# Draft Minutes

## INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

### SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

**43rd Annual Meeting (16th of SSED)**

held in conjunction
with the 21st ECTP-2017
Graz, Austria
2nd September 2017

Prepared By: Earle Waghorne, SSED Secretary
Clara Magalhães, SSED Chair

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
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| 1. | Introduction of participants and welcome to the new members  
The list of participants is appended to these minutes |
| 2. | In memorium George Nancollas  
Clara Magalhães gave a brief history of Professor Nancollas's contribution to the establishment of the IUPAC Solubility Data Commission. The meeting observed a minute’s silence.  
In memorium Heinz Gamsjäger  
Earnst Gamsjäger presented a short history of his father’s career including involvement in IUPAC and the SSED. The meeting observed a minute’s silence. (Copy attached) |
| 3. | Approval of Minutes of the 42nd Annual Meeting (15th of SSED) in conjunction with the 17th ISSP, Geneva, Switzerland Czech Republic  
The minutes had been circulated previously and were accepted. |
| 4. | Information  
Clara Magalhães presented a list of meetings taking place in  
Earle Waghorne, Clara Magalhães  
Contact project group |
conjunction with the ECTP, in particular an IUPAC Division 1, project meeting on recommending reference materials for solubility measurements.

This initiative was discussed and it was decided to request that the SSED be allowed to make input to the project.

The need for annual project reports was discussed. It was decided that the secretary would develop a short report form that would be circulated to project leaders; reports were to be sent to sub-committee chairs and would form the basis of the SSED chair's report to Division V.

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<thead>
<tr>
<th>5. Chair’s Report</th>
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<tr>
<td>Clara Magalhães provided a detailed report of the SSED’s activities and publications over the past year. A copy of this report is appended to these minutes.</td>
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</table>

There was a discussion of contributions that the SSED could make to IUPAC’s 100th anniversary celebrations. The possibility of writing a short piece (500 words) on the importance of solubility, written for laymen, was one suggestion.

It was agreed to propose the translation of Clara Magalhães's book on solubility for young school children should be proposed as an IUPAC project.

<table>
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<tr>
<th>6. SSED Website</th>
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<tr>
<td>David Shaw outlined the history of the development of the website and demonstrated the current, much improved, site. A request was made that SSED members check that they are listed on the website and that their entries in the IUPAC</td>
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</table>

David also asked anyone who had photographs from SSED activities, that were suitable for inclusion on the website, to forward copies to him.

<table>
<thead>
<tr>
<th>Earle Waghorne - prepare form, regarding this proposal</th>
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<tr>
<td>These to include the project numbers. Distribute these to sub-committee chairs and task group leaders</td>
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<table>
<thead>
<tr>
<th>Earle Waghorne</th>
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<tr>
<td>Include a request for SSED members to check their entries with the distribution of the minutes</td>
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<tr>
<td>Also to ask for photos.</td>
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7. Brief outline of the current situation of the IUPAC – Springer negotiations

Earle Waghorne briefly outlined the current state of negotiations with Springer for the use of the SDS volumes in their database. It was noted that IUPAC had ceded their copyright to the publishers of JPCR D and that the insistence of the AIP on very substantial licensing fees for use of material from JPCR D had essentially blocked the Springer project.

It was also explained that IUPAC was open to providing technical support for SSED work, both by trying to provide tools that would assist in the extraction of data from papers and by providing data table templates that were usable both as tables for journal articles and as inputs to data bases.

7.2 Discussion of procedures for publication of future volumes in the SDS.

There was a lengthy discussion of the ways in which the SDS series should be published in the future. The outcomes of this discussion are summarized as:

- The current method of producing large volumes arose from the beginning of the SDS project where books were published and is no longer mandated.
- Modern systems of data handling are computer, rather than paper, based and generally involve data bases.
- The SSED should move to having its work available through data base systems.
- The publication of journal articles, reporting the SDS volumes should be continued in some form, both to ensure rigorous review and to provide contributors with publications and citations.
- The possibility that IUPAC might request SDS volumes be published through PAC.
- It was emphasized that the work of the SSED in compiling and evaluating data was a service to the chemical community and not, fundamentally, a commercial undertaking.
- It was also emphasized that, in the event that IUPAC eventually reaches an agreement to monetize the outputs from the SSED, that some of this income should be directed to support the work of the SSED.

8. Projects – analysis of the running projects (Financial report)

Clara Magalhães presented the current list of proposals
It was decided that the remaining funds for the Wiley Royalties fund should be added to the Franzosini fund.

8.2 Future projects
The possibility of new projects in the area of supercritical fluids, possibly in conjunction with Division 1, was discussed. Participation in the Division 1 initiative relating to reference materials for solubility measurements was discussed

8.3 Formulation of a proposal for future publication of SDS volumes
It was proposed to initiate an interdivisional IUPAC project to look at the future publications and to develop electronic tools to assist in the capture and publication of data (see discussion above also).

