Minutes

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

38th Annual Meeting (11th of SSED)

held in conjunction
with the 15th ISSP,
Xining, China
21st and 22nd July 2012

	Saturday, July 21, 2012	
	Morning Session 9:00 – 12:30	
1.	Introduction of participants and welcome to the new members A list of participants is appended to these minutes.	C. Magalhães
2.	Approval of Minutes of the 37th Annual Meeting (10th of SSED) in conjunction with the 32nd ICSC, La Grande-Motte, France, These minutes were approved with two minor corrections.	Earle Waghorne
3.	In memoriam Larry Clever Clara Magalhães presented a brief history of Larry Clever's contributions to the IUPAC Solubility Data Commission and the SSED. (Document 1) The members of the SSED observed a minute's silence in memory of Larry Clever. It was agreed that Clara Magalhães would write to Larry's widow, Ruth Clever conveying the symapthy of the members of the SSED. Clara Magalhães read a letter she had received from Rubin Battino (this letter is appended to these minutes). (Document 2) It was agreed that Rubin Battino would write to Chemistry International regarding Larry's contributions. Clara Magalhães was to write to confirm this.	C. Magalhães
4.	Information	C. Magalhães
	On the actions taken after the last meeting	

	ï - "Guidelines for reporting of phase equilibrium measurements" Clara Magalhães reported that she had written to R. D. Chirico, the chair of the project "Guidelines for reporting of phase equilibrium measurements" that was under public analysis until the end of October 2011, expressing the Subcommittee's views on the proposed guidelines (ths letter is appended to these minutes, together with the document written and sent also by Heinz Gamsjäger). (Documents 3 & 4) The SSED noted that some minor changes had been encorporated (*e.g.* the inclusion of peritectics in the example solid/liquid phase diagram); it was also noted that the guidelines were restricted to certain systems, ï Analytical Chemistry Division Terms of reference The Analytical Chemistry Division (ACD) process of electing members is based in a representation of the main branches of Analytical Chemistry that are currently focussed on analytical methods and their applications, described in the Terms of Reference. In order to include new areas of expertise and to broaden the field of action, the revision of the Terms of Reference is under discussion. Suggestions of new fields of expertise are welcomed from all the SSED members, that can send the suggestions directly to the ACD secretary. (Document 5) ï Orange Book Clara Magalhães reported that work on the Orange Book was continuing and that David Shaw was the SSED representative to the project. It is expected that SSED participates at least in the glossary, but also in some particular chapter if somebody is expert in a specific analytical technique. ï The definitions of kilogram and mole The SSED discussed the currrent moves to change the definitions of the kilogram and mole. It was noted that anyone can participate in this discussion. Heinz Gamsjäger wrote the attached comment sent to the ACD vice-president (Brynn Hibbert). (Documents 6 & 7) ï The gas-liquid subsubcommittee Clara Magalhães explained that the current chair of the gas-liquid subcommittee had not been able to carry out this role because of their changed working situation. Alex De Visscher was appointed to the chair of the gas-liquid subcommittee with unanimous support.	

	ï IUPAC/NIST agreement Clara Magalhães explained that Alan Hrvey had been unable to attend this meeting but, hopefully,	
5.	Representatives in and from other IUPAC divisions Clara Magalhães read out a letter from Tony Goodwin explaining that the Division I – Physical and Biophysical Chemistry Division sought representation on the SSED. After discussion the SSED accepted the principle of representatives, from all Divisions of IUPAC, should be welcomed. It was noted that this didn't change the status of the SSED which is within the Analytical Division. The possibility of the presence of SSED representatives in other Divisions and Commissions was also suggested, and the Clara Magalhães must address an email letter about this subject to the Divisions presidents. (Document 8)	
6.	Projects: 6.1 The gas-liquid subsubcommittee Alex De Visscher appointed Chair. 6.2 Analysis of the present projects Clara Magalhães presented an analysis of the current status of SSED projects (a copy is appended to these minutes). (Document 9) 6.3 New projects Clara Magalhães presented a list of new projects (the list is appended to these minutes). (Document 10) David Shaw has undertaken a project to update the SSED web-site. Earle Waghorne was requested to provide updated information; he is to contact David Shaw. It was noted that the 100th volume in the Solubility Data Series will be published in the next year or two. Alan Harvey had suggested an editorial in JPCRD to mark this. Other suggestions to mark this milestone were: an article in PAC giving the history of the Solubiity Data Project, a cumulative index of the existing volumes in the series and a brief note regarding the project to be pubished in the Journal of	C. Magalhães

Solution Chemistry.
It was noted that new projects were being submitted without reference to the SSED although the SSED's terms of reference indicate that it should assume responsibility in the area of solubility and equilibrium data. (Documen 11)
Clara Magalhães also explained that new projects were not being accepted in a timely manner; this is a change from previous years.
It was agreed that Clara Magalhães should discuss this matter with the president of the Analytical Division.

6.4 IUPAC-NIST agreement (old solubility volumes)
Clara Magalhães presented a letter from Alan Harvey outlining the proposal to make out of print volumes available electronically (a copy of this letter is appended to these minutes). (Documents 12 & 13) Clara Magalhães demonstrated some of the features of the web based system being developed.
The SSED agreed that the Clara Magalhães should discuss with IUPAC the possibility of some funding being made available to the SSED (as opposed to funding for specific projects) either from NIST as part of the agreement. The point was strongly made that the operation of the SSED and continuation of the Solubility Data Project regularly requires sall outlays, most often but not exclusively, to support travel; for example, by scientist who are interested in the work of the SSED but have not yet involved in a project.
The SSED expressly gave the Chair (Clara Magalhães) permission to agree to the IUPAC-NIST proposal in the event that no funding was forthcoming from NIST.
It was also agreed that Clara Magalhães should discuss with IUPAC (Fabienne Mayer) the possibility of direct support to SSED from IUPAC.

6.5 Electronic database
Clara Magalhães explained that 2 data bases had been discussed at the Division level and that the Analytical Division analysed the possibility to establish a group to discuss electronic data bases.
It was agreed to propose Jim Sangster as a member of this group.
Glenn Hefter enquired whether Academic Software was still the owner of the rights to the Stability Constant database.
(Document 14)

7.	Division Financial matters	C. Magalhães
	Clara Magalhães explained that the SSED had around €12,000 in an account (NIST account) under the responsibility of Heinz Gamsjäger, that exoplained the history of this account. It was decided that this account should be under the responsibility of the SSED Chairs. It was noted that there should be a clear plan for these funds. The actual financial situation of each project under SSED members responsibility was analysed thoroughly, and the old projects chairs's were advised to spend the respective remaining budget. In relation to the project 2002-044-1-500 whose chair, Pirketta Scharlin retired from IUPAC, and will be continued by Alex de Vissher, the SSED chair will approach Pirketta Scharlin about her substitution in this project by Alex de Vissher.	
8.	Chairman's Report from 2011 – 2012 SSED visibility – Chemistry International and JPCRD articles	C. Magalhães
	The Chair's report is appended to these minutes. (Document 15) Under this point was analyzed the usual advertisement in Chemistry International (CI) of the publication of the SSED projects in the Journal of Physical and Chemical Reference Data, that has failed for the last year projects. It was suggested that the editor in chief should send a note to the CI editor about the SSED publications.	
9.	Franzosini Award	C. Magalhães
	Wolfgang Voigt introduced this year's Franzosini Award winner Julia Schmitt Julia Schmitt and Wolfgang were asked to send informations to the SSED chair to write a report to be published in Chemistry International. It was agreed that an updated document describing the conditions of the Franzosini award should be prepared by Clara Magalhães and Earle Waghorne. It was noted that these should not be unduly restrictive but should provide clear guidance. It was agreed that Clara Magalhães should write to the Franzosini family giving details of the awardees. It was noted that the current financial situation, with very low interest rates, had reduced the amount of funding available for the award (which is supported by the interest on the trust fund held through IUPAC).	
10.	Editor-in-Chief's Report for 2011 – 2012 (Document 16)	M. Salomon

