

# Minutes

## INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

### 37<sup>th</sup> Annual Meeting (10<sup>th</sup> of SSED)

to be held in conjunction  
with the 32<sup>nd</sup> ICSC,  
la Grande-Motte, France  
2<sup>nd</sup> September 2011

**Friday, September 2, 2011**

**Morning Session 10:30 - 12:30**

**A. Subsubcommittees meetings**

Subsubcommittee: Gas-liquid Solubilities

J. Salminen (Chair)

Subsubcommittee: Liquid-liquid Solubilities

D. Shaw (Chair)

Subsubcommittee: Solid-liquid Solubilities

W. Voigt (Chair)

Subsubcommittee: Stability Constants

G. Hefter (Chair)

**Afternoon Session, (14:00 - 19:00)**

**1. Introduction of participants**

C. Magalhães

The list of participants is attached to these minutes

**2. Approval of Minutes of the 36<sup>th</sup> Annual Meeting (9<sup>th</sup> of SSED) in conjunction with the 14<sup>st</sup> ISSP, Leoben, Austria,**

Earle Waghorne

The minutes of the previous meeting were accepted with one minor change (ACSC to ICSC in 15)

**3. Informations**

C. Magalhães

Clara Magalhães asked the Subcommittee members to provide details of events organized in conjunction with the International Year of Chemistry.

Clara Magalhães asked members to consider the Analytical Chemistry Division

terms of reference where are described its main goals, focus and activities, and to suggest changes to these terms of reference. It was pointed out that the terms of reference are traditionally used to select division members.

4. Thermodynamic analysis of solubility data, Guidelines for reporting of phase equilibrium measurements. H. Gamsjäger

Heinz Gamsjaeger made a presentation regarding the proposed "Guidelines for Reporting of Phase Equilibrium Measurements". This clearly indicated a number of deficiencies in the Guidelines. It was agreed to circulate the guidelines to the SSEED members for comments and to respond to IUPAC. The proposed Guidelines were circulated and recirculated with the minutes..

Glenn Hefter requested that the Chair write asking that the SSEED have a preview of such guidelines before they are published.

Wolfgang Voigt pointed out that guidelines and recommendations need to be compatible and that electrolyte systems should be included.

5. Projects: C. Magalhães

5.1 The gas-liquid subcommittee

Clara Magalhães noted that currently not active and requires a new chair.

Glenn Hefter suggested contacting Larry Clever, Peter Fogg, Rubin Battino and Bernard Wolfe.

The current manuscripts are detailed in the EiC's report.

5.2 Analysis of the present projects

Clara Magalhães explained that currently there are ten active projects.

The transfer of funding from 2011 to 2012 may be problematic.

5.3 New projects

Clara Magalhães explained that projects can claim up to \$5,000 and, because there is a limited amount of money available the recommendation is that SSEED projects should apply for a maximum of \$2,500. The money can be used for travel to progress the project.

New projects were referred: Berilium sulfides and selenides (Jiri Hála), Potassium Sulfate in Water (Jitka Eysseltova), Lithium Sulfate in Water (Wolfgang Voigt) in solid- liquids equilibria, and ternary systems of water with alcohols and hydrocarbons (Marian Goral) in liquid-liquid equilibria but many others are welcome.

#### 5.4 IUPAC-NIST agreement (old solubility volumes)

After a lengthy discussion the SSED didn't accept the current proposal although there was support for the principal objective.

The SSED felt that it had insufficient information. In particular there was not sufficient clarity regarding the method of publication (facsimile or OCR) and how errata would be dealt with.

The question of whether there would be a financial aspect to the project was raised.

It was noted that the copyright might be shared between IUPAC and the previous publisher.

It was agreed that the Chair should contact the EiC.

#### 5.5 Division Financial matters

Clara Magalhães reported that she had received no report.

### 6. Chairman's Report from 2010 - 2011

C. Magalhães

The chairman's report is attached.

