure anhydrous HF at four temperatures between 289.0 and 303.4 K. The XeF_6 reacts to form complex ions and the solution conductivity increases with conentration. The enthalpy of solution is 75 kJ mol^{-1}.

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COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Xenon fluoride; XeF_2; [13709-36-9] (2) Water; H2O; [7732-18-5]	E. H. Appelman and J. G. Malm *J. Am. Chem. Soc.* **86**, 2297 - 98 (1964).
VARIABLES: *T*/K = 273	**PREPARED BY:** H.L. Clever

EXPERIMENTAL VALUES

The authors report a solubility of 5 mg $(mL)^{-1}$ in water at 0^oC. This corresponds to a solubility of 0.148 mol L^{-1} (compiler).

AUXILIARY INFORMATION

The authors report xenon difluoride persists in slightly acidic solutions and decomposes at 0^oC to O_2 and HF with a half life of 7 hours. The authors used photochemically prepared XeF_2 , froze samples of about 0.5 g in liquid nitrogen, pipetted in 20 ml of ice on 20 mL of ice water and brought the system to 0^oC. Sample larger than 25 mg $(mL)^{-1}$ did not dissolve completely.

No other information given.

Components:	**Original Measurements:**
(1) Lithium azide; LiN_3; [19597-69-4] (2) Solvents	T. Curtius and J. Rissom, J. Prakt. Chem. **58**, 261-309 (1898).
Variables: *T*/K: 283 - 289	**Prepared by:** **J. Hála**

Experimental Data

Solubility of LiN_3 in water or ethanol at different temperatures[a]

Solvent	Temperature (t/°C)	LiN_3 (g/100 g solvent)	LiN_3 (m_1/mol kg^{-1})[b]
Water; H_2O; [7732-18-5]	10	36.12	7.377
	15.5	62.07	12.68
	16	66.41	13.56
Ethanol; C_2H_6O; [64-17-5]	16	20.26	4.14

[a]Solid phases were not investigated.
[b]Calculated by compiler.

Additional information: Saturated solutions of LiN_3 in water showed alkaline reaction.

iary Information

Method / Apparatus / Procedure:
Isothermal method used. Excess salt was kept in contact with the solvent for several weeks under occasional stirring in a room with constant temperature. Equilibrium temperature was measured in the saturated solutions prior withdrawal of the samples. A weighed amount of the saturated solution was then evaporated in a platinum dish, and dried in a dessicator until constant weight was attained.

Source and Purity of Materials:
LiN_3 was prepared from Li_2SO_4 and $Ba(N_3)_2$ as colorless hygroscopic crystals. The product was recrystallized from water, and analyzed after prolonged drying over concentrated H_2SO_4 in a vacuum desiccator. Found/calculated for LiN_3 (%): N 85.67-86.02/85.71, Li 14.09-14.18/14.29. The barium azide used was prepared by dissolving $Ba(OH)_2$ in 8% aqueous solution of HN_3. The latter was obtained by distillation with dilute H_2SO_4 of either $Pb(N_3)_2$ or NH_4N_3 according to Ref. 1. Purity of water not specified. Absolute ethanol was used.

Estimated Error:
Temperature: not reported.
Solubility: insufficient data given to allow for error estimate.

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Item 8 on the Agenda: New Projects for Future Publications

The list of volumes expected to be completed in 2005 is difficult to predict. Most information will be available by the subcommittee chairmen and chairwoman at and subsequent to this SSED meeting. At this time, I would only like to report on the existing project for hydrocarbons in water, and three projects on actinides, sugars and oxygen.

1. Hydrocarbons in Water and Seawater. Eight volumes were submitted in 2004, and the final four volumes expected to be submitted in 2005 are:

Part 9: C_{10} Hydrocarbons with Water (19 systems, 10 evaluations)
Part 10: C_{11} and C_{12} Hydrocarbons with Water and Heavy Water (22 systems,: 11 evaluations).
Part 11: C_{13} - C_{36} Hydrocarbons with Water (46 systems; 18 evaluations)
Part 12: C_5 - C_{26} Hydrocarbons with Seawater (in preparation)

2. Jiri Hála is working on a new volume on "Solubilities of Inorganic Actinide Compounds," and completion date of mid 2005 is anticipated.

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 Aveiro.

4. 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 (email from Larry dated 16 June 2004).