	Volumes for next year's SDS proposals	
	Wolfgang Voigt explained that he had not seen a copy of the K_2SO_4 volume although it was customary for the appropriate subcommittee chair to see each volume. Clara Magalhães agreed to write to Mark Salomon. Clara Magalhães explained Peter Fogg's volume requires reformatting for publication and agreed to write to IUPAC for funding to support this. She noted that the project has been cost-free so far. It was noted that there was a new document relating to the formatting of articles for JPCRD. (Document 17)	
	Afternoon Sessions, (14:00 - 19:00)	
	Subsubcommittees meetings, (14:00 – 16:00)	
	Subsubcommittee: Solid-liquid Solubilities (Document 18)	W. Voigt (Chair)
	Subsubcommittee: Stability Constants (Document 19)	G. Hefter (Chair)
	Plenary meeting afternoon session (16:30 – 19::00)	
11.	Subsubcommittees reports Subcommittee reports are appended to these minutes. In spite of its absence David Shaw sent the liquid-liquid solubilities activity report (Document 20)	G. Hefter; W. Voigt; D. Shaw
12.	Report on the 15th ISSP – Xining, China, 2012	D. Zeng
	Dewen Zeng made a presentation about the upciming ISSP highlighting the strong support of the Institute for the ISSP; which has around 100 participants, with around half coming China.	
13.	Future International Symposia on Solubility Phenomena	C. Magalhães
	One proposal for the next ISSP was received from the Karlsruher Institut für Technologie, Germany. This proposal was wlecome by all the presents. The official presentation will be done at the end of the 15th ISSP meeting by Marcus Altmaier.	
14.	Adjournment	C. Magalhães

Attendees at the Meeting

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Remembering H. Lawrence Clever (1923 – 2012)

Larry, as we use to call him, belongs to the group of founders of the Solubility Data Project. He was a very nice person.
He was present in all important moments of the Commission V.8 (Solubility Data) and now Subcommittee on Solubility and Equilibrium Data.
He had the repository of all the Solubility Data Project history and, fortunately for us, he wrote its history until 2001.
He is the editor of the two first volumes written under the IUPAC Solubility Data Series that appeared already in 1979 when the existence of Commission V.8 was approved by IUPAC bodies.
But he participated in many others – to the moment he participated in 10 volumes.

Volumes where Larry Clever participate:

Published by Pergamon Press, Oxford, UK: Editor-in-Chief A.S. Kertes

Vol. 1	H.L. Clever, *Helium and Neon* (1979), *xxi* + 393 pp
Vol. 2	H.L. Clever, *Krypton, Xenon and Radon* (1979), *xx* + 357 pp
Vol. 4	H.L. Clever, *Argon* (1980), *xviii* + 331 pp
Vol. 14	H. Miyamoto, M. Salomon and H.L. Clever, eds., *Alkaline Earth Metal Halates* (1983), *xx* + 332 pp
Vol. 27/28	H.L. Clever and C.L. Young, *Methane* (1987), *xviii* + 783 pp
Vol. 29	H.L. Clever, *Mercury in Liquids, Compressed Gases, Molten Salts and Other Elements* (1987), *xii* + 255 pp

Published by Pergamon Press, Oxford, UK: Editor-in-Chief J.W. Lorimer

Vol. 52	I. Lambert and H.L. Clever, *Alkaline Earth Hydroxides in Water and Aqueous Solutions* (1992), *xxiv* + 365 pp

Published by Journal of Physical and Chemical Reference Data. Editor-in-Chief M. Salomon

Vol. 76	P.G.T. Fogg, S.A. Bligh, M.E. Derrick, Y.P. Yampol'skii, H.L. Clever, A. Skrzecz and C.L. Young, *Solubility of Ethyne in Liquids*. J. Phys. Chem. Ref. Data **30**, 1693-1875 (2001).
Vol. 80	H.L. Clever, *Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon, and Silicon and Solid Xenon fluorides in all solvents*, J. Phys. Chem. Ref Data **34**, 201-438 (2005).

From Rubin Battino we know:
Larry had in effect completed an **update volume on Oxygen and Ozone solubilities**. I have his materials and will get them into publishable form this coming Fall. Larry also had almost completed an **update volume on the solubilities of the rare gases**.

Remembrance of H. Lawrence (Larry) Clever
June 14, 1923 - May 15, 2012

I may be one of the few people who know what the "H" in Larry's name stands for, and I would occasionally use that name in my occasionally erratic way. I never did find out from him why he preferred Larry over "H" – some things are best left as mysteries.

When I arrived at Duke University in February of 1953 I was the last of a long line of chemistry majors from The City College of the College of the City of New York to become a graduate student there. New students get to find out about the research interests of the faculty so they can choose a faculty member to work with, and a dissertation topic. Larry was a post-doctoral Fellow working for Paul Magnus Gross, the former head of the department who was then Dean of the Graduate School. The topic Larry was working on was the solubility of gases in liquids; I found that to be of interest and chose it. He had built the apparatus, which was working well. He would soon be completing his time as a post-doc and would move on to a faculty position at Emory University. Larry served with distinction there for forty years, retiring as a Professor Emeritus of Chemistry. My immediate faculty supervisor was the then head of department, John Henry Saylor.

Larry had a great deal of experience in the practical matters of doing physical chemistry research. He was my mentor and taught me many skills. In those days in physical chemistry you could not succeed in laboratory work unless you had skills in carpentry, machining, glass-blowing, electronics (vacuum tube!), solvent purification, vacuum pumps, and how to clean glassware. My meager skills were quickly advanced by Larry. Aside from practical laboratory skills, Larry taught me how to drive a stick-shift car. I believe it was the summer following his going to Emory that he returned to Duke and we worked together doing many experiments. In fact, we worked 12 hour shifts around-the-clock as long as the apparatus was functioning. Then, we would take a few days off and travel somewhere, only to return to our 24-hour research. Needless to say, we became fast friends and accomplished much research.

In my first academic position at the Illinois Institute of Technology I returned to research on the solubility of gases in liquids (amongst other areas). Larry and I continued making contributions in this field for the rest of our lives, sometimes in joint research and sometimes independently. Indeed, the review article we wrote on the subject is our most widely cited paper.

This interest in the solubility of gases in liquids got us invited to a meeting in Canada that led to the formation of the Solubility Data Commission (V.6.1) of IUPAC (International Union of Pure and Applied Chemistry). The organizer of this group was Professor E. S. (Steve) Kertes of the Hebrew University in Jerusalem. We both served as members of this Commission for many years. For a time Larry was the Chair of the Gas Solubility Subcommission. I edited two volumes for the series and Larry edited many more. We also contributed to the volumes of other members of our Commission. Via this activity we got to attend international meetings almost annually, and also to make friends with scientists from many countries. (Larry and Ruth attended more of these meetings than I did.) This international chemistry fraternity was a close-knit group, and we enjoyed each other's company over the years.

For the record Larry was born in Mansfield, Ohio, to Vance and Leona. He received three degrees in chemistry from the Ohio State University: BS, 1945; MS, 1949; and PhD, 1949. He held various positions over the years: Junior Chemist, Shell Development Co., 1945-1947; Instructor and Research Associate, Duke University, 1951-1954; instructor to professor, Emory University, 1954-1992; Participant, Oak Ridge National Laboratory, 1957; Research Associate, University of Michigan, 1963-1964; Polymer Research Institute, University of Massachusetts (Amherst), 1972-1973; Director Solubility

Data Project, Emory University, 1981-1992; Visiting Professor, University of Melbourne (Australia), 1988; Professor Emeritus of Chemistry, Emory University, 1992-2012.

In his retirement Larry was actively working on "update" volumes involving various gases. At his death the one on the solubility of oxygen and ozone was essentially complete. I have all of his relevant materials for this volume and plan on submitting it soon. I am also seeking someone to do the same thing for the volume on the solubility of the rare gases in liquids – that volume is also close to completion.

Although you might consider the solubility of gases in liquids to be his passion, Larry also published papers in many other areas. He was an excellent teacher who inspired many students. He published a number of articles in chemical education. Larry's interest in surface tension led him to recently write an article on the parachor. A search under H. Lawrence Clever in *Chemical Abstracts* came up with 268 entries. The following is a summary of the areas to which he contributed: calorimetry; the solubility of sparingly soluble salts of metals such as Pb, Hg, Zn, and Cd; excess Gibbs energies and refractive indexes of various systems; the solubility of gases in liquids; several review articles on the solubility of gases in liquids; the Setchenov salt-effect parameter; many critical evaluations in the *Solubility Data Series* volumes; surface tension and density of many solvents and mixtures; Rayleigh scattering and the thermodynamic properties of systems; phase studies; and the ion product of water.

Ruth and Larry have a loving and close family in their many relatives and, especially in their son John, his wife Anne, and their two grand children, Faye and David. I know from our correspondence that Ruth and Larry have actively visited with family their whole lives. Over the years I have had occasion to meet some of their family and they are a wonderful loving group.