It was noted that Leslie Petit has offered the Equilibrium Constant database to IUPAC. The Chair was asked to write to the Secretariat seeking further information.

James Sangster's LOGKOW project was discussed. It was noted that Jim Sangster had mentioned an agreement with a US company. It was agreed that this needed clarification before a proposal can be made to IUPAC. It was also noted that, so far, a satisfactory candidate to join the project had not been found.

It was agreed that the Chair would contact Jim Sangster again, to seek clarification of the role of the American company and to continue to seek a candidate to work on the project. It was also agreed that this should be an item for discussion at the Xining meeting.

It was suggested that LogKOW database could be considered to be part of the more general problem of the IUPAC databases along with the "Stability Constants Database".

### 7. Franzosini Award

C. Magalhães

Clara Magalhães asked that nominations for the next Francosini awards be made by

February 2012.

8. Editor-in-Chief's Report for 2010 - 2011 M. Salomon  
Clara Magalhães presented the EiC's report.  
The EiC report is attached.
  
9. Subsubcommittees reports G. Hefter; W. Voigt;  
D. Shaw; J. Salminen  
Justin Salminen sent no report on the gas-liquid subsubcommittee activities.  
David Shaw reported that the only on-going projects by the liquid-liquid subsubcommittee are those proposed by Marian Goral; all the others have been published or sent for publication.  
Wolfgang Vogt had meetings with the chairs of the projects on solid-liquids solubilities present in La Grande-Motte.  
Glenn Hefter reported in the meeting that the only stability constants project is the project 2008-025-1-500:Humic-metal binding constants database that sent a report of their activities, once the project 1999-050-1-500:Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands has met its objectives. A new project will be presented.
  
10. Report on the 15<sup>th</sup> ISSP - Xining, China, 2012 D. Zeng  
Dewen Zeng presented the current state of the organization for the 15<sup>th</sup> ISSP.
  
11. Future International Symposia on Solubility Phenomena C. Magalhães  
It was agreed that the 2013 SSED meeting would be held in conjunction with the IUPAC General Assembly in Istanbul (end of July)  
Several VENUES for the next ISSP and SSED meetings were presented; they will be considered at the 2012 SSED meeting in Xining, China.
  
12. Adjournment C. Magalhães

### Attendees at the Meeting

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# **Subcommittee on Solubility and Equilibrium Data**

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Chair's Activity Report  
since March 2010

# The Subcommittee on Solubility and Equilibrium Data (SSED)

- Coordinates projects in the area of compilation and critical evaluation of published experimental data on the **chemical solubility** of well defined substances and other equilibrium systems;
- coordinates the dissemination of evaluated solubility data through traditional (journal) and electronic (internet-accessible database) means;
- works with the Analytical Chemistry Division and the US National Institute of Standards and Technology (NIST, the Solubility Data Series publisher) in the selection of chemical systems for analysis;
- encourages the formation of Task Groups to perform compilation, evaluation, improve the existing theories, present new theories, and collaborate with other Divisions' groups.



# Meetings and Conferences

- **SSED meeting** - The 36<sup>th</sup> solubility committee annual meeting (9<sup>th</sup> of SSED) occurred in Leoben on the 24<sup>th</sup> and 25<sup>th</sup> July 2010 in conjunction with the 14<sup>th</sup> ISSP.
- **14<sup>th</sup> ISSP** - The 14<sup>th</sup> International Symposium on Solubility Phenomena and Related Equilibrium Processes occurred in Leoben, Austria, at the Montanuniversitaet from the 25<sup>th</sup> to the 30<sup>th</sup> July 2010.

