# Minutes

**INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY**

**SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA**

**39th Annual Meeting (12th of SSED)**

to be held in conjunction
with the IUPAC General Assembly,
Istanbul, Turkey
11th August 2013

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**Sunday, August 11, 2013**

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**Morning Session 9:00 - 12:30**

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1. **Introduction of participants and welcome to the new members**

   A list of participants is appended to these minutes.

   **C. Magalhães**

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2. **Approval of Minutes of the 38th Annual Meeting (11th of SSED) in conjunction with the 15th ISSP, Xining, China**

   The minutes were accepted without changes.

   **Earle Waghorne**

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3. **Information**

   Clara Magalhães explained that the approval of projects had been difficult and, in response, she had “frozen” several project proposals. These had been submitted and accepted at the Istanbul meeting.

   Clara Magalhães outlined the history of the SSED, explaining that it had developed from the merging of the Solubility and Equilibrium Data Commissions, both within the Analytical Division. She introduced a discussion about expanding the formal links of the SSED within IUPAC and this initiative was discussed and supported.

   **C. Magalhães**

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**On the actions taken after the last meeting**

- **On glossary of medical terms**

  The Medicinal Chemistry Division recently asked for input from the SSED on solubility related terms that appear in their glossary of terms. Clara Magalhães explained that she had asked the authors of the "Glossary of..."
terms related to solubility (IUPAC Recommendations 2008)” for help on this matter. The Medical Chemistry has some specific terms that SSED should analyze.

• From the draft of the minutes of the 93rd Bureau meeting
  o New strategic plan
    Clara Magalhães reported that the Vice-President of UPAC had established a task group to develop a new IUPAC strategic plan. There will be consultation and the intention is implementation after the 2015 GA.
  o Projects - revision of old unfinished projects
    Clara Magalhães discussed the situation regarding unfinished projects. The unfinished projects without any progress in the last years must be given as closed. This is described in the chairman’s report (appended).
  o Ideas to draft guidelines for the publication of books
  o Digital IUPAC - futuristic area
• From the Analytical Chemistry Division meeting
  o Project publication should be in Pure and Applied Chemistry unless good reason. Meetings with David Martinsen and René Deplanque were booked and occurred during the IUPAC General Assembly.
  o The secretary of the Analytical Chemistry Division (ACD) want to get information from NIST on the solubility papers data access statistics.

4. Questions seeking input for creation of the **new strategic plan**
   • Is IUPAC infrastructure adequate?
   • Can we evaluate our goals to determine in which direction to go?
   • Are we addressing diversity?
   • How can we use the National Subscriptions, publications, investments and fundraising to keep IUPAC on a strong financial base?

It was agreed that these topics would be discussed at the SSED meeting in 2014 in Karlsruhe.

5. **IUPAC publications**
   • Chemistry International
• PAC
• JPCRD – IUPAC-NIST agreement
• Books

SSED members must make an effort to write small papers to be published in Chemistry International, about their IUPAC project. SSED members should think about new book proposal. David Fellhauer made a presentation before the CPEP members about a possible new book. Other publications were analyzed in the Chair's report (copy appended).

6. Projects:

6.1 Revision of the current projects and termination of those that are not expected to be completed. The following decisions were taken in the ACD meeting

2002-009-2-500 Gauglitz (terminate)
2002-044-1-500 Scharlin (extended 2015) Alex de Vischer
2006-034-1-500 Clever and Battino (extended 2015)
2007-045-1-500 Fogg (extended)
2007-047-1-500 Sazonov (terminate)
2008-025-1-500 Filella (extended)
2010-050-1-500 Goral (extended)
2011-031-1-500 Voigt (extended)
2011-043-1-500 Chair changed from Goral to David Shaw (extended)
2012-006-1-500 Lorimer (extended)
2012-025-1-500 Acree
2011-065-3-500 Bendová extend

6.2 New rules for project presentation

Dated from February 2013 there is a new project submission form, as well as some changes in the process of submission. The projects' submission forms must be sent to IUPAC by the chair of SSED, after consultation of the chairs of the respective subsubcommittees