One thing that Ruth and Larry and my wife Charlotte and I have shared is a love of hiking and spending time in Nature. For fifteen or more years we would meet annually in Gatlinburg, rent a chalet for a few days, and hike in the Smoky Mountains. Typically, we would do one favorite old hike, and one new one. The hot tub on the porch of the chalets was invariably used after a long day's hiking. In 1988 Ruth and Larry joined us in New Zealand with a group of New Zealand friends, my nephew Robert, my mother-in-law Ellie, and Ellie's friend Carol, to hike the Milford Track. This track is 33.5 miles long and winds through the Southern Alps. There are endless waterfalls, and great vistas from MacKinnon Pass. At the end of the hike at Sandfly Point you are ferried to Milford Sound. (Sandflies bite if you are standing still, so you have to keep moving!) There was a boat ride on Milford Sound the following day. This was a great and unforgettable trip.

I miss my friend and colleague of 59 years. He and Ruth have always been "family," and it is hard to lose a brother. Knowing him has enriched my life and that of many others, and that is an accomplishment towards which we all can strive. Thank you, Larry.

Rubin Battino
May 21, 2012
rubin.battino@wright.edu

Dear Dr. Chirico

The Provisional IUPAC Recommendation, "Guidelines for Reporting of Phase Equilibrium Measurements" is of particular interest for the IUPAC Subcommittee on Solubility and Equilibrium Data and I am a member of this group. Find below some critical comments regarding the examples selected in general and the 4 Figures in particular.

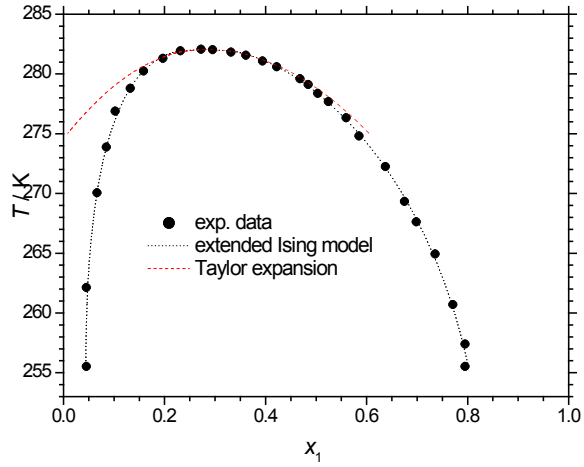
- Why are there no examples of electrolyte + water, metallurgical, ceramic or molten salt systems? Phase equilibria are by no means a solely organic chemistry domain.
- Fig. 1: All 1- and 2-phase regions should be labelled, consequently cr(1, II) and cr(1, I) should be distinguished and the area above the dashed line should be labelled cr(1,I) + liquid.
- Fig. 2: The melting point of decylamine, cr(2), can be found in Tab. 7, but is missing in Fig. 2. The second 2-phase region to the left of the inter-component compound is not indicated.
- Fig. 3: A horizontal line indicating the monotectic invariant is missing. The 2-phase region cr(1) + liquid above the monotectic line is not indicated. Again the freezing point of ethanonitrile, cr(2), is given in Tab.8, but missing in Fig. 3. The eutectic line is also missing, thus the phase diagram looks incomplete. As data listed in Tab. 6, Tab.7, Tab. 8 and Tab. 9 could be used in thermodynamic courses for teaching purposes it should be emphasized that in the liquid + liquid 2-phase region the critical index

$$\beta = \lim_{T \to T_c} \left(\frac{\partial \ln(x_1^h - x_1^l)}{\partial \ln|T - T_c|} \right) \neq 1/2 .$$

At present the maximum looks as if it could be approximated by a Taylor expansion.

- Fig. 4: It should be explicitly stated that open symbols are assigned to data belonging to lower temperature phase boundaries.

Figure 3.



Best regards,

Heinz Gamsjäger

Dear Dr. Chirico

The members of the Subcommittee on Solubility and Equilibrium Data (SSED) present in the last meeting, held in La Grande-Motte, France, on the 2nd of September 2011 supported the suggestions made by Prof. Heinz Gamsjäger in previous emails and documents sent by him to you, to improve the "Guidelines for Reporting of Phase Equilibrium Measurements" still under analysis of the scientific community for comments.
As you know SSED published in 2010, in Pure and Applied Chemistry [Gamsjäger H, *et al*., *PAC* **82**(5) 1137-1159] the technical report "The IUPAC-NIST Solubility Data Series: A guide to preparation and use of compilations and evaluations" where a detailed description of the criteria and procedures to be used in data compilation, evaluation and presentation in the special features of solubility was presented. The guidelines presented in the 2010 document are similar to those now presented by the Physical Chemistry Division to a broader range of phase equilibrium measurements.
Phase equilibrium measurements can be calculated from solubility measurements and some examples related only with organic mixtures are presented in the present Guidelines, but no reference exist to the broad range of inorganic salts, molten salts, ionic liquids, etc. that originated the need to create other bodies of theories besides the classical thermodynamic assumptions. References to this possibility are written in the text but no example is presented.

Besides the suggestions already sent to you by SSED members here we suggest that you make, at least, reference to the document

Heinz Gamsjäger, John W. Lorimer, Mark Salomon, David G. Shaw and Reginald P. T. Tomkins, The IUPAC-NIST Solubility Data Series: A guide to preparation and use of compilations and evaluations (IUPAC Technical Report), *Pure Appl. Chem*. **82** 1137 (2010)

which can be done, at least, in three paragraphs of the text now available for comments.

At least the books
The Experimental Determination of Solubilities, G. T. Hefter, R. P. T. Tomkins (Eds.), John Wiley, Chichester (2003) and
Methods for Phase Diagrams Determinations, J. C. Zhao (Ed.), Elsevier, Amsterdam (2002) (with the support of the American Society for Materials)
should also be quoted in the Guidelines.

Yours sincerely
Clara Magalhães
Chair of SSED

Terms of Reference

The goal of the Analytical Chemistry Division is the promotion of the principal branches of analytical chemistry. In many instances this is achieved in collaboration with other Divisions.

This includes the critical and comparative evaluation of established and emerging analytical methods, to enable analytical chemists to choose those best suited for specific applications. These activities include:Â

- harmonisation and proposal of rules for interlaboratory comparisons,
- recommendations for sample collection, preparation, storage and handling,Â
- the compilation of data used in analytical chemistry and their critical evaluation,Â
- the definition of recommended methods and proper application of QC and QA procedures.

The Division encourages interactions between the basic and applied disciplines.Â Its work is currently focussed on analytical methods and their applications, as follows:

1. General aspects of analytical chemistry. This includes all matters relating to terminology in analytical chemistry, chemometrics, figures of merit, quality assurance, and fundamental data including those for solubility and chemical equilibria.

2. Separation methods.Â This includes the development of critical guidelines, definition of terms, and recommendations for the operation of analytical separation methods.

3. Spectrochemical methods. This includes the critical assessment of spectrochemical methods of analysis involving electromagnetic radiation and compilation of fundamental data.

4. Mass spectrometric methodsÂ for elemental and molecular analysis.

5. Electrochemical methods. This includes the critical assessment of electroanalytical methods. Recommendations for standardisation and measurement procedures, development of critical guidelines, compilation of essential data and assessment of terminology are considered.

6. Nuclear chemistry methods. This includes analytical methods based on the measurement of isotopes and isotope ratios, and radiochemical methods and their applications.Â

Proposed changes to the SI – position paper for the Analytical Chemistry Division on the kilogram and mole

Drafted by D B Hibbert, P De Bièvre, Z Mester

February 2012

Preamble

In response to a presentation from Ian Mills, President of the Consultative Committee for Units, the meeting of ICTNS in Glasgow (2009) resolved

> Given that:
>
> (a) definition of the mole in a way that is independent of mass is desirable;
>
> (b) the mole is often thought of by chemists as an Avogadro number of entities; and
>
> (c) the name of the ISQ base quantity "amount of substance" has been a source of much confusion,
>
> ICTNS recommends to the [IUPAC] Bureau that:
>
> the recommendation of the CCU (Consultative Committee on Units) of the BIPM, that the mole be defined as follows:
>
> > "The mole, unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles, is such that the Avogadro constant is equal to exactly $6.022\ 141\ 79 \times 10^{23}$ per mole.
> >
> > Thus we have the exact relation $N_A = 6.022\ 141\ 79 \times 10^{23}\ mol^{-1}$. The effect of this definition is that the mole is the amount of substance of a system that contains $6.022\ 141\ 79 \times 10^{23}$ specified elementary entities."
>
> be supported by the IUPAC, with the following suggestions:
>
> 1. the greatest effort should be made to change the name of the ISQ base quantity "amount of substance" at the same time that a new definition of the mole is approved
> 2. a note should accompany the new definition to explain that the molar mass of ^{12}C will be an experimental quantity, with a relative measurement uncertainty of about 1.4×10^{-9}

ITCNS expressed no view on the redefinition of the kilogram, although this has been interpreted as support (minutes of San Juan meeting).