# Franzosini Award

Two Franzosini Awards were attributed to:

- Professor Jitka Eysseleva, Charles University, Prague, the Czech Republic, and
- Professor Stanislav Frančisković Bělinski, Ruder Bosković Institute, Zagreb, Croatia

# Visibility of SSED within IUPAC 2010/2011

- **CI, 32, No. 1, January – February 2010**
  - ◆ ***Mark Your Calendar***
    - ♣ Pg. 36: 25-30 July 2010, 14th ISSP, Leoben, Austria.
- **CI, 32, No. 2, March – April 2010**
  - ◆ ***Mark Your Calendar***
    - ♣ Pg. 32: 25-30 July 2010, 14th ISSP, Leoben, Austria.
- **CI, 32, No. 3, May – June 2010**
  - ◆ ***IUPAC WiRE***
    - ♣ Pg. 16: In Memoriam - Ari Horvath.
  - ◆ ***Mark Your Calendar***
    - ♣ Pg. 34: 25-30 July 2010, 14th ISSP, Leoben, Austria.

# Visibility of SSED within IUPAC 2010/2011 (continued)

- **CI, 32, No. 3, May – June 2010**
  - ◆ ***Making an imPACt***
    - ♣ Pg. 20: Chemical speciation of environmentally significant metals with inorganic ligands. Part 3: the  $\text{Pb}^{2+} + \text{OH}^-$ ,  $\text{Cl}^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ , and  $\text{PO}_4^{3-}$  systems (IUPAC Technical Report), K. J. Powell, et al, *Pure and Applied Chemistry*, 2009, **81**(12) pp. 2425-2476.
    - ♣ Pg. 22: Rare Earth metal chlorides in water and aqueous systems, IUPAC-NIST Solubility Data Series 87.
- **CI, 32, No. 4, July – August 2010**
  - ◆ ***The Project Place***
    - ♣ Pg. 22-24: Analytical Chemistry in Action, Brynn Hibbert.
  - ◆ ***Making an imPACt***
    - ♣ Pg. 26-27: The IUPAC-NIST Solubility Data Series: A guide to preparation and use of compilations and evaluations (IUPAC Technical Report), H. Gamsjaeger, J. W. Lorimer, M. Salomon, and R. P. T. Tomkins, *Pure and Applied Chemistry*, 2010, **82**(5) pp. 1137-1159.

# Visibility of SSED within IUPAC 2010/2011 (continued)

- **CI, 32**, No. 6, November – December 2010
  - ◆ **Features**
    - ♣ Pg. 6-9: A Place in the Salt: learning and playing with salt in Aveiro, Portugal, M. C. F. Magalhães, C. Sampaio, P. Trincão.
  - ◆ **IUPAC WIRE**
    - ♣ Pg. 18: Two Franzosini Awards in 2010.
  - ◆ **Conference call**
    - ♣ Pg. 24-25: Solubility Phenomena, H. Gamsjaeger.
- **CI, 33**, No. 2, March – April 2011
  - ◆ **The Project Place**
    - ♣ Pg. 24: Rare earth metal (Sc, Y, lanthanoids) bromides and iodides in water and aqueous systems (Solubility Data Series), C. Guminsky.

# Completed SDS Volumes

## IUPAC-NIST Solubility Data Series

- **Volume 88:** Marian Goral *et al.*,
  - ◆ “Esters with water - Revised and Updated. Part 1. C2 to C4 esters ”, *J. Phys. Chem. Ref. Data* (2009), **38**(4), 1093. (Published December 2009).
  - ◆ “Esters with water - Revised and Updated. Part 2. C5 and C6 Esters”, *J. Phys. Chem. Ref. Data* (2010), **39**, online. (Published March 2010).
  - ◆ “Esters with water - Revised and Updated. Part 3. C7 and C9 Esters”, *J. Phys. Chem. Ref. Data* (2010), **39**, online. (Published June 2010).
  - ◆ “Esters with water - Revised and Updated. Part 4. C10 and C12 Esters”, *J. Phys. Chem. Ref. Data* (2010), **39**, online.
- **Volume 89:** Jitka Eysseltoová *et al.*
  - ◆ "Alkali metal nitrates. Part 1. Lithium nitrate." *J. Phys. Chem. Ref. Data* **39**, (2010).