6.3 Analysis of the present projects

This is presented in the Chairman's report (Appended).
### 6.4 New projects

<table>
<thead>
<tr>
<th>Project #</th>
<th>Task group Chair</th>
<th>Submitted</th>
<th>Budget request</th>
<th>comments</th>
<th>Awarded</th>
</tr>
</thead>
<tbody>
<tr>
<td>2013-034-1</td>
<td>Mutual solubility of Rare Earth Metals (Sc, Y, Lanthanoids) bromides in molten alkaline bromides</td>
<td>Marcelle Gaune-Escard</td>
<td>11/07/2013</td>
<td>$5,000</td>
<td>SSED $4,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Also sent to Div. 2</td>
<td></td>
</tr>
<tr>
<td>2012-030-1</td>
<td>Rare Earth Metals (Sc, Y, Lanthanoids) fluorides in water and aqueous systems - IUPAC NIST Solubility Data Series</td>
<td>Guminski</td>
<td>03/02/2012</td>
<td>$2,000</td>
<td>SSED $2,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Awaiting Division Assessment</td>
<td></td>
</tr>
<tr>
<td>2012-022-1</td>
<td>Solubility in systems with lithium and/or sodium nitrates. Part 2. Sodium nitrates</td>
<td>Eyssel-tova</td>
<td>25/04/2012</td>
<td>$2,000</td>
<td>SSED $2,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Awaiting Division Assessment</td>
<td></td>
</tr>
</tbody>
</table>

### 6.5 Databases

There was a brief discussion prior to the meeting with the CPEP.

### 7. Division Financial matters

The task group chairs should spend the project budget before declare it finished. IUPAC bodies will collected the not spent budgets of the projects declared finished.

### 8. Chairman's Report from 2012 – 2013

SSED visibility - Chemistry International and JPCRD articles

The Chairman's report is appended.

### 9. Subsubcommittee reports

Reports from the Chairs of the solid/liquid subcommittee (Wolfgang Voigt) liquid/liquid subcommittee (David Shaw) gas/liquid subcommittee (Alex de Vischer) and Equilibrium subcommittee (Glenn Hefter) are appended.
10. **Editor-in-Chief’s Report for 2012 - 2013**  
   
   Volumes for next year’s SDS proposals  
   The EiC’s report is appended.  
   Following discussion it was agreed that Volume 100 would be held for publication in 2014 to maintain the rate of production at close to four volumes per year.  
   Clara Magalhães will contact the EiC.  

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

**Meetings with Divisions I and VII presidents and members**  
Members of the SSED (Clara Magalhães, Earle Waghorne, Jim Sangster, Cezary Guminski, Magdelena Bendová and Zdenik Wagner) met with the Division I president and other division I members. Linkages between the SSED and Division I were discussed and it was agreed that project level links and Division I representation on the SSED would be maintained.  

**Meeting on databases**  
Clara Magalhães, Earle Waghorne, Jim Sangster, Magdelena Bendová and Zdenik Wagner met with the CPEP. A representative of the publisher de Gruyter made a brief presentation on the way that they might assist IUPAC in the development of data-bases.  
There was also a discussion of the new procedures for submission of books as IUPAC projects. David Fellauer made a presentation of the proposed book on analytical and thermodynamic chemistry as applied to the nuclear waste industry. It was agreed that this would provide a test case for the new IUPAC procedures.  

**Meeting on the IUPAC-NIST agreement and publication in JPCRD**  

Dr. David Fellhauer made a presentation outlining the plans for the 16th ISSP to be held in Karlsruhe. The proposed dates for the meeting are July 21 – 25, 2014 at the Karlsruhe Institute of Technology (KIT) and the web site will open in September 2013.  

M. Salomon

M. Altmaier
<table>
<thead>
<tr>
<th></th>
<th>Future International Symposia on Solubility Phenomena</th>
<th>C. Magalhães</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Adjournment</td>
<td>C. Magalhães</td>
</tr>
</tbody>
</table>

**Attendees at the Meeting**

**BELAREW, Prof. Christo**  
Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchevstr Bl 11, 1113 Sofiam Bulgaria  
TEL: +359 (2) 979-3925  
TEL: +359 (2) 870-5024  
FAX: +1 (403) 284-4852  
EMAIL: Balarew@svr.igic.bas.bg

**BENDOVA, Prof. Magdalena**  
Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic  
Email: bendova@icpf.cas.cz

**FELLHAUER, Dr. David**  
Email: David.fellhauer@kit.edu

**GUMINSKI, Dr. Cezary**  
Department of Chemistry, University of Warsaw, Pasteura 1, 02093 Warszawa, Poland  
Tel: +48 (22) 8220211, ext. 331  
Fax: +48 (22) 8225996  
Email: cegie@chem.uw.edu.pl