5. I assume updated information on other volumes will be forthcoming during the Aveiro meeting.

A4

Item 9 on the Agenda: New Procedures for Data Evaluation

presented by A. Maczynski, M. Goral & A. Skrzecz

New Procedures for Data Evaluation

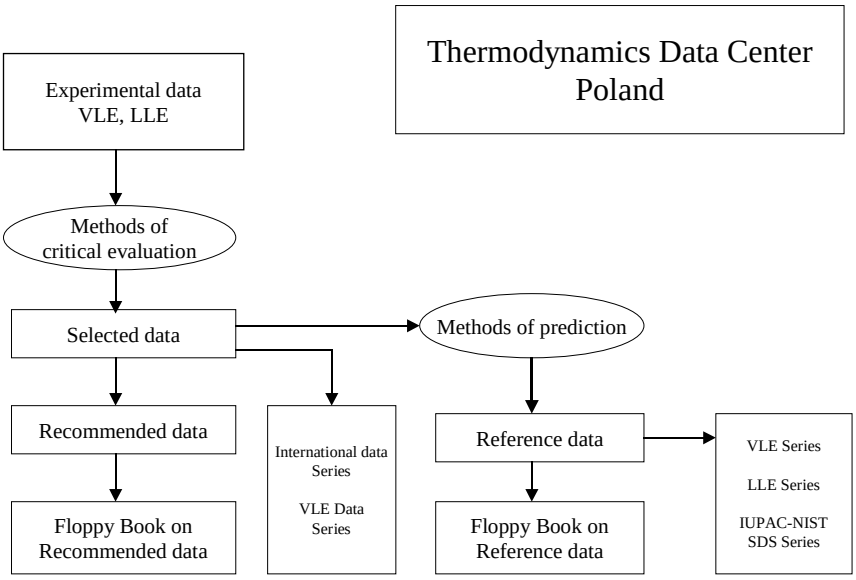
A. Maczynski, M. Goral, and A. Skrzecz

Thermodynamics Data Centre, Warsaw. Poland

Presented at the 30th Annual Meeting of
the IUPAC Subcommittee on Solubility and Equilibrium Data
Portugal, Aveiro, July 24, 2004

The Thermodynamics Data Centre, TDC, is a common laboratory of the Institute of Physical Chemistry PAS, Institute of Coal Chemistry PAS, Warsaw University, and Warsaw Technical University.

All activities of the TDC are showed on the figure below:



An important part of TDC is the Data Bank containing ***experimental*** phase equilibrium data (mainly VLE and LLE) and related thermodynamics properties, mainly heat of mixing.

This Data Bank contains over 32000 VLE and 6000 LLE data sets, predominantly isotherms or isobars, updated by about 2000 data sets per year.

Various methods are used for the critical evaluation of experimental data and for obtaining ***Selected Data***. It was found, that criteria of critical evaluation are fulfilled by about 30 % data only. These can be used for further work.

Selected Data obtained at TDC are published since 1993 in the International Data Series - Selected Data on Mixtures by the Thermodynamics Research Center, National Institute for Standards and Technology, USA.

The twelve Volumes of Vapor-Liquid Equilibria Series have been published by TDC in1998-2002. A CD version has been also provided.

As a next step ***Recommended Data*** are obtained by the selection of only one single data set for a given system, at the reported temperature and pressure. Such a data are used for instance for the calculations of BiP's – Binary Interaction Parameters, required in the Process Simulators. At the TDC ***Recommended Data*** are being prepared in an electronic form as a floppy book.

An Important area of the TDC activity is the development of methods for the prediction of phase equilibrium data.

Most of these methods are based on an Equation of State where use is made of an association term developed by Goral. It was found that for VLE data systems containing alcohols and hydrocarbons the accuracy in predicting these data is close of the best experimental data. These results have already been published in a series of articles in the Journal of Physical and Chemical Reference Data. The predicted ***Reference Data*** can be used for critical evaluation of experimental data as well as for obtaining new data.

We consider this as an important step in the development of thermodynamics of phase equilibria.

Similarly an important step has been done for solubility and liquid-liquid equilibrium data.

The method used for the prediction of mutual solubility data for systems containing water and hydrocarbons was developed and already published in a series of articles in the Journal of Physical and Chemical Reference Data. Similarly as for VLE data the predicted LLE data for water - hydrocarbons systems are on the level of accuracy of the best experimental data and, as ***Reference Data***, can be used for the critical evaluation of experimental data as well as for obtaining new data.

On the basis of this method the IUPAC SDS Volumes 37 and 38 on Hydrocarbons with Water and Seawater have been recently updated and prepared for publication as 12 Parts of the IUPAC-NIST Solubility Data Series, Volume 81. The compilations has been updated with new published data, and evaluations have been prepared all over again using our new methods of critical evaluation.

The ***Reference Data*** have also been prepared in an in electronic form as a floppy book.

Method of correlation and critical evaluation of solubility data in hydrocarbon + water systems.

The solubilities of binary systems of C_5-C_{36} hydrocarbons with water were reviewed in 1989 in the Volumes 37 and 38 of the IUPAC Solubility Data Series, refs 1 and 2. The solubilities of hydrocarbon+water systems are of considerable importance and of widespread interest among several groups including industrial and environmental chemists. The volumes mentioned above are now difficult to obtain and nearly 20 years out of date. New technique of data evaluation has been developed in the mean–time. Therefore, the decision was made to revise and update this work as a new volume 81, refs 1 and 2.