# Completed SDS Volumes

## IUPAC-NIST Solubility Data Series (continued)

- **Volume 90:** Ayako Goto *et al.*,
  - ◆ “Hydroxybenzoic Acid Derivatives in Binary, Ternary, and Multicomponent Systems. Part I. Hydroxybenzoic Acids, Hydroxybenzoates, and Hydroxybenzoic Acid Salts in Water and Aqueous Systems”, *J. Phys. Chem. Ref. Data* (2011), **40**(1). (Published February 2011).
  - ◆ “Hydroxybenzoic Acid Derivatives in Binary, Ternary, and Multicomponent Systems. Part II. Hydroxybenzoic Acids, Hydroxybenzoates, and Hydroxybenzoic Acid Salts in non Aqueous Systems”, *J. Phys. Chem. Ref. Data* (2011), **40**(2). (Published May 2011).

# Other publications

- H. Gamsjaer, J. W. Lorimer, M. Salomon, D. G. Shaw, R., T. Tomkins “The IUPAC-NIST Solubility Data Series: A guide to preparation and use of compilations and evaluations” was published on the same time, as a technical Report in the *Pure Appl. Chem.*, 2010, Vol. **82**, No. 5, pp. 1137-1159 and in the *Journal of Physical Chemical Reference Data*, 2010, Vol. **39**, 23101-1.
- A. H. Harvey and M. Salomon, “Editorial IUPAC-NIST Solubility Data Series”, *Journal of Physical Chemical Reference Data*, 2010, Vol. **39**, 20401-1.



# Completed SDS Projects

- Project number: 2008-008-1-500
  - ◆ Project Title: **An introduction to the IUPAC-NIST Solubility Data Series: Preparation and use of compilations and evaluations**
  - ◆ Task Group lider: *David Shaw*
  - ◆ Starting date: July 2006, finished April 2010
- Project number: 2007-046-1-500
  - ◆ Project Title: **Solubility data related to industrial processes. Mutual solubility of esters with water**
  - ◆ Task Group lider: *Marian Goral*
  - ◆ Starting date: October 2007, finished March 2011

# Completed SDS Projects (continued)

- Project number: 2007-044-1-500
  - ◆ Project Title: **Solubility data related to industrial processes. Solubility in systems with lithium and/or sodium nitrates**
  - ◆ Task Group lider: *Jitka Eysselová*
  - ◆ Starting date: October 2006, finished March 2011
- Project number: 2006-033-1-500
  - ◆ Project Title: **Solubility data related to industrial processes. Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems**
  - ◆ Task Group lider: *Cezary Guminski*
  - ◆ Starting date: August 2005, finished December 2009

# Completed SDS Projects (continued)

- Project number: 2005-033-1-500
  - ◆ Project Title: **Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates**
  - ◆ Task Group lider: *H. Miyamoto*
  - ◆ Starting date: October 2005, finished May 2008
- Project number: 2002-036-1-500
  - ◆ Project Title: **Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates**
  - ◆ Task Group lider: *Ayako Goto, H. Miyamoto*
  - ◆ Starting date: January 2003, finished March 2011

# SDS Projects in Progress

- 10 projects still ongoing
  - ◆ Project number: 1999-050-1-500
  - ◆ Project number: 2002-031-1-500
  - ◆ Project number: 2002-032-1-500
  - ◆ Project number: 2002-035-1-500
  - ◆ Project number: 2002-044-1-500
  - ◆ Project number: 2005-014-1-500 (IUPAC Stability Constants database)
  - ◆ Project number: 2006-034-1-500
  - ◆ Project number: 2007-045-1-500
  - ◆ Project number: 2007-047-1-500
  - ◆ Project number: 2008-025-1-500

# New SDS and other Projects

- Project number: 2010-047-1-500
  - ◆ Project Title: Mutual solubility of phenols with water. Solubility Data Series.
  - ◆ Task Group lider: *Marian Goral*
  - ◆ Task group members: A. Maczynski, M. Salomon, D.G. Shaw, and B. Wisniewska-Gocłowska.
- Project number: 2010-050-1-500
  - ◆ Project Title: Mutual solubility of aliphatic and non aliphatic amines with water. Solubility Data Series.
  - ◆ Task Group lider: *Marian Goral*
  - ◆ Task group members: A. Maczynski, M. Salomon, D.G. Shaw, and B. Wisniewska-Gocłowska.