At the ICTNS meeting in San Juan the following minute was taken

RW presented the report of BIPM made available to the participants as attachment to the Agenda (Attachment 1, item 8.1) and answered comments and questions. During the ensuing discussion, the support of ICTNS for the proposals for the redefinition of SI units including the mole, decided in the Glasgow meeting (item 8.2.4 of the Glasgow minutes) was reiterated.

AF [Ales Fajgelj] expressed his wish to propose an interdivisional project in order to evaluate the consequences of the new definition of the mole for the various branches of Chemistry. *RDW* [Ron Weir, President of ICTNS] informed that anyone might submit a project proposal. All relevant divisions can be included, but ICTNS would have to judge the output.

Attached is a presentation from Ian Mills which gives his view on the problems of the kg and mole.

The present paper is in response to discussion at the Division V meeting in Antwerp, February 2012, and will form the basis of the ACD response to ICTNS/IUPAC and the proposed project.

Present SI definitions

The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.

1. The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12.
2. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

Proposed "New SI" definitions

The kilogram, kg, is the unit of mass; its magnitude is set by fixing the numerical value of the Planck constant to be equal to exactly 6.626 06X × 10^{-34} when it is expressed in the unit s^{-1} m^2 kg, which is equal to J s.

The mole, mol, is the unit of amount of substance of a specified elementary entity, which may be an atom, molecule, ion, electron, any other particle or a specified group of such particles; its magnitude is set by fixing the numerical value of the Avogadro constant to be equal to exactly 6.022 14X × 10^{23} when it is expressed in the unit mol^{-1}.

Proposal from Commission on Isotopic Abundances and Atomic Weights (CIAAW)

In its 2011 meeting in Calgary (CA), the Commission examined the on-going approaches to redefine the mole, unit of the amount-of-substance.

The CIAAW, **noting**

1. the request of CCQM for "open debate …" so as to enable the preparation of an informed proposal by the CCU of a future redefinition of the mole by the CGPM,
2. the 2009 statement by ICTNS that "the name of the ISQ base quantity 'amount of substance' has been a source of much confusion" and that "the greatest effort should be made to change the name … at the same time that a new definition of the mole is approved",
3. the ICTNS (2009) is of the opinion that the mole is often thought of by chemists as an Avogadro number of entities,
4. a unanimous opinion of the WG on the mole has not yet been attained for submission to

CCQM,

and **considering** that

1. the non-SI unit of mass, the dalton (symbol Da), is defined as 1/12th of the mass of a single ^{12}C atom,
2. atomic mass values for the elements are commonly expressed in daltons, not in kilograms,
3. all atomic-weight values of the elements are also expressed in daltons,
4. all molecular-weight values for large molecules such as proteins are also expressed in daltons,
5. numerous chemical measurements consist of measurement of ratios of number of entities (atoms, molecules, …),

recommends

1. changing the name of the quantity "amount of substance" to "number of entities",
2. the following future definition of the mole:

   Mole, the unit of number of entities, symbol 'mol', is a number of specified entities equal to 6,022 14xy ·10^{23} entities exactly.

3. that any decision on redefinition of the mole be deferred until full consideration is given to the interests of the chemical and isotopic measurement communities.

and **suggests**

that together with the fixed value of the Avogadro constant, the dalton could serve to redefine the kilogram in a way that would suit the needs of the chemists:

Kilogram, the unit of mass, symbol 'kg', is the mass of 6,022 14x yz ·10^{23} atoms of ^{12}C in their nuclear ground state multiplied by 1000/12,

or

Kilogram, the unit of mass, symbol 'kg', is the mass of one mole of ^{12}C atoms in their nuclear ground state multiplied by 1000/12.

A proposal from Division V

As chemists we should support a 'dalton' approach to defining the kilogram, and I see merit in fixing the Avogadro number to define the mole.

I (DBH) do not think 'number of entities' is an appropriate term for the quantity for which mole is unit. The phrase in English has a meaning so it could lead to the sentence "The number of entities [*usual English*] is 6.022 14xyz × 10^{23} for which the number of entities [*quantity*] is 1 mol." This in my view dos not aid clarity.

We have discussed 'chemical amount', but I ask if we need a quantity at all? 1 mol of an entity is simply N_A of the entities if N_A is a number (and not of dimension mol^{-1}). I think this is behind the 'number of entities' suggestion.

Maria Magalhães

From: heinz.gamsjaeger@mu-leoben.at
Sent: terça-feira, 13 de Março de 2012 14:35
To: Brynn Hibbert; Maria Magalhães; A.Fajgelj@iaea.org; lorimer@uwo.ca
Subject: Re: FW: ACD position on the "New SI"

Dear Brynn,

I strongly support the ACD proposal
Note 2: ....the present quantity 'amount of substance' is renamed 'chemical amount'.

There are two arguments in favour of the ACD proposal.
1) The CIAAW proposal to rename the present quantity 'amount of substance' as 'number of entities' will be confusing for all chemists which have been quite happy with 'amount of substance', because 'number of entities' requires no associated unit other than '1'. thus the mole is in fact the chemist's glorified dozen.
2) To maintain continuity with the present ISQ is also quite important, as anybody engaged in chemical education or in editing chemical journals will confirm.

Best regards,

Heinz

Date sent: Thu, 08 Mar 2012 10:57:45 +0000
Subject: FW: ACD position on the "New SI"
From: Clara Magalhães <mclara@ua.pt>
To: SSED member <mclara@ua.pt>
Copies to: Brynn Hibbert <b.hibbert@unsw.edu.au>

> Dear SSED members
> There is a public discussion of new definitions of mass unit and mole,
> as well as a proposal for a new name for the amount of substance. Some
> people are proposing that the unit of mass could be the gram instead
> of the kilogram. It turned the new definition of mass unit less
> complicate. Those of you that would like to express your opinion on
> this subject please send an email to Brynn Hibbert before the 16th
> MARCH. Yours sincerely Clara Magalhães
>
>
>
> ------ Forwarded Message
> From: Brynn Hibbert <b.hibbert@unsw.edu.au>
> Date: Sat, 3 Mar 2012 10:50:17 +0000
>
> Conversation: ACD position on the "New SI"
> Subject: ACD position on the "New SI"
>
> Dear Titular members, Associate members and National Representatives
> Following instructions from our ACD meeting in Antwerp, Paul De
> Bièvre, Zoltan Mester and I put together a position paper on the ³New
> SI². You may be aware that there is a proposal to redefine four out of
> the seven base units of the Si (kg, mol, K, A). As the mole is the
> Œchemists¹ unit we are particularly sensitive to the proposed changes.
> The initial reaction of IUPAC (at the Glasgow GA) was for ICTNS to
> offer endorsement, but since then there has been growing disquiet that
> there was not sufficient level of discussion. Recently the CIAAW has
> published a statement, and Division 2 is also coming to a new
> position. We wish to offer our opinion and need to have an agreed
> position within two weeks so that Filomena can take it to the Bureau
> meeting in May and before that the CCQM meeting in April. So could I
> ask you to read the attached paper and decide whether you support the
> recommendations, and offer any amendments or changes by FRIDAY 16th
> MARCH I will collate the responses and circulate the final paper.
> Please contribute (even if you simply agree). This is both important
> and a good opportunity for members to work on a project together.
> Thanks to all Brynn Hibbert
>

> Vice President IUPAC Division V
>
>
> D. Brynn Hibbert,
> Professor of Analytical Chemistry
> School of Chemistry
> University of New South Wales
> Sydney, NSW 2052 Australia: CRICOS Code 00098G
>
> Tel: +61 2 9385 4713 Fax: +61 2 9385 6141 mobile: 0411
> 286 480 http://www.chem.unsw.edu.au <http://www.chem.unsw.edu.au/>
> http://www.chem.unsw.edu.au/research/groups/hibbert/
> <http://www.chem.unsw.edu.au/research/groups/hibbert/> Book: *****
> Quality Assurance for the Analytical Chemistry Laboratory, OUP, New
> York, 2007 *****
>
>
>
>
> ------ End of Forwarded Message
>
>

em.O.Univ.Prof. Dr. Heinz Gamsjaeger
Lehrstuhl fuer Physikalische Chemie
Montanuniversitaet Leoben
A-8700 Leoben, Austria
Tel:+43 (0)3842 402 4804
FAX:+43 (0)3842 402 4802
e-mail: gamsjaeg@unileoben.ac.at