Procedures used in critical evaluation

When each system is evaluated separately the estimation of data quality can be difficult. For example, plots of the solubility versus temperature from two studies of the same system can yield two smooth but disagreeing curves, with the reason for the systematic difference not being clear. In other systems, only a few experimental points may be available. Moreover, solubilities in hydrocarbon water systems are very low and consequently even small experimental errors may lead to substantial relative errors in measured solubilities, which in some cases reach 100 % or more. To help clarify these uncertainties this work presents a new approach to the critical evaluation of the solubility data of the hydrocarbon-water systems. This approach involves the calculation of “reference data” using smoothing equations that incorporate solubility information from many systems. The calculation of reference data includes two steps:

1. Approximation of solubilities of hydrocarbons in water using a smoothing equation described in the next section. This equation depends on the hydrocarbon properties and contains also empirical coefficients. The same values of these coefficients are used for

mixtures of various hydrocarbons in water. These are derived from a regression making use of all the hydrocarbon solubility data.

2. Liquid-Liquid Equilibrium (LLE) calculations yielding solubility of water in various hydrocarbons. The input data for these calculations are the hydrocarbon– in–water solubilities predicted by the smoothing equation mentioned above The LLE calculations use an equation of state (ESoC) modified so as to account for the role of hydrogen bonding.

In these two steps an extensive body of experimental data is described using only a few adjustable parameters. This provides an additional framework for comparison of experimental data and helps in the recognition of systematic errors. The hydrocarbon solubilities calculated from the smoothing equation and the calculated water solubilities are used as the reference data in evaluations. The calculations and examples of evaluation of data are given in refs 3 – 8.

Derivation of reference data for solubility of hydrocarbons in water

The mole fraction of hydrocarbons in water (x_1) at temperature (T) along the three phase equilibrium exhibits a minimum ($x_{1,\min}$) near room temperature $T_{\min}$. The solubility curve can be approximated with an equation derived in refs. 5–8:

$$\mathbf{ln}(x_1 / x_{1,\min}) = C\, \mathbf{f}(T / T_{\min}), \qquad (1)$$

where C is an adjustable parameter dependent on hydrocarbon, and $\mathbf{f}(T/T_{\min})$ is a function, described in refs. 5–8, which achieves a minimum value equal to zero at $T = T_{\min}$. Altogether Eq. 1 depends on three parameters: $T_{\min,}$ C and $x_{1,\min}$. It was found that $T_{\min.}$= 305 K for *n*–alkanes and *i*–alkanes, $T_{\min.}$= 298 K for cycloalkanes and unsaturated hydrocarbons and $T_{\min.}$= 290 K for benzene and alkyl benzenes.

It was found that both $\mathbf{ln}x_{1,\,\min}$ and C depend linearly on excluded volume, b, used in equation of state of van der Waals type. These dependences for aromatic hydrocarbons are shown in Figs 1 and 2.

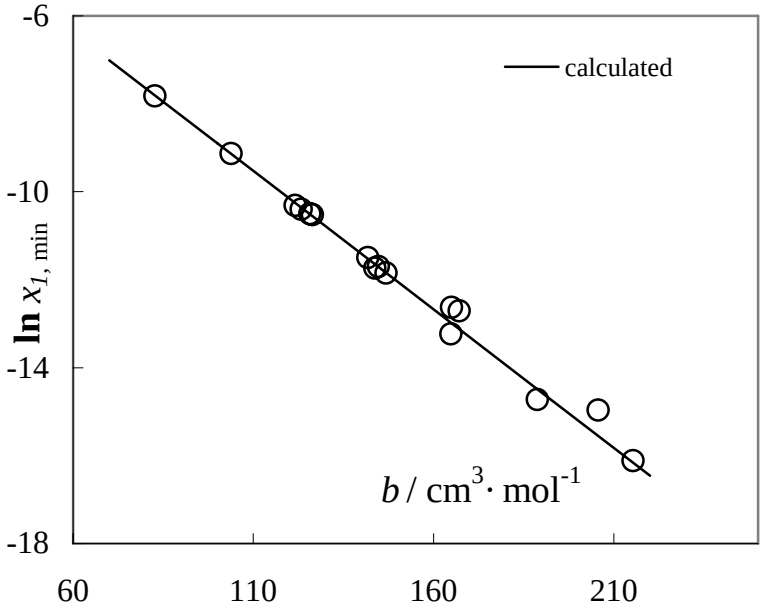


Fig. 1 Minimum solubilities ($x_{1,\,min}$) of arenes *vs.* excluded volume (*b)*.