- Project number: 2010-005-2-500
  - ◆ Project Title: Rare Earth Metal (Sc, Y, Lanthanoids) Bromides and Iodides in Water and Aqueous Systems. Solubility Data Series.
  - ◆ Task Group lider: *Cezary Guminski*
  - ◆ Task group members: H. Voigt and Dewen Zeng.
- Project number: 2011-007-1-500
  - ◆ Project Title: Solubility of potassium sulphate in water. Solubility Data Series.
  - ◆ Task Group lider: *Jitka Eysseltová*
  - ◆ Task group members: R. Bouaziz.
- James Sangster
  - ◆ Proposed an ongoing project to maintain the database of octanol/water partition coefficient that he has developed.
  - ◆ Website for access to the database:
    - ◆ <http://logkow.cisti.nrc.ca/logkow/>.

# International Symposium on Solubility Phenomena and Related Equilibrium Processes

- 15th ISSP
  - ◆ Local: Qinghai Institute of Salt Lakes, Xining, China
  - ◆ Date: July/August 2012
  - ◆ Organizer: Dewen Zeng
  
- 16th ISSP
  - ◆ To be proposed in the 10<sup>th</sup> SSED meeting, on the 2<sup>nd</sup> September, held together with the 32<sup>nd</sup> International Conference on Solution Chemistry, in La Grande-Motte, France

## E-i-C Report 2010 – July 2011 (Mark Salomon)

The following is a summary of publications and manuscripts in course of publication which Allan Harvey and I have been working on.

- Editorial: IUPAC-NIST Solubility Data Series (see Appendix)

Allan H. Harvey and Mark Salomon

J. Phys. Chem. Ref. Data, 39, 20401-1 (2010)

- The IUPAC-NIST Solubility Data Series: A Guide to Preparation and Use of Compilations and Evaluations

Heinz Gamsjäger, John W. Lorimer, Mark Salomon, David G. Shaw, and Reginald P. T.

Tomkins, J. Phys. Chem. Ref. Data, 39, 23101-1 (2010)

- **IUPAC-NIST Solubility Data Series. 89. Alkali Metals Nitrates Part 1. Lithium Nitrates**  
**J. Phys. Chem. Ref. Data, Vol. 39, No. 3, 2010**

Jitka Eysseltova, Editor, Evaluator<sup>a)</sup>

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Violetta Timofeevna Orlova, Compiler

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This paper is the first part in the nitrate solubility series. The solubility data for lithium nitrate are reviewed. Where appropriate, binary, ternary, and multicomponent systems are critically evaluated. Most of the solubility results were obtained in water or aqueous solutions. The solubility in ethanol alcohol and alcohol + water solvent mixtures is also included in this volume. All data were critically examined for their reliability. The best values were selected on the basis of critical evaluations and presented in tabular form. Fitting equations and graphical plots are also provided. The quantities, units, and symbols used in this volume are in accord with IUPAC recommendations. The original data have been always reported and, if necessary, transferred into the IUPAC recommended units and symbols. The literature on the solubility data was researched through 2006. Lithium salts are important in the physical chemistry of electrolytes because of the strong hydration of the cation as well as in biochemical and pharmacological applications. In other areas, mixtures of lithium nitrate with other lithium salts have been investigated in connection with absorption heat pump systems in the areas of refrigeration and air conditioning.