8.4 Projects with CODATA and other organizations
It was decided to explore whether there were areas of activity where the SSED could collaborate with CODATA

9.1 Editor-in-Chief's Report.
Mark Salomon (EiC) reported that there are currently no SDS volumes waiting to be published.

9.2 Subcommittee Reports
The Equilibrium subcommittee reported that there were currently four ongoing projects. Solid - Liquid and Gas - Liquid subcommittee chairs reported no now activities

9.3 IUPAC reporting procedures, Division V report

9.4 Data Base on Ionic Liquids
Johan Jacquemin presented a report on the status of the Ionic Liquids data base

Clara Magalhães to discuss at IUPAC meeting at ECTP

Earle Waghorne/Clara Magalhães
Check the current membership of the CODATA committee and approach.

Glenn Heftet, Wolfgang Voigt, David Shaw, Alex de Vissher

David Shaw/Clara Magalhães

Magdalena Bendová/ Johan Jacquemin
| 10. | Report of meeting on critical evaluations and future developments  
David haw presented a summary of the meeting held in Sao Paolo  
(Copy attached) | D. Shaw |
|---|---|---|
| 11. | Franzosini Award  
Clara Magalhães explained that the terms of the Franzosini award might be taken to indicate that the award would cover travel expenses to an ISSP while the amounts available now made this impossible. It was agreed to confirm the wording and, if necessary, to have it amended to indicate that the award would contribute to travel costs.  
Johan Jacquemin reported that three nominations had been received in response to the advertisement on the ISSP-2018 website. | Clara Magalhães |
| 12. | Next SSED meetings and possible conferences to link  
The 2018 SSED meeting will be in Tours in conjunction with the ISSP.  
The 2019 meeting will be in Paris, in conjunction with the IUPAC General Assembly.  
The 2020 meeting will be in Los Alamos in conjunction with the 2020 ISSP. | Earle Waghorne, Clara Magalhães |
| 13. | Contributions of SSED to the celebration of the IUPAC 100 years.  
Essential tools for the next century  
There was a discussion of contributions that the SSED could make to IUPAC's 100th anniversary celebrations. The possibility of writing a short piece (500 words) on the importance of solubility, written for laymen, was one suggestions.  
It was agreed to propose the translation of Clara Magalhães's book on solubility for young school children should be proposed as an IUPAC project. | Clara Magalhães and others  
Prepare proposal to IUPAC |
| 14. | Next ISSP 2018  
Johan Jacquemin described the current state of preparation for the 3028 ISSP. The website is fully functional. Two innovations for the 2018 meeting are the introduction of flash presentations and two discussion sessions modeled on Faraday discussions. Abstracts for the discussion sessions will have a deadline this autumn and a deadline | |
for full papers late in the year.

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<tr>
<th>15.</th>
<th>Any other business</th>
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<tbody>
<tr>
<td></td>
<td>There was no other business.</td>
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<thead>
<tr>
<th>16.</th>
<th>Adjournment</th>
<th>Clara Magalhães</th>
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</table>
List of Participants

**ATANASSOVA, Dr. Maria**  
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In memorium George H. Nancollas

Born in Wales, UK, received a Ph.D. from the University of Wales and a D.Sc. from the University of Glasgow. He published more than 450 scientific documents.

George H. Nancollas was the Chair of Commission V.6 (Equilibrium Data), in 1972, when A. Stevan Kertes proposed that Commission V.6 started a project on collecting and evaluating Solubility data.

This idea was strongly supported by George H. Nancollas that also participated, in 1974, in the called first Solubility Data project meeting. He participated also in ISSP.

In memoriam

Heinz Gamsjäger

Emeritus Professor
Chair of Physical Chemistry,
Montanuniversität Leoben, Austria
IUPAC Satellite meeting Aims

Ala Bazyleva email:
I will be happy to meet with your and other SSED members in Graz!
I am sending you our rough selection of phase equilibria reference systems for LLE, SLE, and VLE. These are just preliminary results of the project, not yet discussed. During our project meeting, we are planning to discuss the selection, possible additional candidates to include or exclude from the list, modeling issues (since we need to provide interpolation capabilities for experimentalists). We will demonstrate our ThermoData Engine software as well as one more piece of software developed by one of the project members (Prof. Kang from Korea).
Your feedback will be highly appreciated.

Books
David Fellhauer
I would like to inform you, that we will meet our SSED colleague Taishi Kobayashi from Kyoto University mid of September 2017 in order to discuss the next steps of the (SSED) book project on "Analytical methods relevant for nuclear waste disposal" which we have proposed recently.

Chemistry International
Chairs of IUPAC projects, particularly at completion, must write brief pieces about them for CI
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GUIDELINES FOR REPORTING OF SOLUBILITY DATA

The following describes requirements necessary for manuscripts reporting solubility data of solid solutes in solvents or solvent mixtures to be published in the Journal of Chemical and Engineering Data JCED. These guidelines are given as a supplement to the general Author Guidelines for JCED (see http://pubs.acs.org/paragonplus/submission/jceaax/jceaax_authguide.pdf).