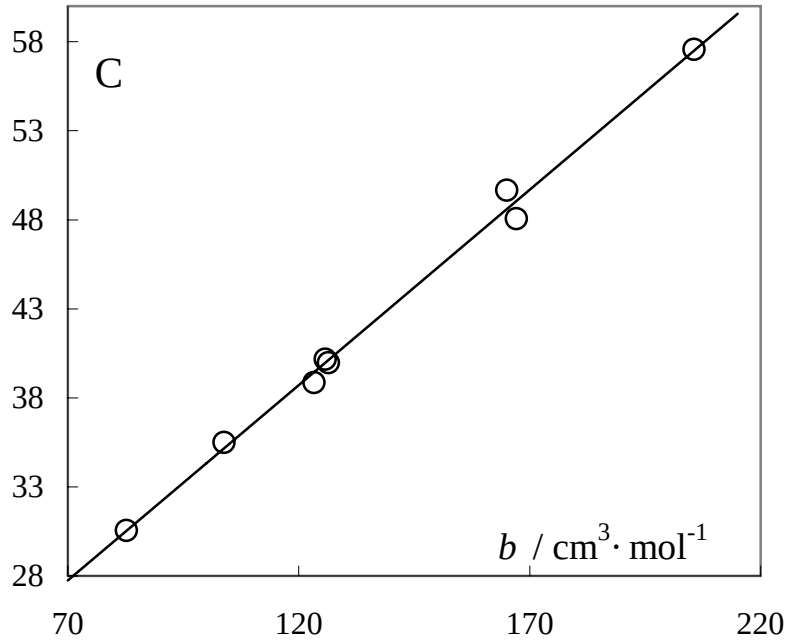


Fig. 2. Coefficient *C vs.* excluded volume of aromatic hydrocarbons (*b*).

The linear relations shown in Figs 1 and 2 suggest that Eq. 1 can be rewritten in the form

$$\ln x_1 = (c_1 + c_2\, b) + (c_3 + c_4\, b)\, \mathbf{f}(T/\, T_{\min.}). \qquad (2)$$

The coefficients c_1, c_2, c_3 and c_4 were found by simultaneous regression of all solubility data for benzene and alkyl benzenes. It was found that solubilities of non–aromatic hydrocarbons can be described by an analogous equation:

$\ln x_1 = (c_5 + c_6\, b + c_7\, L) + c_8\, b\, \mathrm{f}\,(T / T_{\min.})$, (3)

where L is the number of –bonds e.g. L=0 for alkanes, L=1 for alkenes and so on.

Equations 2 and 3 with constants c_1 to c_8 allow to reproduce the solubility data for 157 hydrocarbons; these were taken from 1037 data sets and 218 references. The equations are valid up to the three–phase critical temperature (T_{3c}). Once the constants c_i are determined, Eq. 1 can be used for the prediction of the hydrocarbon solubility even in the absence of experimental data. Statistical analysis of the deviations for the investigated systems shows that they are random and can be ascribed to error of the data. The standard error of the calculated x_1 is in the range of 1% to 5% at room temperatures and does not exceeds 10% at T_{3c}. These values are smaller than the standard error of the experimental x_1–values, which is about 30%.

Derivation of reference data for solubility of water in hydrocarbons

The solubility of water in hydrocarbons was calculated using LLE calculations by a method developed by Góral, ref. 8. This method of phase equilibrium calculations (EoSC) is based on the Redlich–Kwong EoS with an added term accounting for hydrogen bonding. Application of the EoSC for water systems is described in refs 5 – 8. In the LLE correlation the input data the is the solubility of the hydrocarbons in water, as calculated by Eq. 1. The output is water solubility (x_2) in a given hydrocarbon as a function of temperature (T).

To perform these calculations a model of association was developed. This model uses one equilibrium constant of self–association for water and two constants of cross–association of water with an aromatic ring and with a –bond. Because these constants are temperature dependent altogether 8 parameters had to be used in the model of association. With these 8 parameters solubility data for water in 157 hydrocarbons were calculated. The accuracy of the calculated solubility of water was similar to that of the solubility of hydrocarbons.

Floppy Book on Recommended Solubility Data

The Floppy book is a form of presentation for large amounts of experimental data sets. The corresponding data base may contain both experimental data and equation parameters or equation parameters only.

The Floppy book contains both management software and databases. The area of interest to TDC are mainly data bases relating to thermo physical properties, namely VLE, LLE, HE, etc. The data sets are indexed so as to enable rapid searching under various aspects such as: required property, substance, system, data record, reference, etc. The data records found are always displayed on the screen. To make comparison easier, it is also possible to display on one screen up to 10 records of the same system. The respective numerical data are displayed in

the left window. This packet allows to find very quickly the needed information in the data base.

The Floppy Book on Recommended Solubility Data is part of TDC Floppy Book project on recommended VLE, LLE and solubility data. Up to now, the Recommended Solubility Data Floppy Book contains 305 recommended data sets on mutual solubility of hydrocarbon - water systems.

In all these systems large miscibility gaps are present; i.e. both components are nearly mutually insoluble. Therefore each side of solubility curve, the hydrocarbon-rich and the water-rich phases are presented independently. In each particular system, the curve shown describes the temperature dependence of the reference solubilities while the points shown represent the recommended experimental solubilities

Keep in mind that the reference solubilities are those calculated by the same model for all hydrocarbon – water data accepted after critical evaluation. The body of all available experimental data form the background of these investigations. They are collected for the new updated NIST-IUPAC SDS volume 81 on solubility of water and hydrocarbons.

The sample screens shown hereafter present the most important steps in using our Floppy Book.

- opening screen, Fig. 3;
- selection of the compound and system, Fig. 4;
- graphical presentation of water – rich phase, Fig. 5
- graphical presentation of hydrocarbon – rich phase, Fig. 6.