- IUPAC-NIST Solubility Data Series. 90. Hydroxybenzoic Acid Derivatives in Binary, Ternary, and Multicomponent Systems. Part I. Hydroxybenzoic Acids, Hydroxybenzoates, and Hydroxybenzoic Acid Salts in Water and Aqueous Systems

J. Phys. Chem. Ref. Data 40, 013101 (2011); doi:10.1063/1.3525876 (130 pages)

Ayako Goto, Editor<sup>1</sup>, Hiroshi Miyamoto, Editor<sup>2</sup>, Mark Salomon, Editor<sup>3</sup>, Rensuke Goto,

Evaluator<sup>1</sup>, Hiroshi Fukuda, Evaluator<sup>4</sup>, Erich Königsberger, Compiler<sup>5</sup>, and Lan-Chi

Königsberger, Compiler<sup>5</sup>

Abstract. The solubility data for well-defined binary, ternary, and multicomponent systems of solid-liquid type are reviewed. One component, which is 2-, 3-, and 4-hydroxybenzoic acids, 4-hydroxybenzoate alkyl esters (parabens), or hydroxybenzoic acid salts, is in the solid state at



room temperature and another component is liquid water, meaning that all of the systems are aqueous solutions. The ternary or multicomponent systems include organic substances of various classes (hydrocarbons of several structural types, halogenated hydrocarbons, alcohols, acids, ethers, esters, amides, and surfactants) or inorganic substances. Systems reported in the primary literature from 1898 through 2000 are compiled. For seven systems, sufficient binary data for hydroxybenzoic acids or parabens in water are available to allow critical evaluation. Almost all data are expressed as mass and mole fractions as well as the originally reported units, while some data are expressed as molar concentration.

- IUPAC-NIST Solubility Data Series. 90. Hydroxybenzoic Acid Derivatives in Binary and Ternary Systems. Part II. Hydroxybenzoic Acids, Hydroxybenzoates, and Hydroxybenzoic Acid Salts in Nonaqueous Systems

J. Phys. Chem. Ref. Data 40, 023102 (2011); doi:10.1063/1.3569816 (116 pages)

Ayako Goto<sup>1</sup>, Hiroshi Miyamoto<sup>2</sup>, Mark Salomon<sup>3</sup>, Rensuke Goto<sup>1</sup>, Hiroshi Fukuda<sup>4</sup>, Erich Königsberger<sup>5</sup>, Lan-Chi Königsberger<sup>5</sup>, and Pirketta Scharlin<sup>6</sup>

Abstract. The solid-liquid solubility data for well defined nonaqueous binary and ternary systems are reviewed. One component includes hydroxybenzoic acid, hydroxybenzoate, and hydroxybenzoic acid salt, and another component includes a variety of organic compounds (hydrocarbons, alcohols, halogenated hydrocarbons, carboxylic acids, esters, et al.) and carbon dioxide. The ternary systems include mixtures of organic substances of various classes and carbon dioxide. The total number of compilation sheets is 270 for six types of system. Almost all data are expressed as mass percent and mole fraction as well as the originally reported units, while some data are expressed as molar concentration. Critical evaluation was carried out for the binary nonaqueous systems of 2-, 3-, and 4-hydroxybenzoic acids and hydroxybenzoates (methylparaben, ethylparaben, propylparaben, and butylparaben) in alcohols, 1-heptane, and benzene.

- A complete guide to the preparation and use of compilations and evaluations for the *IUPAC-NIST Solubility Data Series* were jointly published by IUPAC and NIST.

H. Gamsjäger, J.W. Lorimer, M. Salomon, D.G. Shaw and R.P.T. Tomkins in Pure Appl. Chem., **82(5)**, 1137 (2010)

And published simultaneously in

J. Phys. Chem. Ref. Data, **39(2)**, 023101 (2010)

### Volumes In Press

- Phenols with Water, Part 1. C<sub>6</sub> and C<sub>7</sub> Phenol and Methylphenols with Water and Heavy water. Volume 91.

Volume Editors: Marian Góral and David G. Shaw. The manuscript is in press.

Abstract. The mutual solubilities and related liquid-liquid equilibria of nine binary systems of C<sub>6</sub> and C<sub>7</sub> phenols with water are exhaustively and critically reviewed. Reports of experimental determination of solubility that appeared in the primary literature prior to the end 2009 are compiled. For four systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units.