From: "Anthony R. H. Goodwin" <AGoodwin@slb.com> <mailto:AGoodwin@slb.com>
Date: Tue, 12 Jun 2012 01:17:44 +0000
To: "mclara@ua.pt" <mailto:mclara@ua.pt> <mclara@ua.pt> <mailto:mclara@ua.pt>
Cc: Kaoru Yamanouchi <kaoru@chem.s.u-tokyo.ac.jp> <mailto:kaoru@chem.s.u-tokyo.ac.jp> , "Wilson, Angela" <akwilson@unt.edu> <mailto:akwilson@unt.edu>
Conversation: Divisional Rep. for Subcommitte on Solubility and Equilibrium Data
Subject: Divisional Rep. for Subcommitte on Solubility and Equilibrium Data

Dear Clara,
At the Division I (Physical and BioPhysical) meeting last weekend, the topic of Divisional Representatives was discussed. The Subcommittee on Solubility and Equilibrium Data webpage does not specifically identify Representatives from other Divisions, however, if your Subcommittee has these I was asked to serve that role for Division I. Could you let me, and those copied on this, know the situation with regard to representatives and if you are able to accept the role proposed?

Best regards,

Tony

Anthony R. H. Goodwin

Projects

1999-050-1-500: Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands – not yet finished

2001-032-1-500: Metal and ammonium formate systems Series: Solubility Data Series - volume 73

2001-033-1-500: Actinide carbonates and carbon-containing compounds - volume 74

2001-034-1-500: Non-metals in liquid alkali metals Series: Solubility Data Series - Guminski Is it already published??

2001-037-1-500: Chemicals in the atmosphere: Solubilities in aqueous Media - Book - finished

2001-052-1-500: Solubility of volatile and gaseous fluorides in all solvents Series: Solubility Data Series; editor-in-chief: Mark Salomon - Volume 80

2001-084-1-500: Experimental determination of solubilities - Book - finished

2001-085-1-500: IA and IIA azides, cyanates, cyanides and thiocyanates - published

2002-004-1-500: Solubility Data Series To see what to do with this project that is a collction of projects

2002-025-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds - Volume 36

2002-031-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates Published this year – Volume 94

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) - Reconverted. Published cadmium carbonate – Volume 92

2002-033-1-500: Solubility data related to oceanic salt systems. Part I - Binary systems containing sodium, potassium, and ammonium sulfate abandoned

2002-034-1-500: Solubility data related to oceanic salt systems. Part II - magnesium chloride-water and calcium chloride-water and their mixtures abandoned

2002-035-1-500: Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis Erich Koenigsberger – it will continue

2002-036-1-500: Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates Volume 90

2002-037-1-500: Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons abandoned

2002-038-1-500: Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics abandoned

2002-039-1-500: Solubility data of compounds relevant to human health. Antibiotics: macrocyclic lactone antibiotics Series: Solubility Data Series; editor-in-chief: Mark Salomon abandoned

2002-040-1-500: Solubility data of compounds relevant to human health. Noble gases Series: Solubility Data Series; editor-in-chief: Mark Salomon Project suspended???

2002-041-1-500: Solubility data of compounds relevant to human health. Gaseous compounds of carbon, hydrogen, fluorine, chlorine, bromine and iodine Series: Solubility Data Series; editor-in-chief: Mark Salomon It should be abandoned

2002-042-1-500: Solubility data related to industrial processes. Lead sulfate Series: Solubility Data Series; editor-in-chief: Mark Salomon abandoned

2002-043-1-500: Solubility data related to industrial processes. Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane Alex will see about it

2002-044-1-500: Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions Alex will see the status

2002-045-1-500: Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide Project terminated

2002-050-1-500: Solubility data related to industrial processes. Acetonitrile: ternary and other multicomponent systems Volume 78

2003-018-1-500: Mutual solubility of hydrocarbons and water (update of SDS Vol 37 & 38) Series: Solubility Data Series; editor-in-chief: Mark Salomon already published

2005-006-1-500: Mutual solubility of alcohols and water (update of SDS Vol 15) Volume 82

2005-014-1-500: IUPAC Stability Constants Database - completion of data collection up to 2006 already finished

2005-017-1-500: Glossary of terms related to solubility - updates and revisions to the Orange Book Published in PAC

2005-033-1-500: Transition and 12 to 14 main group metals, lanthanide, actinide and ammonium halates Volume 85

2006-032-1-500: Solubility data related to industrial processes. Mutual solubility of ethers and ketones with water Volume 86

2006-033-1-500: Solubility data related to industrial processes. Rare earth metal chlorides (Sc, Y, lanthanoids) in water and aqueous systems Volume 87

2006-034-1-500: The solubility of oxygen and ozone in all solvents (update of SDS vol 7. 1981) almost finished

2007-044-1-500: Solubility data related to industrial processes. Solubility in systems with lithium and/or sodium nitrates Volume 89

2007-045-1-500: Solubility data related to industrial processes. Solubility of higher alkynes in liquids still running

2007-046-1-500: Solubility data related to industrial processes. Mutual solubility of esters with water already published

2007-047-1-500: Solubility data related to industrial processes. Nitriles C+3: binary and multicomponent systems ??

2008-008-1-500: An introduction to the IUPAC-NIST Solubility Data Series: Preparation and use of compilations and evaluations already published

2008-025-1-500: Humic-metal binding constants database until 2014

2010-005-2-500: Rare Earth Metal (Sc, Y, Lanthanoids) Bromides and Iodides in Water and Aqueous Systems (Solubility Data Series) already published

2010-047-1-500: Mutual Solubility of Phenols with Water.Â Solubility Data Series. Volume 91

2010-050-1-500: Mutual Solubility of aliphatic and non aliphatic amines with Water. (Solubility Data Series) ??

2011-017-1-500: Solubility of Potassium Sulfate in Water (Solubility Data Series) Volume 93

2011-043-1-500: Solubility data related to Industrial Processes. Solubility data in ternary systems containing water alcohol, and hydrocarbon ??

New SSED projects 2012

Project name	number	date of approval	Chair
Solubility of lithium sulfate in aqueous solutions	2011-031-1-500	22 March 2012	Wolfgang Voigt
Solubility data in ternary systems containing water, alcohol and hydrocarbon	2011-043-1-500	29 September 2012	Marian Goral
Database on solubility and liquid–liquid equilibria of binary mixtures of ionic liquids and molecular compounds	2011-065-1-500	June 2012	Magdalena Bendová
Solubility of lead carbonates	2012-004-1-500	22 March 2012	Heinz Gamsjäger
The solubility of beryllium sulfate and other beryllium compounds in aqueous and non-aqueous media	2012-006-1-500	22 March 2012	John Lorimer
Critical evaluation of thermodynamic data of sulfate complexes in solution	2012-008-1-500	5 March 2012	Glenn Hefter
Solubility in systems with lithium and/or sodium nitrates. Part 2. Sodium nitrates	2012-022-1	submitted 25 April 2012	Jitka Eysseltova
Polycyclic aromatic hydrocarbons in pure and binary solvent mixtures	2012-025-1	submitted 30 April 2012	William E. Acree, Jr
The solubility of rare earth metal (Sc, Y, Lanthanoides) fluorides in water and aqueous systems	2012-030-1	submitted 03 July 2012	Cezary Guminski
Modernizing the website of the SSED	2012-031-1	submitted 07 July 2012	David Shaw
Simultaneous phase and chemical equilibrium in multicomponent liquid – liquid systems including critical phenomena	??	not yet	Maria Toika
Solubility of rare earth metal (Sc, Y, lanthanoides) bromides in alkali metals bromides	2011-058-1	suspended	Marcelle Gaune-Escard

REVISED VERSION

TERMS OF REFERENCE

Subcommittee on Solubility and Equilibrium Data

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. The SSED also coordinates the dissemination of evaluated solubility data through traditional (journal) and electronic (internet-accessible database) means. The SSED 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 treatment, encourages the formation of Task Groups to perform compilation and evaluation, and assists Task Groups in carrying out their projects.