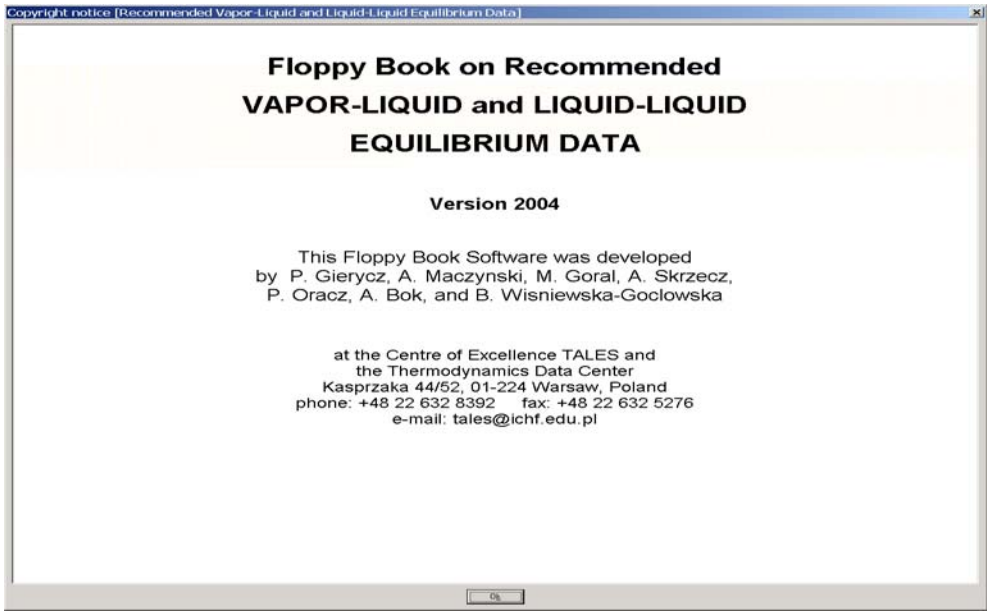


Fig. 3. Title screen

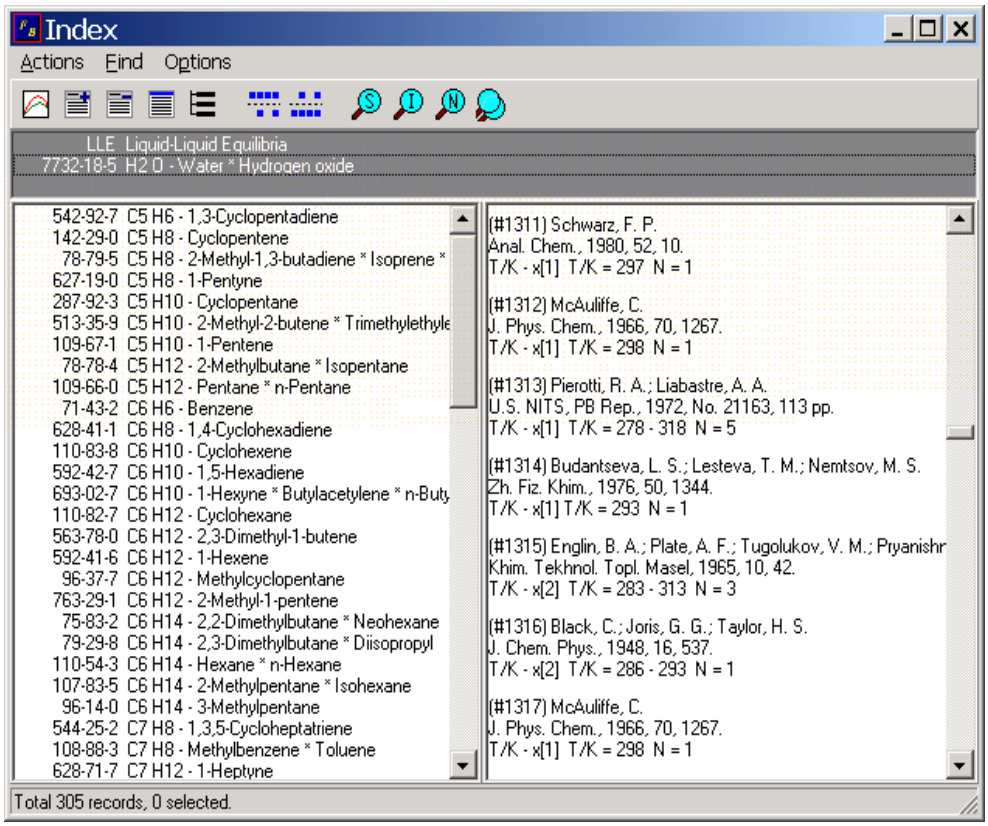


Fig. 4. Selection of system and record