- Phenols with Water, Part 2. C<sub>8</sub> to C<sub>15</sub> Alkane Phenols with Water. Volume 91.

Volume Editors: Marian Góral and David G. Shaw. The manuscript is in press.

Abstract. The mutual solubilities and related liquid-liquid equilibria of forty three binary systems of C<sub>7</sub> to C<sub>15</sub> phenols with water are exhaustively and critically reviewed. Reports of experimental determination of solubility that appeared in the primary literature prior to the end 2009 are compiled. For eleven systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. The standard evaluation criteria used throughout the Solubility Data Series were applied.

### Volumes In Progress

- Oxygen and Ozone Update. Latest communication from Larry Clever indicates that his update on oxygen and ozone is essentially complete. The manuscript needs extensive editing, and a co-editor with experience in formatting manuscripts for submission to Allan Harvey is needed.

- Solubility of the Higher Acetylenes and other Acetylenic Compounds. Peter Fogg is preparing this update on acetylenes. A Project Proposal Form has not yet been submitted to IUPAC. I anticipate that the manuscript will require extensive editing, and a co-editor with experience in formatting manuscripts for submission to Allan Harvey is needed.

- Potassium Sulfate

Jitka Eysseltová, Editor, Evaluator<sup>a)</sup>

*Department of Inorganic Chemistry, Charles University, Faculty of Science, Albertov 2030, 12840 Prague, Czech Republic*

Roger Bouaziz, Compiler

*Laboratory of Inorganic and Structural Chemistry, Faculty of Sciences, Rouen University Haute Normandie 76130 France*

Draft manuscript received and reviewer comments forwarded to Jitka.

- Mutual Solubility of aliphatic and non aliphatic amines with Water. Marian Góral, Editor. A Project Proposal Form has been submitted.

- Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates (Project number: 2002-031-1-500)

A. De Visscher, E. Königsberger, H. Gamsjäger, J.W. Lorimer

No information available.

### Proposed New Volumes

- Allan Harvey, editor of JPCRD, has put forward a proposal to publish out of print SDS volumes. The proposal is to scan these volumes and using OCR technology republish in JPCRD. Permission from the copyright holder (IUPAC) is required, and this is being pursued by the SSED Chair. An outline by Allan Harvey is presented below.

“We request that, as the copyright holder to Volumes 1-65 of the IUPAC Solubility Data Series, IUPAC grant NIST permission to place scanned and OCR'd copies of this material, organized

appropriately for web access, on one or more public websites maintained by NIST. Acknowledgment of IUPAC as the source would be made.

We will certainly provide a way for any Errata provided by the SSED to any of these volumes to be made available at the same web location as the original volume. We will need to explore one or two different ways of doing that. If there is an existing list of Errata for any volume, please send it to me and we will work on incorporating it.”

- Marian Góral has proposed a new volume on multicomponent systems containing water, hydrocarbons and alcohols updating the early volume on water + hydrocarbon + alcohol as well as extension of this work with systems water + two alcohols and water + two hydrocarbons.

## Appendices

### Editorial: IUPAC-NIST Solubility Data Series

J. Phys. Chem. Ref. Data, 39, 20401-1 (2010)

#### Allan H. Harvey

*Co-Editor, Journal of Physical and Chemical Reference Data, Thermophysical Properties Division, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305-3337, USA*

#### Mark Salomon

*Editor-in-Chief, IUPAC-NIST Solubility Data Series, 2 Eastborne Drive, Little Silver, New Jersey 07739, USA*

This issue of *Journal of Physical and Chemical Reference Data* (JPCRD) contains not only a guide to preparation and interpretation of articles in the IUPAC-NIST Solubility Data Series (SDS; see the article by Gamsjäger *et al.*), but also the latest contribution to the SDS (see the article on solubility of esters in water by Góral *et al.*). It is therefore an opportune time to reflect on the history and value of the SDS.