**KURODA, Prof. Yutaka**  
Tokyo University of Agriculture and Technology, Tokyo, Japan  
Email: ykuroda@cc.tuat.ac.jp

**MAGALHÃES, Prof. Clara**  
University of Aveiro, Department of Chemistry, P-3810 Aveiro, Portugal  
Tel: +351 (234) 401518  
Fax: +351 (234) 370084  
Email: mclara@ua.pt

**SANGSTER, Dr. James**  
Sangster Research Laboratories  
P.O. Box 49562  
5122 Côte des Neiges, Montreal, Canada H3T 2A5  
Tel: +1 (514) 340 4711 (ext. 3922)  
Fax: +1 (514) 340 5840  
Email: james.sangster@polymtl.ca

**TEPAVITCHAROVA Dr. Stefka**  
Bulgarian Academy of Sciences  
Email: stepav@svr.igic.bas.bg
WAGHORNE, Prof. Earle W.
UCD School of Chemistry and Chemical Biology, University College Dublin, Belfield, Dublin 4, Ireland
Tel: +353 (87) 989 2930
Email: earle.waghorne@ucd.ie

WAGNER Zdenik
Institute of Chemical Process Fundamentals, of the Academy of Science, Czec Republic
Email: wagner@icpf.cas.cz
Subcommittee on Solubility and Equilibrium Data

Chair’s Activity Report from February 2012 to July 2013
Visibility of SSED within IUPAC 2012/2013

• CI, 34, No. 1, January – February 2012
  ♦ Where 2B & Y
  • Pg. 37: Solubility and Equilibria, 23-27 July 2012, Xining, China.
  ♦ Mark Your Calendar
    ♣ Pg. 39: 22-27 July 2012, 15th ISSP, Xining, China

• CI, 34, No. 2, March – April 2012.
  ♦ Mark Your Calendar
    ♣ Pg. 32: 22-27 July 2012, 15th ISSP, Xining, China

• CI, 34, No. 3, May – June 2012.
  ♦ Mark Your Calendar
    ♣ Pg. 34: 22-27 July 2012, 15th ISSP, Xining, China
Visibility of SSED within IUPAC 2012/2013 (continued)

- **CI, 34, No. 4, July – August 2012**
  - ♦ *Mark Your Calendar*
  - ♣ Pg. 40: 22-27 July 2012, 15th ISSP, Xining, China

- **CI, 34, No. 5, September – October 2012.**
  - ♦ *IUPAC Wire*
  - ♣ Pg. 15: In Memoriam Prof. H. Lawrence Clever

- **CI, 34, No. 6, November – December 2012.**
  - ♦ *Making an impact*
  - ♣ Pg. 25: IUPAC-NIST Solubility Data Series – Recent Volumes

- **CI, 35, No. 3, May – June 2013.**
  - ♦ *Conference Call*
  - ♣ Pg. 32-33: Solubility Phenomena by Dewen Zeng
Completed SDS Volumes
IUPAC-NIST Solubility Data Series

• **Volume 93**: Jitka Eysseltová, Roger Bouaziz.

• **Volume 94**: Tomasz Mioduski, Cezary Gumiński, Dewen Zeng. “Rare Earth Metal Iodides and Bromides in Water and Aqueous Systems.”

• **Volume 95**: “Alkaline Earth Carbonates in Aqueous Systems,
Completed SDS Volumes
IUPAC-NIST Solubility Data Series

- **Volume 96**: M. Góral, D. G. Shaw, A. Maczynski, B. Wisniewska-Gocłowska and P. Oracz, “Amines with Water”


- **Volume 98**: W. E. Acree, “Solubility of Polycyclic Aromatic Hydrocarbons in Pure and Organic Solvent Mixtures: Revised and Updated”
## Projects already finished

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012-025-1-500</td>
<td>Polycyclic Aromatic Hydrocarbons in Pure and Binary Solvent Mixtures (Update of Volumes 54, 58 and 59)</td>
</tr>
<tr>
<td>2011-017-1-500</td>
<td>Solubility of Potassium Sulfate in Water</td>
</tr>
<tr>
<td>2010-050-1-500</td>
<td>Mutual Solubility of aliphatic and non aliphatic amines with Water</td>
</tr>
<tr>
<td>2010-047-1-500</td>
<td>Mutual Solubility of Phenols with Water</td>
</tr>
<tr>
<td>2010-005-2-500</td>
<td>Rare Earth Metal (Sc, Y, Lanthanoids) Bromides and Iodides in Water and Aqueous Systems</td>
</tr>
<tr>
<td>2007-045-1-500</td>
<td>Solubility data related to industrial processes. Solubility of higher alkynes in liquids</td>
</tr>
<tr>
<td>2007-039-1-500</td>
<td>Extension of ThermoML - the IUPAC standard for thermodynamic data communications</td>
</tr>
<tr>
<td>2005-033-1-500</td>
<td>Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates</td>
</tr>
</tbody>
</table>
Projects in progress