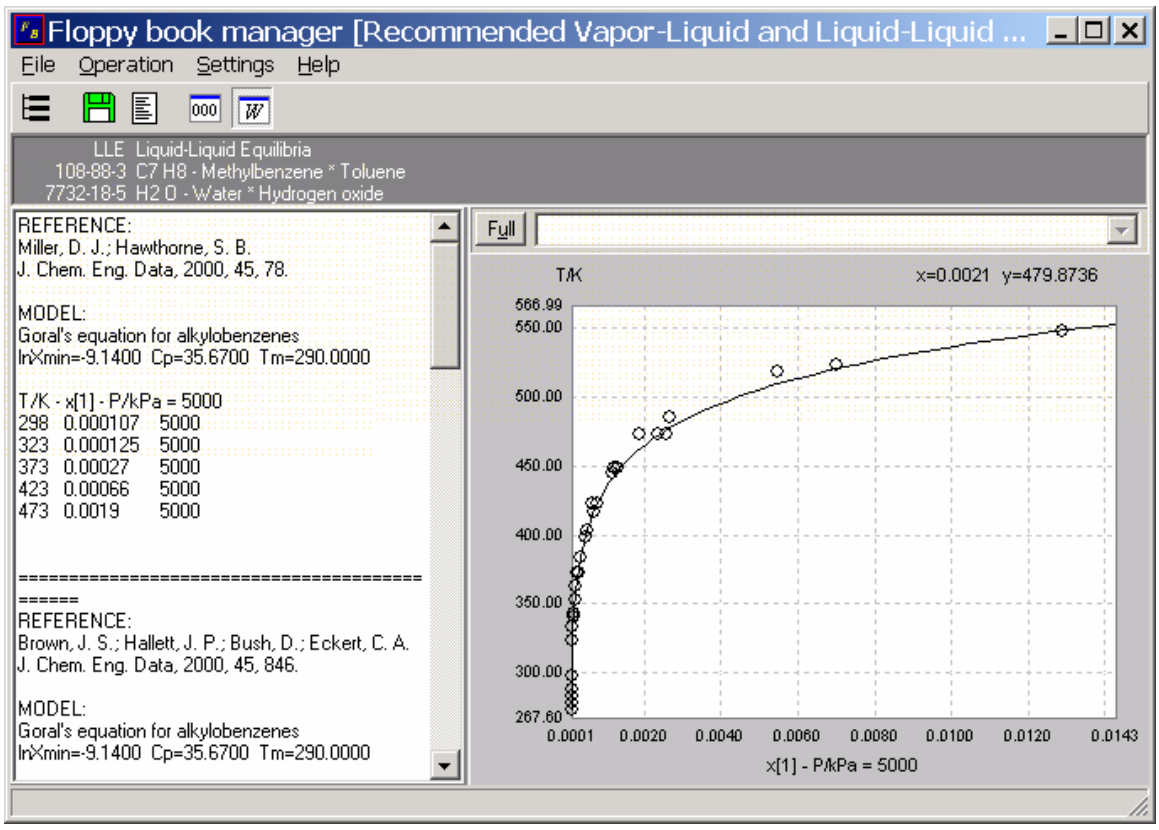


Fig. 5. Graphical presentation of water – toluene system (water-rich phase)