Solubility data have been published for over 100 years. Because solubility is important in many different disciplines, these data have been reported in a wide variety of journals and other publications, with widely varying units and nomenclature. This has resulted in the unfortunate situation that workers in one field often may not be aware that the data they need have been published in a journal devoted to a different field, and sometimes in the even more unfortunate situation where erroneous information is used because of misunderstandings concerning the sometimes obtuse units in which solubility may be reported.

The IUPAC Solubility Data Series was the brainchild of the late Prof. A. S. Kertes, who envisioned a venue for collecting and publishing all available solubility data on important systems, with data converted to a common set of units and the data sources documented as to methods, purity of chemicals used, and uncertainties to the extent possible. Critical evaluations are also produced when there are enough

independent data sources to justify such evaluation. The efforts to produce these compilations were carried out by the Commission on Solubility Data of the International Union of Pure and Applied Chemistry (IUPAC), which has since become the Subcommittee on Solubility and Equilibrium Data of the IUPAC Analytical Chemistry Division.

The first volume in the SDS, on the solubility of helium and neon in liquids, was published as a monograph in 1979. Publication of these compilations as monographs by commercial publishers, with camera-ready copy supplied by IUPAC, continued through Volume 65 in 1996. In the 1990s, IUPAC became interested in publishing these data in a journal, both to improve accessibility and to allow the flexibility to produce volumes in multiple parts. This coincided with the interests of NIST's Office of Standard Reference Data (now subsumed in NIST's Measurement Services Division), whose mission was to support the dissemination of critically evaluated data of importance to science and industry. As a result, it was decided that these compilations would henceforth be published in JPCRD, and renamed the IUPAC-NIST Solubility Data Series. Volume 66, the first published in JPCRD, appeared in 1998, and publication has continued at the rate of approximately two volumes per year.

The IUPAC Subcommittee continues to support projects on collection and evaluation of data on solubilities for a variety of systems. Upcoming volumes include one on alkali metal nitrates, one on oxygen and ozone (an update of a previous volume), and one on hydroxybenzoic acid derivatives. Compounds of interest for human health and environmental concerns are of particular interest for future volumes. Additional participation in these efforts is welcomed; interested parties should contact either Mark Salomon or the Chair of the IUPAC Subcommittee on Solubility and Equilibrium Data (currently Prof. Maria Clara F. Magalhães, mclara@ua.pt).

This partnership between IUPAC and NIST has been fruitful, and both partners look forward to continued success of these efforts to provide science and industry with reliable information about

### **Some notes on the General Structure of Volumes.**

General JPCRD requirements for submission of volumes are the is the following  
**all in one single file and in the following order.**

1. Title Page with volume title, authors and abstract and key words
2. Table of Contents (includes a list of tables only for the critical evaluations and a list of figures).

3. Preface. Note that references in the preface are numbered accordingly but full references are not entered in the preface. The full reference is given in the Cumulative References section at the end of the manuscript. Note that all equation numbers are sequential throughout the volume.

~~Note: Introduction to the solubility of solids in liquids—this introduction is no longer being used.~~

4. Logical entry of data starting with Binary Systems starting with the critical evaluation followed by compilations (each compilation on a separate page). . Please note that references are not given at the end of each critical evaluation, just the reference number continuing, in order, from reference numbers which were given in the Preface. These full references are given in the Cumulative References section at the end of the manuscript in the order as they appear in the Preface and the following evaluations and compilations

5. Logical entry of data for multicomponent systems (see 4 above).

8. Cumulative References

9. Figures are submitted separately as high definition jpg or tiff files.

Check to make sure that all equations are entered using the Equation Editor macro found in Microsoft Word and data tables are prepared using the “Insert Table” macro in Word with all data inserted in appropriate rows and columns. Also check that symbols are in italics (e.g. molality is  $m$  and mass fraction is  $w$  or in percent, it is  $100w$ ), and subscripts and superscripts are in Roman. Units (e.g. kg) are always in Roman. For example:  $m_1/\text{mol kg}^{-1}$  and  $100w_1$ .