- Projects number: 1999-010-1-500 and 2012-008-1-500
- Project number: 2002-031-1-500
- Projects number: 2002-032-1-500 and 2012-004-1-500
- Project number: 2002-035-1-500
- Project number: 2002-044-1-500
- Project number: 2005-006-1-500
- Project number: 2006-034-1-500
- Project number: 2008-025-1-500
- Project number: 2011-031-1-500
- Project number: 2011-065-1-500
- Project number: 2012-006-1-500
- Project number: 2012-031-1-500
- Project number: 2013-018-1-500
Projects for publication


2002-031-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates. Part 3

2013-018-1-500: Solubility of benzoic acid and substituted benzoic acids in both neat organic solvents and organic solvent mixtures
Meetings and conferences

**SSED meeting** - The 38th solubility committee annual meeting (11th of SSED) occurred in Xining, China on the 21st July 2012 in conjunction with the 15th ISSP

**15th ISSP** - The 15th International Symposium on Solubility Phenomena and Related Equilibrium Processes occurred in Xining, China, at the Qinghai Institute of Salt Lakes from the 22nd to the 27th July 2012.
Next meetings and conferences

**SSED meeting** - The 39th solubility subcommittee annual meeting (12th of SSED) will occur in Istanbul, Turkey on the 11st August 2012 in conjunction with the IUPAC General Assembly.

**16th ISSP** - The 16th International Symposium on Solubility Phenomena and Related Equilibrium Processes will occur in Karlsruhe, Germany, from the 21st to the 25th July 2014.

**SSED meeting** - The 40th solubility subcommittee annual meeting (13th of SSED) will occur in Karlsruhe, Germany, on the 20th July 2014 in conjunction with the 16th ISSP.
Projects publications (1)

- 1999-050-1-500 – Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands – published Hg$^{2+}$, Cu$^{2+}$, Pb$^{2+}$, Cd$^{2+}$, and Zn$^{2+}$ (to be published in PAC in 2013)

- 2002-031-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates – published: JPCRD IUPAC-NIST SDS Vol 95 - Part 1 – 41(1) 2012 (67 pages); Part 2 - 41(2) 2012 (137 pages); Part 3 – to be published in 2013

- 2002-032-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb) – published Cd$^{2+}$ in JPCRD

2010-005-2-500 – Rare Earth Metal (Sc, Y, Lanthanoids) Bromides and Iodides in water and aqueous systems – published: JPCRD IUPAC-NIST SDS Vol 94 - Part 1 – 41(1) 2012 (63 pages); and Part 2 – 42(1) 2013 (35 pages)

Projects publications(3)


Editor-in-Chief Report for 2012-2013

To date, the Subcommittee on Solubility and Equilibrium Data (SSED) has published 99 volumes in the *Solubility Data Series*. Volumes 66 to 99 were published in the *Journal of Physical and Chemical Reference Data* (JPCRD) under the title of the *IUPAC-NIST Solubility Data Series*. From 2012 to 2013, seven new volumes were published either as a single manuscript or in parts making a total of 12 articles published in JPCRD during this period. Citations to these 12 publications are presented in the table below.

<table>
<thead>
<tr>
<th>Volume</th>
<th>Authors, titles and references to recent publications in J. Phys. Chem. Reference Data</th>
</tr>
</thead>
</table>

Volumes 100 and 101 are presently scheduled for publication either late this year or mid 2014. The status of Volume 102, *Hydrocarbon-Alcohol-Water Systems*, is not yet resolved as discussed by David Shaw in his Activity Report of the Liquid-Liquid Group.

**Volume 100.** Larry Clever and Rubin Battino with contributions from Alex De Visscher, *Oxygen Update*. This volume is in an advanced state of final editing and may be published late 2013.

**Volume 101.** Bill Acree, *Solubility of Non-steroidal Anti-inflammatory Drugs in Both Neat Organic Solvents and Organic Solvent Mixtures*. While a draft volume in under preparation, the Project Proposal Form has only recently been submitted to IUPAC.
completed project

2010-50-1-500  amines with water, published in three parts in jpcrd in 2012.

current project

2011-43-1-500  hydrocarbon-alcohol-water systems  part 1 is in draft form and has been reviewed internally. revisions are currently in progress.