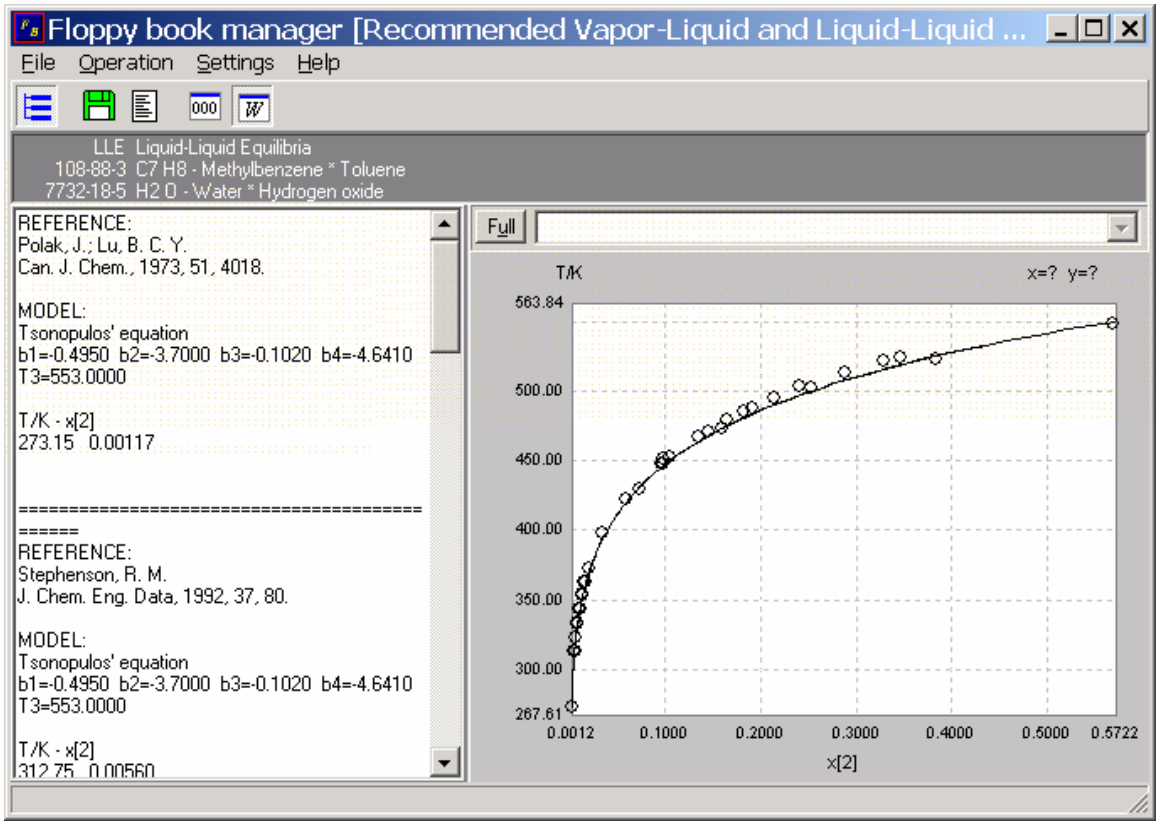


Fig. 6. Graphical presentation of water – toluene system (toluene-rich phase)

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9. M. Góral, Fluid Phase Equilibria **27,** 118 (1996).

A5

Item 12 on the Agenda: Reports of Subcommittees and Projects

Report of the Liquid-Liquid Subcommittee Meeting

Aveiro, Portugal, 24 July 2004

Present: Marian Goral (2004 Franzosini Award Recipient), Andrzej Maczynski, Mark Salomon, Valerii Sazonov, David Shaw (Chairman), Adam Skrzecz

Participants in the Liquid-Liquid Subcommittee of the SSED have been active in the last year and project work has progressed very well. Specific projects in progress and planned for the immediate future are summarized below.

Active Projects

Project 2002-050-1-500; Solubility data related to industrial processes; Acetonitrile: ternary and other multicomponent systems.

Task Group: Valerii Sazonov (Leader), Mark Salomon, David Shaw, Adam Skrzecz

This project is at an advanced stage. All compilations and most evaluations have been prepared and reviewed internally. Volume completion is expected by the end of 2004.

Project 2003-018-1-500; Mutual solubility of hydrocarbons with water (update and revision of SDS Volumes 37 and 38)

Task Group : Andrzej Maczynski (Leader), Marian Goral, Mark Salomon, David Shaw, Adam Skrzecz, Barbara Wisniewska-Goclowska

In view of the size of this update project (Volumes 37 and 38 have a combined page count of over 1100) the decision was made to submit the revised work to JPCRD as a series of 12 parts. Parts 1-8 have been submitted to JPCRD. Parts 9-12 have all compilations and evaluations complete. Remaining tasks include review of some evaluations and preparation of preface and indices. Submission to Editor in Chief will be in October 2004. All parts will be published as volume 81.

Project 2003-011-3-600; A critical compendium of pesticide physical data

Task Group: Don Wauchope and David Shaw (Co-Leaders)

This project is at an early stage. Task Group members are being recruited; discussions are continuing about the scope of the project , data presentation formats, and collaboration with other similar projects.

New Projects (accepted by the SSED; Project Proposals will be prepared)

Mutual Solubility of Alcohols and Water (update and revision of SDS Volume 15)

Proposed Task Group: Andrzej Maczynski (Leader), Marian Goral, Mark Salomon, David Shaw, Adam Skrzecz, Barbara Wisniewska-Goclowska

This project will be similar to the hydrocarbon/water update volume now nearing completion. Scope of the volume will include benzyl alcohol and its derivatives, which were not covered in Volume 15. Compilations published in Volume 15 will be incorporated by reference, rather than republished. New evaluations will be prepared. Volume completion is estimated to require 30 months.

C-3 and Higher Nitriles: Binary and Multicomponent Systems

Proposed Task Group: Valerii Sazonov (Leader), Mark Salomon, David Shaw, Adam Skrzecz

This project will complete the sub-series on nitrile solubility and is expected to be completed in 30 months.

Future Projects (seriously contemplated but not formally proposed)

Solubilities of Carboxylic Esters in Water: Binary Systems; Andrzej Maczynski

Solubilities of Furfural and Derivatives: Binary and Multicomponent Systems; Valerii Sazonov

Report of the Subcommittee on Solid Solubilities
W. Voigt

Aveiro, July 2004

At present nine projects listed as being active. Situation within the individual projects is as follows:

Solubility data related to oceanic salt systems

1. and 2.)
Part I. Binary systems containing sodium, potassium, and ammonium sulfate (2002-033-1-500) C. Balarew, R. Bouaziz, R. Cohen-Adad, J.W. Lorimer, N. Ariguib. Part II. Magnesium chloride-water and calcium chlorides-water and their mixtures (2002-034-1-500) W. Voigt

Established working principles of compiling and evaluating data within the task groups dealing with the oceanic salt systems have to be reconsidered, mainly because of the reduced manpower and too limited time frame. Thus, the simultaneous generation of compilation sheets of binary and multi-component systems has to be substituted in a first step by an isolated collecting and extracting of only binary system data. The consequences on the evaluation procedure is still under discussion.
R. Bouaziz is not longer an active task member. Since R. Cohen-Adad has serious health problems at present it is not possible to communicate with him***)**. W. Voigt will initiate with help of N. Ariguib to contact M.-Th. Cohen-Adad in order to discuss the problem how to proceed with the alkaline metal sulfate systems including all the material R. Cohen-Adad has collected and evaluated.
Evaluated solubility data of the oceanic salt systems are of extraordinary importance for science and technology. However, considering the task members situation the completion of the two projects has to be postponed.