- Article Title
  - Name of the solute must be given, and the identity of the solvent(s) should be given, if practical. Abbreviations should not be used.
  - Temperature range of solubility measurements should be mentioned, if practical.

- Abstract
  - All of the following must be mentioned.
    - Chemical systems
    - Experimental methods
    - Variable ranges (temperature and pressure)
    - Modeling approaches

- Substance Information
  - Description of chemical substances must conform to the Author Guidelines cited above.
  - Melting temperature and melting enthalpy (with uncertainties), based on new measurements or from the literature, should be reported if possible.

- Experimental Data
  - The experimental method must be fully described and validated.
    - The method must be validated by measurements for, at least, one system for which multiple consistent data are available in the literature. The validation measurement results must be presented in tabular form, and deviation from literature values must be given in numerical or graphical form.
  - For the studied systems, graphical comparison must be provided for all available literature data, as described in the Author Guidelines.
  - Solubility data involving various polymorphs, amorphous solids, hydrates, complexes, etc., require experimental proof of the identity of the solid in equilibrium with the saturated solution (e.g., via x-ray diffraction).
  - The amount of experimental solubility data presented should be substantial.
    - Specifically, the number of solutes times the number solvents should be at least 12. (For example, 3 solutes in 4 solvents, or 2 solutes in 6 solvents.) A binary solvent system with results for at least three different solvent compositions, in addition to the pure solvents, counts as three solvents.
    - The temperature interval for solubility measurements should be at least 40K.
SSED Webpage
https://iupac.org/who-we-are/divisions/division-details/?body_code=502

Updating of personal pages
Please check if your name is included in the SSED members’ roster in the right. If you find your name, click on it and check that your contact information is correct and up to date. If your entry is missing or needs updating, contact

Enid Weatherwax  ewatherwax@iupac.org
New Projects

2016-041-1: Montserrat Filella - Critical evaluation of homogeneous equilibrium and solubility constants of pentavalent technology-critical elements (Nb, Ta, Sb) in environmental and biological-relevant conditions – 1000 US$

2016-042-1: Montserrat Filella - Critical evaluation of homogeneous equilibrium and solubility constants of tellurium in environmental and biological-relevant conditions (14th October) – 2000 US$

2017-022-1: Pawel Oracz - Halogenated Aliphatic Hydrocarbons C₁₋C₁₄ with Water - 2000 US$

2017-025-1: Solubility in Systems with Potassium Nitrate (Part 3 of Volume 89 of the Solubility Data Series) – 3000 US$
Volumes Published Since Last Meeting:

None

Current Projects

2012-31-1-500 Web-site Modernization Project

This project was funded in February 2013 and is essentially complete. In the last year the new IUPAC web site has gone live and numerous updates and expansions of the SSED page have been made. This page should now serve as a source of information for current SSED participants and a recruiting tool to explain the SSED to prospective new participants. Suggestions and ideas for further changes, corrections and updates (ideally with proposed content in good form!) should be sent to Clara Magalhaes or David Shaw.

New Project

Pawel Oracz and Marian Goral have submitted a proposal, “Halogenated Aliphatic Hydrocarbons C_1-C_14 with Water”. A proposal is currently under review.
Interdivisional Discussion of Critical Evaluation

An Open Meeting
IUPAC General Assembly
July 11, 2017

Meeting Report September 2017

Franzosini Award

nomination for the Franzosini Award is already open see

http://issp18.org/topics/call-for-nomination-for-the-franzosini-award
Next SSED meetings

<table>
<thead>
<tr>
<th>Year</th>
<th>Place</th>
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<tbody>
<tr>
<td>2018</td>
<td>ISSP18 - Tours, France</td>
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<tr>
<td>2019</td>
<td>100 IUPAC General Assembly - Paris, France</td>
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<tr>
<td>2020</td>
<td>ISSP19 - Los Alamos, USA</td>
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<tr>
<td>2021</td>
<td>IUPAC General Assembly – Montréal, Canada</td>
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<td>2022</td>
<td>ISSP20 - Bragança, Portugal</td>
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IUPAC 100 years celebration
A Common Language for Chemistry

1. Women celebrating a chemical moment in time – Mary garson
2. IUPAC100 for Africa: postgraduation summer school on green chemistry – Pietro Tundo
3. Creating the common language for chemistry: a visual of how IUPAC made history – Fabienne Meyers
4. IUPAC Periodic table competition: Jan Apotheker, Juris Meija
5. Providing Essential tools for the next century – Laura McConnell
6. IUPAC next centenary: World Chemistry Leadership Meeting (WCLM) at IUPAC’s centenary 2019

Plan your own event or activity   Website: IUPAC100