2012-31-1-500  web-site modernization project

this project was funded in february 2013 and is underway. the task group has communicated by email and skype conference call. at present work is delayed because the secretariat is unable to implement changes in the ssed web pages while migrating the iupac website to a new server. i ask you to enquire during the general assembly when we can expect support from the secretariat.
Volumes published since August 2012

From list of EIC, Mark Salomon:

<table>
<thead>
<tr>
<th>Volume</th>
<th>Reference</th>
</tr>
</thead>
</table>

For the compounds in the volumes of Acree it is not always clear whether the compounds are liquids or solids (mostly solids).

In addition, for this type of compounds the typical evaluation procedure was not applicable, since only one or two sets of independent measurements were published. Acree applied a correlation model and reported the deviations from it. Again, I would like to stress that in my opinion, such correlations can help to identify outliers, but not give an explanation for the deviation. There could be a less accurate measurement, but also the only correct measurement, in a structural situation, where the correlation fails. Thus, I ask the question, which line we will follow in future: will we set in our expertise to evaluate the measurements from the descriptions in the papers, the knowledge of the groups, which had been working or are working on solubilities or shall we trust only on statistics (in case of several experiments) or (more or less accepted) correlations. This issue is not limited to the organic compounds, we have these problems also for carbonates with application of Pitzer’s equations as a mean to perform a thermodynamic analysis. After all the years I tend to more point out the papers with accurate experimental deteminations and in addition to consider correlations, but to make clear for the reader, that the latter is not the deciding criterion for the data quality.
On-going projects

2011-031-1-500 / 22 March 2012
Solubility of lithium sulfate in aqueous solutions: W. Voigt, J. Schmitt, D. Zeng
⇒ Project is in an advanced state, Compilation is ready and already prepared in the required format, evaluation is still under way, should have been ready in July this year, but will take until the end of the year.

2012-004-1-500 / 22 March 2012
Solubility of lead carbonates: H. Gamsjäger, C. Maghães,
???

25 April 2012 / 2012-022-1 / submitted
Solubility in systems with lithium and/or sodium nitrates. Part 2. Sodium nitrates:
J. Eysseltova
⇒ from communications with J.E. it was pointed out that it will become an extensive part, exact state of preparation unknown, because J.E. could not be present at the meeting
No new information since last year.

03 July 2012 / 2012-030-1 / submitted 03 July 2012
The solubility of rare earth metal (Sc, Y, Lanthanoides) fluorides in water and aqueous systems:
⇒ first results of evaluation were presented at the 15th ISSP in Xining

2011-058-1 / suspended due to health problems of the task chair

Solubility of rare earth metal (Sc, Y, Lanthanoides) bromides in alkali metals bromides: M. Gaune-Escard

The Solubility of Beryllium Sulfate and Other Beryllium Compounds in Aqueous and Non-aqueous Media
John Lorimer

New projects

Recommended by Mark, Project form filed
IUPAC-NIST Solubility Data Series. XX. Solubility of Non-steroidal Anti-inflammatory Drugs (NSAIDs) in Both Neat Organic Solvents and Organic Solvent Mixtures
William E. Acree, E. Königsberger
Marcelle Gaune-Escard

**Mutual Solubility of Rare Earth Metal (Sc, Y, Lanthanides) Bromides in Molten Alkali Bromides.**

It seems it is the same proposal as in 2012. In my opinion it is not solubility, but solid-liquid phase diagram investigations, which is not quite the same as a typical (isothermal) solubility investigation. The volumes of Cesary were maybe most similar to this proposal, but it contained also isothermal equilibrium experiments, which I not expect from the work proposed here.

Wolfgang Voigt

Solid-liquid solubility chair
The National Institute of Standards and Technology (NIST, an agency within the U.S Department of Commerce) requests from the International Union of Pure and Applied Chemistry (IUPAC) a non-exclusive release of copyright for Volume 1 to Volume 65 of the Solubility Data Series originally published by Pergamon Press and Oxford University Press and for which IUPAC is the copyright holder for the purpose of electronic re-publication. NIST intends to make these volumes available for public download at no cost at an unrestricted website.
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.

In return, NIST will supply a copy of the scanned and OCR’s material to IUPAC that it can use on its own website. Acknowledgment will be given to NIST for digitizing the materials.