Proposed Initial Membership

H. Gamsjaeger (Austria), Chair
P. May (Australia)
M. Salomon (USA)
P. Scharlin (Finland)
D. Shaw (USA)
S. Sjoberg (Sweden)

Subject: RE: IUPAC/NIST and projects
Date: Wednesday, March 14, 2012 00:10
From: Harvey, Allan H. Dr. <allan.harvey@nist.gov>
To: Mark Salomon <marksalomon@comcast.net>, "mclara@ua.pt" <mclara@ua.pt>
Cc:

Conversation: IUPAC/NIST and projects

From the NIST perspective – our goal is dissemination of the information. While I cannot speak 100% with authority for NIST, I think I can say with 99.9% confidence that the intention is to put this material up on the web in a way that is freely available to all. As such, it would be fine for there to be a link to the material from some IUPAC site. I would have to think about whether it would make sense for the files to be duplicated and stored on both sites.
We have already done a large fraction of the scanning work at NIST (I would have to check with my colleague to find out what fraction), and also a significant fraction of dividing the scans into appropriate sections. Completion for all the volumes would of course depend on further availability of NIST resources – the project was suspended in Fall 2011 because we had not heard any reply about getting permission from IUPAC. Possibly some SSED people can help in checking the quality of the project output to make sure files are in the right place, etc.

In summary, the position of NIST for this has been (and continues to be) that we are willing to make the scanned information from these old volumes freely available to the public on a NIST website, as long as IUPAC (as the copyright holder) gives the appropriate permission.

I see reference to an "IUPAC/NIST agreement". Of course some NIST input would be needed before finalizing any such document – is this agreement envisioned as only covering the permission for the old volumes, or as something with a wider scope?

Best Regards,
Allan Harvey, Co-Editor, JPCRD

Dr. Allan H. Harvey, aharvey@boulder.nist.gov
Thermophysical Properties Div., National Institute of Standards & Technology
325 Broadway, Boulder, CO 80305 USA
Phone: (303)497-3555, Fax: (303)497-5044

From: Mark Salomon [mailto:marksalomon@comcast.net]

Sent: Tuesday, March 13, 2012 9:08 AM
To: mclara@ua.pt
Cc: Harvey, Allan H. Dr.
Subject: Fwd: IUPAC/NIST and projects

Dear Clara,

I think NIST has the final word on how the old IUPAC SDS volumes are to be disseminated. I know that IUPAC holds the copyrights to the old volumes, but if NIST is to scan these volumes at great expense and effort, I don't know if they will agree to give the ACD unlimited free access to these old volumes. Perhaps a link to the NIST web site for access to the volumes would be appropriate. Bottom line: I'm not sure how to proceed without the advice of Allan Harvey.

More to come later on how the agreement should be finalized (after we hear from Allan).

Cheers,
Mark

-------- Original Message --------
Subject: IUPAC/NIST and projects
Date: Sun, 11 Mar 2012 20:17:47 +0000
From: Clara Magalhães <mclara@ua.pt> <mailto:mclara@ua.pt>
To: Mark Salomon <mark.salomon@maxpowerinc.com>
<mailto:mark.salomon@maxpowerinc.com> , Mark Salomon
<marksalomon@comcast.net> <mailto:marksalomon@comcast.net> , David Shaw
<dgshaw@alaska.edu> <mailto:dgshaw@alaska.edu>

Dear Mark and David

In the Antwerp Analytical Chemistry Division (ACD) meeting the SDS IUPAC/NIST agreement was one of the subjects analysed.

The ACD Vice-president (Brynn Hibert) suggested that in the IUPAC/NIST agreement we consider the possibility to make the old SDS volumes also available by the ACD web page. In order to finish the IUPAC/NIST agreement I
would like to know if you both together with Brynn from IUPAC developed the final text of the agreement to be present in China meeting and finally we have an official document. I know that David will not be present in China but I hope that Mark will be. We need the editor in Chief present in the

next meeting.

The proposal of allowing access to all the old SDS texts in the IUPAC web page in conjunction with NIST came from the experience with some documents that are available in different institutions web pages and in some of them they are for free and in others they have to be bought.

Please let me know what you think of the idea that with Brynn we finish the writing of the agreement. Brynn has easier access to the bureau than us. I think this could be a good way to see the data finally available.

Many thanks by your precious help
Clara

NIST-Related items for 2012 SSED meeting

prepared by Allan Harvey, JPCRD Co-Editor (aharvey@boulder.nist.gov)

ONLINE AVAILABILITY OF OLD SDS VOLUMES

- Old printed volumes are in a few libraries, generally difficult for many to access.
- NIST has scanned all the printed volumes, done some work to organize into sections and link together in HTML pages.
- Sample (Volume 2) can be seen at http://www.iapws.org/drafts/SDS2/SDS-2-contents.htm
- NIST would plan to make them all available on a NIST website, for free.
- Official permission from IUPAC desired.
- NIST would like the SSED to officially request that IUPAC give this permission.
- NIST would also give IUPAC copies of these files, in case some IUPAC project wanted to use them.

Subject: Clarification of LOGKOW Databank
Date: Friday, June 29, 2012 15:41
From: James Sangster <James.Sangster@polymtl.ca>
To: Clara Magalh‹es <mclara@ua.pt>, <Earle.Waghorne@ucd.ie>, David Shaw <DavidShaw@post.harvard.edu>, <g.hefter@murdoch.edu.au>
Conversation: Clarification of LOGKOW Databank

Hi Clara,

I received the Minutes of the SSED meeting of September last (10 months late).

Under item #6 I noticed that you require clarification of my agreement with the U. S. company.
Not to waste any more time, I give details here. As stated in my draft Proposal, the databank is
currently distributed in two ways:

(1) Technical Database Services, Inc., New York (TDS)

I have a legal contract agreement with TDS (signed December 2010). Under this agreement, TDS
has exclusive rights for the distribution (sale and lease) of the ASCII flat file of the complete databank.

(2) National Research Council of Canada, Ottawa (NRC)
As part of the formal agreement with TDS, I have a verbal agreement with NRC (dating from approximately 1995). In this agreement, NRC hosts the LOGKOW database on its server

http://logkow.cisti.nrc.ca

NOTA BENE: LOGKOW is accessible free of charge from this internet site, however the user can
retrieve data for only one substance at a time.

Neither Sangster Research Laboratories nor NRC is permitted to distribute LOGKOW in any form,
except as provided in the contract agreement with TDS.

I hope this is sufficient clarification to allow further discussion leading to a proposal submission to
IUPAC.

I update LOGKOW 2 or 3 times a year. The complete updated ASCII file is sent to NRC at these times and the internet site is thereby updated at this frequency. A complete ASCII flat file is also
sent to TDS, upon the request of TDS.

Concerning my draft Proposal (which you have had for some time), we have not yet recruited a chemist(s) to continue the updating of LOGKOW. However, this is to be the job of the Project's
Task Group: I have specified who the members would be and have acquired their agreement to collaborate. I have also secured the expressed interest for collaboration of a number of colleagues (not members of the Task Group).

I noticed that LOGKOW could be considered together with the Stability

Constants Database
as IUPAC projects. I understand that the Stability Constants Database is not updated, but would be
- I assume - simply archived. Is this correct?

I believe that both LOGKOW and the Stability Constants Database would fit into IUPAC's mandate.
Both are valuable resources for chemists. At this point I do not know of what significance (if any)
is the fact that LOGKOW is actively updated, whereas the Stability Constants Database is not.

I expect that I will be able to attend a meeting of the SSED in 2013. Please keep me informed on
details when these are available.

Jim

QuickTime™ and a
decompressor
are needed to see this picture.

Subcommittee on Solubility and Equilibrium Data

Chair's Activity Report

from August 2011 to July 2012

QuickTime™ and a
decompressor
are needed to see this picture.

Terms of reference

- 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.

QuickTime™ and a
decompressor
are needed to see this picture.

Meetings and conferences

- **Last SSED meeting** - The 37th solubility subcommittee annual meeting (10th of SSED) occurred in La Grande-Motte, France, on the 2nd of September 2011 in conjunction with the 32nd International Conference on Solution Chemistry (ICSC).

- **Annual meeting of the Analytical Chemistry Division** - occurred in Antwerpen, Belgium, from the 5th to the 8th February 2012.

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decompressor
are needed to see this picture.

Next meetings and conferences

SSED meeting - The 38th solubility subcommittee annual meeting (11th of SSED) will occur in Xining, China on the 21st and 22nd July 2012 in conjunction with the 15th ISSP.

15th ISSP - The 15th International Symposium on Solubility Phenomena and Related Equilibrium Processes will occurr in Xining, China, from the 23rd to the 27th July 2012.