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

3.)
Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb) C.Magalhães, H. Gamsjäger and K. Sawada (2002-032-1-500)
Project status is in accordance with the plan. Compilation sheets are ready, half of the data are evaluated. A new member will enter the task group to perform modelling of carbonate solubilities. The material will be send to Prof. W. Hummel (Switzerland) as an end-user of such data for possible advices in the preparation of the volume.

4.)
Alkaline earth metal carbonates. E. Königsberger and J. Vanderdeelen J. Lorimer (2002-031-1-500)
The volume is ready from in respect to compilation sheets and critical evaluations. The subcommittee members agreed to complement the critical evaluation with thermodynamic modelling on the basis of work, which had been done by E. Königsberger. The corresponding calculations has still to be performed. Also the preface of the volume has to be rewritten.
J. W. Lorimer asked to replace his responsibility by E. Königsberger and at the same time to involve A. de Visscher, a colleague of J. Vanderdeelen. A. de Visscher was a speaker on the

11th ISSP and demonstrated high professionality in applying thermodynamic modelling in electrolyte solutions combined with specific background in carbonate systems.

5.)

Inorganic actinide compounds. J. Hala , M. Salomon (2002-025-1-500)

The work on this volume is proceeding as expected.

Solubility data of compounds relevant to human health.

6.)

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

Progress is made in accordance with the schedule.

7.)

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

Nearly all compilation sheets are ready. Critical evaluations been done for aqueous and alkoholic solvents. Evaluation of amide containing solvents seems to be difficult. A suggestion will be made by A. Goto and sent to W. Voigt until the end of 2004. Thus the volume can be completed until the end of 2005.

8.)

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

The compilation sheets are ready. The volume will be quite small (approx. 85 compilation sheets). Only a very limited evaluation can be done on the basis of very few and scattered data. However, it was agreed to complete the volume on this basis. Until the end of the year 2004 a proposal of an evaluation will be sent to the subcommittee chair.

Solubility data related to industrial processes.

9.)

Lead sulfate. J.W. Lorimer (2002-042-1-500)

J. W. Lorimer does not see the possibility of finishing this volume within the next two years.

Additional activities

***a) Solubility of Sugars in Aqueous and Nonaqueous Solutions*, João AP Coutinho**, editor.

At the SSED meeting J. A.P. Coutinho presented the compilation sheets and questions of an evaluation strategy have been discussed. It is proposed to initiate the formal procedure for getting a project number within the phantom proposal under the aspect of “Solubility data of compounds relevant to human health”.

***b) Transition and 12 to 14 Main Group Metals, Lanthanides, Actinides and Ammonium Halates*. H. Miyamoto, R. Miyamoto, C. Guminski, M. Salomon**

This up-date volume is in essence ready and was delivered as an pdf file at the SSED meeting. It is proposed to complete the work on this volume as a substitute of the “lead sulfate volume“ under the sub-title “Solubility data related to industrial processes” of the phantom proposal.

c) J. Eysseltova has started with compilation work on solubility of alkaline metal nitrates in water and is willing to propose an appropriate project in 2005.

*) Roger Cohen-Adad could not recover and died at August the 17th .

A6

Item 15 on the Agenda: Address by Hiroshi Miyamoto

May I thank the chairman for his kind cooperation.

Now, I am remembering how I took part in many activities of the IUPAC Solubility Data Project (SDP).

First, I attended the meeting on SDP from 1979 through 2004 almost every year. My attendance at the meeting held in Davos, Switzerland in 1979 was my first chance to meet the SDP members. This chance was provided by the invitation from Prof. Steven Kertes and Dr. Mark Salomon.

Later, I stayed in the Solubility Data Center at Emory University in Atlanta, GA from September 1981 until the summer of 1982. While staying at the Center, I completed the manuscripts of the first halate volume which compiled and evaluated the solubility data of alkaline earth metal halates. I would like to thank the hospitality of Prof. Larry Clever.

Next, the 8th ISSP was held in Niigata, Japan in 1998, which reported in IUPAC magazine "Chemistry International" by Prof. Jack Lorimer. I would like to thank the distinguished guests and all attendees who traveled great distances and took valuable time from their very busy schedules to express their great interest in the scientific program and help us make the conference possible.

Finally, we (Ryo and I) have already finished the preparation of the manuscripts of the 4th and final halate volume including transition metals and lanthanide halates. Today, we discussed with Mark and Cezary concerning the final editorial work of the volume. As the result, the manuscripts of our final volume of CD style will be sent to Mark the Editor-in-Chief soon after this meeting.

Now, I am seventy-five years old. Soon, it will be difficult for me to take a long flight to attend the meetings. So, I would like to thank you very much for your kind advice and comments on my SDP activities.

Thank you very much to Heinz and all IUPAC friends!