SSED meeting - The 39th solubility subcommittee annual meeting (12th of SSED) will occur in Istambul, Turkey in conjunction with the IUPAC General Assembly

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decompressor
are needed to see this picture.

Franzosini Award

The Franzosini Award is attributed biannually, under proposal, to two researchers that had contributed with their work to the development of solubility field of knowledge, and that assures their participation in the SSED projects.

The proposals are analysed by a commission that includes the chair of the subcommission.

The award helps the travel of the nominee to the ISSP

The nominees have, the right to participate in the SSED meetings, and to present an invited lecture in the ISSP

QuickTime™ and a
decompressor
are needed to see this picture.

Visibility of SSED within IUPAC 2011/2012

- ***CI*, 33,** No. 4, July – August 2011
  - ***IUPAC Wire - In Memoriam***
    - Pg. 66: reference to the dead of Ari Horváth
  - ***Making an Impact***
    - Pg. 22: Chemical speciation of environmentally significant metals with inorganic ligands. Part 4: the Cd^{2+} + OH^-, Cl^-, CO_3^{2-}, SO_4^{2-} and PO_4^{3-} systems (IUPAC technical report), Kipton J. Powell *et al*. PAC **83**(5) 1163-1214
    - Pg. 23: IUPAC-NIST Solubility Data Series - Volume 88: Esters with water - revised and updated (4 parts series) and Volume 89. Alkali metal nitrates. Part 1. Lithium nitrate

QuickTime™ and a
decompressor
are needed to see this picture.

Visibility of SSED within IUPAC 2011/2012

- ***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 - Solubility Phenomenon, Xining, China
- ***CI*, 34,** No. 2, March – April 2012
  - ♦ ***Reports from San Juan, Part II***
    - ♣ Pg. 16: Analytical Chemistry by Brynn Hibbert
  - ♦ ***Mark your calendar***
    - ♣ Pg. 32: 22-27 July 2012 - Solubility Phenomenon, Xining, China
- ***CI*, 34,** No. 3, May – June 2012
  - ♦ ***Mark your calendar***
    - ♣ Pg. 34: 22-27 July 2012 - Solubility Phenomenon, Xining, China

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decompressor
are needed to see this picture.

New proposals

- 2011-031-1-500 - Solubility of lithium sulfate in aqueous solutions - W. Voigt
- 2011-043-1-500 - Solubility data in ternary systems containing water alcohol, and hydrocarbon - M. Goral
- 2011-065-1-500 - Database on solubility and liquid–liquid equilibria of binary mixtures of ionic liquids and molecular compounds - Magdalena Bendóva
- 2012-004-1 - Solubility of lead carbonates - H. Gamsjaeger
- 2012-006-1 - The Solubility of Beryllium Sulfate and Other Beryllium Compounds in Aqueous and Non-aqueous Media - J. Lorimer
- 2012-008-1-500 - Critical Evaluation of Thermodynamic data of sulfate complexes in solution - G. Hefter

2012-022-1 - Solubility in systems with lithium and/or sodium nitrates. Part 2. Sodium nitrates - Jitka Eysseltova

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New proposals (continue)

- 2012-025-1 - Polycyclic aromatic hydrocarbons in pure and binary solvent mixtures - William E. Acree, Jr.
- 2012-030-1 - The solubility of rare earth metal (Sc, Y, Lanthanoides) fluorides in water and aqueous systems - Cezary Guminski
- 2012 - ?? - Modernizing the website of SSED - Davis Shaw
- 2011-058-1 - Mutual Solubility of Rare Earth Metal (Sc, Y, Lanthanides) Bromides in Alkali Metals Bromides (melts) - M. Gaune-Escard

Simultaneous phase and chemical equilibrium in multicomponent liquid – liquid systems including critical phenomena - Maria Toikka

- 2011-030-1 - Enlarged Database for Thermodynamic Simulation of Chemical Speciation in Environmental Water Systems - C. Balarev -

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Projects already finished

2011-017-1-500: Solubility of Potassium Sulfate in Water
2010-005-2-500: Rare Earth Metal (Sc, Y, Lanthanoids) Bromides and Iodides in Water and Aqueous Systems
2010-050-1-500: Mutual Solubility of aliphatic and non aliphatic amines with Water.
2010-047-1-500: Mutual Solubility of Phenols with Water.
2007-039-1-024: Extension of ThermoML - the IUPAC standard for thermodynamic data communications
2002-031-1-500: Alkaline earth metal carbonates
1999-050-31-500: Chemical speciation of environmentally significant heavy metals and inorganic ligands

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Projects for publication

2007-045-1-500: Solubility data related to industrial processes. Solubility of higher alkynes in liquids
2006-034-1-500: The solubility of oxygen in all solvents (update of SDS vol 7. 1981)
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) (Cd carbonate published)
2002-031-1-500: Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates

QuickTime™ and a
decompressor
are needed to see this picture.

Projects still running

2008-025-1-500: Humic-metal binding constants database
2007-047-1-500: Solubility data related to industrial processes. Nitriles C+3: binary and multicomponent systems
2007-045-1-500: Solubility data related to industrial processes. Solubility of higher alkynes in liquids
2006-034-1-500: The solubility of oxygen in all solvents (update of SDS vol 7. 1981)
2005-014-1-500: IUPAC Stability Constants Database - completion of data collection up to 2006
2002-044-1-500: Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions
2002-035-1-500: Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis
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)

E-i-C Report 2011 – July 2012 (Mark Salomon)

The following is a summary of publications and manuscripts in course of publication which Allan Harvey and I have been working on. The last E-i-C report left off with the publication of volume 90 on hydrobenzoic acid derivatives. During the last year and starting with volume 91, here are summaries of manuscripts published in J. Phys. Chem. Ref. Data or are in course of publication.

Volumes Published

• **Volume 91**, Phenols with Water & Heavy Water. M. Góral, D.G. Shaw, A. Maczynski and B. Wisniewska-Goclowska.

Part 1. C_6 and C_7 Phenyl and Methylphenols.

Part 2. C_8 too C_{15} Alkyl Phenols.

• **Volume 92**. Metal Carbonates. H. Gamsjäger, M.C.C. Magalhães, E. Königsberger, K. Sawada, B.R. Churagulov, P. Schmidt, D. Zeng. Part 1. Solubility and Related Thermodynamic Quantities of Cadmium(II) Carbonate in Aqueous Systems.

• **Volume 93**. Postasium Sulfate in Water. J. Eysseltová and R. Bouaziz.

• **Volume 94**. Alkaline Earth Carbonates in Aqueous Systems. A. De Visscher, J. Vanderdeelen, E. Königsberger, B.R. Churagulov, M. Ichikuni, M. Tsurumi.

Part 1. Indtroduction, Be and Mg

Part 2. Ca

• **Volume 95.** Rare Earth Metal Iodides and Bromides. T. Mioduski, C. Guminski, D. Zeng.

Part 1. Iodides

Volumes In Press

• **Volume 96.** Amines with Water. M. Góral, D.G. Shaw, A. Maczynski, B. Wisniewska-Goclowska and Paweł Oracz.

Part 1. C_4-C_6 Aliphatic Amines

Part 2. C_7-C_{24} Aliphatic Amines

Part 3. Non-Aliphatic Amines

Volumes In Progress

• Oxygen and Ozone Update. No information available at this time.

• Solubility of the Higher Acetylenes and other Acetylenic Compounds. Peter Fogg is preparing a final draft for this update on acetylenes. Last correspondence was in December, 2011, and the manuscript will be submitted as soon as the final draft is received.

Proposed New Volumes

- 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 extention of this work with systems water + two alcohols and water + two hydrocarbons. A Project Submission Form has been submitted to IUPAC.

- C. Guminski and D. Zeng have proposed a new volume on rare earth metal fluorides. A Project Submission Form has been submitted to IUPAC.

- J. Lorimer, J. Hála and C. Balarew have proposed a new volume on $BeSO_4$ and other Be compounds in aqueous and nonaqueous media. A Project Submission Form has been submitted to IUPAC.

- Bill Acree has proposed a new updated volume polycyclic aromatic hydrocarbons. A Project Submission Form has been submitted to IUPAC.

JPCRD-Related items for 2012 SSED meeting

prepared by Allan Harvey, JPCRD Co-Editor (aharvey@boulder.nist.gov)

GENERAL ISSUES FOR SDS

- SDS papers are an important part of JPCRD content; we look forward to continuing to publish whatever the SSED decides is significant enough for a project.
- No problems anymore with page limits (within reason).
- SDS Volume 100 coming soon – perhaps mark with an Editorial.
- Division of Volumes into "Parts" – OK as long as parts are not too short (maybe 20 published pages minimum) and (more important) the division should make logical sense in terms of subject matter (like one part for lithium compounds, one for sodium compounds, etc.). Best to consult with Mark Salomon and Allan Harvey early in project to discuss such division.

HINTS FOR PREPARING PUBLICATIONS

- See sample manuscript linked at jpcrd.aip.org, and also recent SDS papers in the Journal.
- Failure to follow proper formatting will delay publication of the paper.
- References must be numbered in order of appearance in the paper. May make things easier to do things like "we collected the literature data[1-76] on …". Then list in order in References section at end (no references sections within individual data sheets).
- For references with translation journals (like Russ. J. Phys. Chem. and Zh. Fiz. Khim.), References section should cite the version actually used in preparing the paper. Both may be listed in the data sheet.
- Equations must be numbered individually in order of appearance through the paper, using Mathtype or Word's equation editor.
- Use Table feature of Word for tables. Number tables consecutively, but tables within data sheets are unnumbered.
- Make proper use of italics for variables, roman type for chemical formulas, etc. Use symbols available in Word. Degree sign (°), not superscript letter o. Minus sign (−), not hyphen (-). Middle dot (·) [hydrate formulas], not superscript period. Multiplication sign (×), not letter x.
- Supply figures in PDF, EPS, or TIF.
- Supply complete postal addresses for all authors. If certain authors should be designated "Editor", "Compiler", "Evaluator", etc., make that clear.
- Make section numbering logical and consistent within the paper.
- When listing small numbers of coefficients, etc., do it within the sentence, like:
  The coefficients … are $a_1 = -154.17$, $a_2 = -3.449$, and $a_3 = 140.94$.
  instead of writing each equality like a separate equation on its own line.
- For multi-part papers, only need complete Preface in Part 1, but later Parts should have a brief introductory section putting the part in context. Part 2 should reference Part 1, Part 3 should reference Parts 1 and 2, etc.

Report of the Solid-Liquid Group
Solubility and Equilibrium Data Subcommittee
International Union of Pure and Applied Chemistry

Prepared by W. Voigt
At the 2012 Meeting of SSED

Xining, July 2012

Volumes published since January 2011

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

Ayako Goto, Editor, Hiroshi Miyamoto, Editor, Mark Salomon, Editor, Rensuke Goto, Evaluator, Hiroshi Fukuda, Evaluator, Erich Königsberger, Compiler, and Lan-Chi Königsberger, Compiler

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

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

Ayako Goto, Hiroshi Miyamoto, Mark Salomon, Rensuke Goto, Hiroshi Fukuda, Erich Königsberger, Lan-Chi Königsberger, and Pirketta Scharlin

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

IUPAC-NIST Solubility Data Series. 92. Metal Carbonates. Part 1. Solubility and Related Thermodynamic Quantities of Cadmium(II) Carbonate in Aqueous Systems

H. Gamsjäger, Editor, M. C. F. Magalhães, Editor, E. Königsberger, Editor, K. Sawada, Editor, B. R. Churagulov, Compiler, P. Schmidt, Compiler, and D. Zeng, Compiler

J. Phys. Chem. Ref. Data **40**, 043104 (2011); http://dx.doi.org/10.1063/1.3645087 (*26 pages*)

IUPAC-NIST Solubility Data Series. 93. Potassium Sulfate in Water

Jitka Eysseltová and Roger Bouaziz

J. Phys. Chem. Ref. Data **41**, 013103 (2012); http://dx.doi.org/10.1063/1.3679678 (*48 pages*)

IUPAC-NIST Solubility Data Series. 94. Rare Earth Metal Iodides and Bromides in Water and Aqueous Systems. Part 1. Iodides

Tomasz Mioduski, Cezary Gumiński, and Dewen Zeng

J. Phys. Chem. Ref. Data **41**, 013104 (2012); http://dx.doi.org/10.1063/1.3682093 (*63 pages*)

IUPAC-NIST Solubility Data Series. 95. Alkaline Earth Carbonates in Aqueous Systems. Part 1. Introduction, Be and Mg

Alex De Visscher, Jan Vanderdeelen, Erich Königsberger, Bulat R. Churagulov, Masami Ichikuni, and Makoto Tsurumi

J. Phys. Chem. Ref. Data **41**, 013105 (2012); http://dx.doi.org/10.1063/1.3675992 (*67 pages*)

IUPAC-NIST Solubility Data Series. 95. Alkaline Earth Carbonates in Aqueous Systems. Part 2. Ca

Alex De Visscher, Editor, Evaluator and Jan Vanderdeelen, Evaluator

J. Phys. Chem. Ref. Data **41**, 023105 (2012); http://dx.doi.org/10.1063/1.4704138 (*137 pages*)

New 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 reqired format, evaluation is under way

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

30 April 2012 / submitted 30 April 2012
Polycyclic aromatic hydrocarbons in pure and binary solvent mixtures: William E. Acree, Jr.

- ➔ No further information

2012-030-1 / submitted

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 are 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

From the listing above and the discussion with task chairs (so far as present at the meeting) is can be expected that 2 new volumes and 2 new continuation parts of volumes will be ready until the next SSED meeting.

Wolfgang Voigt

Solid-liquid solubility chair

Report of the Stability Constants Group
Subcommittee on Solubility and Equilibrium Data
International Union of Pure and Applied Chemistry

Prepared by Glenn Hefter

1. Approval was given by IUPAC in March 2012 for a new project titled "*Critical Evaluation of Thermodynamic Data of Sulfate Complexes in Solution*" (Project #2012-008-1-500). Participants are G. Hefter (Task Group Chair) and D. Meyrick from Murdoch University, Perth, Australia and C. Guminski, University of Warsaw, Poland. Preliminary literature and compilation work has commenced.

2. For the project Humic-Metal Binding Constants Database (Project #2008-025-1-500), M. Filella Task Group Chair, progress has been impeded by other commitments of the participants. Most of the data collection is complete and all articles are being screened and classified. The projected completion date is January, 2014.

3. The long-running project on the "*Chemical Speciation of Environmentally Significant Metals with Inorganic Ligands*" (Project #1999-050-1-500; Task Group Chair, S. Sjoberg) is now more or less complete. The last (5th) part in the series, on zinc(II), is just waiting for final input from one of the contributors prior to submission. Previous parts in the series on mercury(II), copper(II), lead(II) and cadmium(II) have all been published as IUPAC Technical Reports in *Pure & Applied Chemistry.*

Report of the Liquid-Liquid Group
Solubility and Equilibrium Data Subcommittee
International Union of Pure and Applied Chemistry

Prepared by D Shaw
Prior to 2012 Meeting of SSED

Volumes Published Since Last Meeting:

Goral, M., D. G. Shaw, A. Maczynski, and B. Wisniewska-Goclowska, 2011, IUPAC-NIST Solubility Data Series. 91. Phenols with Water. Part 1. C_6 and C_7 Phenols with Water and Heavy Water, *Journal of Physical and Chemical Reference Data*, **40**, 033102.
Goral, M., D. G. Shaw, A. Maczynski, and B. Wisniewska-Goclowska, 2011, IUPAC-NIST Solubility Data Series. 91. Phenols with Water. Part 2. C_8 to C_{15} Phenols with Water and Heavy Water, *Journal of Physical and Chemical Reference Data*, **40**, 033103.

Projects Completed:

2010-047-1-500: Mutual Solubility of Phenols with Water.Â Solubility Data Series.

Projects in Preparation:

2007-047-1-500 Nitriles C+3: Binary and Multicomponent Systems, V Sazonov. Valerii Sazonov status: no communication; status unknown; Note—email address given on IUPAC web site for Valerii Sazanov does not work. Information and help from Russian colleagues is needed.

2010-050-1-500: Mutual Solubility of aliphatic and non aliphatic amines with Water. (Solubility Data Series). The volume (3 parts) was sent to JPCRD in June 2012

2011-043-1-500: Solubility data related to Industrial Processes. Solubility data in ternary systems containing water alcohol, and hydrocarbon. This project was discussed in detail during a meeting of Goral, Maczynski and Shaw in Warsaw in February 2012. Compilation and evaluation are underway and the work is progressing well.

New Project:

Proposal for revision of SSED web pages (Task Group: De Visscher, Magalhaes, Salomon and Shaw, Chair) was submitted to the Secretariat in July 2012.