INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
Analytical Chemistry Division
SOLUBILITY DATA COMMISSION (V.8)

Minutes of the 25th Annual Meeting (19th of SDC) to be held in conjunction with the 40th IUPAC General Assembly, at the Freie Universität Berlin, Berlin, Germany August 8 - 10, 1999

The List of Attendees with complete addresses, telephone and fax numbers together with e-mail addresses is attached to these minutes.

1. Introduction of participants

David Shaw, Chairman of Commission V.8., called the meeting to order and welcomed the participants. Attendees were asked to identify themselves and their affiliation. The Chairman welcomed in particular Chiara Milanese, who received the "Franzosini Award 1999".

2. Approval of Minutes of the 24th Meeting held at Bandai Civic Hall, Niigata, Japan

The Niigata Minutes were approved.

3. Other Items for Agenda

Report on the meeting of Titular Members - Monday 9 August 1999 at 12:00 - is scheduled as topic 16.a

4. Announcements by Secretary

The Secretary requests the participants to fill in the attendance list the actual postal and E-mail addresses, fax and phone numbers. The colleagues presently contributing to the activities of Com. V.8 disagree with the members listed in the IUPAC Handbook 1998-1999. An effort will be made to improve the situation before the next edition appears. Contributors to the Commission's activities are requested to provide their text on discs when they want to communicate it via the minutes.

5. Chairman's Report for 1997-1999 - D. Shaw

During this report period the Solubility Data Commission (SDC) has actively continued to pursue its goals of compiling and evaluating published solubility data and fostering international research interest in topics related to chemical solubility.

A new agreement for publication of the Solubility Data Series was negotiated by the SDC with the Journal of Physical and Chemical Reference Data and approved by the Union. Under this agreement publication resumed in mid 1998 after an 18 month interruption. During the first year of this agreement four volumes (the agreed upon number) were submitted:

Vol. 66 Ammonium Phosphates, J. Eysseltová and T.P. Dirkse, editors.

Vol. 67 Aliphatic Halogenated Hydrocarbons in Water: Part II: Halogenated Ethanes and Ethenes with Water, A. Horvath and F.W. Getzen, editors.

Vol. 68 Aliphatic Halogenated Hydrocarbons in Water: Part III: Halogenated Aliphatic Compounds C3-C14 with Water, A. Horvath and F.W. Getzen, editors.

Vol. 69 Ternary Systems Containing Alcohols, Hydrocarbons and Water, A. Skrzecz, A. Maczynski and D.G. Shaw, editors.

Volume 66 has already been published and the remaining three volumes are expected to be published before the end of 1999. Of the four volumes to be submitted between July 1999 and June 2000, Gases in glassy polymers, Yampols'kii and Fogg, eds., has already been submitted. Three additional volumes will be submitted to the publisher by mid 2000.

Negotiations are also underway between the SDC and the US National Institute of Standards and Technology (NIST) concerning electronic dissemination of evaluated solubility data. Although these negotiations are not yet concluded, we are optimistic that the experience of NIST in operating web-based chemical databases can be extremely helpful in making an electronic solubility database a functioning reality.

The SDC continues to organize the International Symposia on Solubility Phenomena (ISSP) with IUPAC sponsorship. These meetings provide opportunities for presentation of original research and the discussion of topics related to solubility. These meetings, held in even numbered years, also provide venues for participants in the work of the SDC to meet and discuss the progress of Commission projects. The Eighth ISSP was held in Niigata, Japan, 5-8 August 1998. Preparations are well underway for the Ninth ISSP to be held in Hammamet, Tunisia, 25-28 July 2000. The Tenth ISSP is tentatively scheduled for Varna, Bulgaria in August 2002.

The SDC has engaged in extensive discussions of its future plans in light of the reorganization of IUPAC scheduled for 2001. The Commission considered three options for its future activities: 1) completion of work in progress by 2001 and disbandment, 2) continuing after 2001 in the present form outside the IUPAC framework, and 3) continuation after 2001 within IUPAC in a form responsive to new structure and mission of the Union. The SDC decided that it is in the best interests of the international scientific community and the participants in the solubility data project to continue within IUPAC in a form which is consistent with the new organization of IUPAC. A proposal to the Union for creation of a new Commission on the Dissemination of Solubility Data was submitted and has received an encouraging

informal response. Efforts are continuing to develop a program of activities and projects related to solubility which is responsive to the new goals of the Union.

6. Editor-in-Chief's Report for 1998-1999 - M. Salomon

1. General comments of the Editor-in-Chief

An agreement with the U.S. National Institute of Standards and Technology (NIST) was concluded in 1998 in which the *Solubility Data Series* will be published in the *Journal of Physical and Chemical Reference Data* (*JPCRD*). For details on the *JPCRD* (publisher, subscriptions, etc.), please refer to The Commission's home page on the internet. Briefly, NIST has agreed to publish four *SDS* volumes per year in *JPCRD*, and in fact one volume (number 66 on Ammonium Phosphates by J. Eysseltová and T.P. Dirkse) has already been published (*JPCRD*, 1998, **27**, 1289-1470). Four more completed volumes are now at the publisher (*JPCRD*) which will be published in 1999. The four volumes are:

Halogenated Ethanes and Ethenes with Water, A. Horvath and F. Getzen, eds.

Halogenated aliphatic compounds C_3 - C_{14} in Water, A. Horvath and F. Getzen, eds.

Ternary Alcohol-Hydrocarbon-Water Systems, A. Skrzecz and D. Shaw, eds.

Gases in Glassy Polymers, Y. Yampol'skii, R. Paterson and P.G.T. Fogg, eds.

The agreement reached with NIST also requires that all volumes prepared by Commission V.8 members be submitted electronically. This is an important requirement as it relates to ease of publication of the *SDS* as well as for future use in electronic dissemination of the *SDS* via the Internet. Finally, there are a number of new formatting procedures to be followed in preparing manuscripts for *JPCRD*, and details are given below.

Prepartion of Manuscripts for *JPCRD*

All manuscripts are initially sent to the Subcommittee Chair. Initial reviews of all materials are the joint responsibility of the Subcommittee Chair and the Editor-in-Chief, and the final review before submission to the Journal of Physical and Chemical Reference Data (JPCRD) is the responsibility of the Editor-in-Chief. For submission to JPCRD, upon approval by the Editor-in-Chief the author(s) can submit the manuscript directly to the Editor of JPCRD. If preferable, the Editor-in-Chief will submit the manuscript to the JPCRD editor. A hard copy (optional) plus an electronic copy of the manuscript should be submitted to:

Editor
Journal of Physical and Chemical Reference Data
Standard Reference Data Program
National Institute of Standards and Technology

Building 820, Room 113
Gaithersburg, MD 20899 e-mail: jpcrd@nist.gov
Telephone: +1 (301)-975-2211
FAX: +1 (301)-926-0416

Page proofs (hard copy) will be sent to both the volume editor and the Editor-in-Chief.

The **Manuscript**, including the abstract, references, and captions should be neatly typed in English, double-spaced, on one side of good white paper with ample margins (both letter size and A4 paper are acceptable as discussed below). It should be carefully proofread by the author. The manuscript must be in good scientific American English; this is the authors' responsibility.

There are two options for formatting manuscripts. Volumes in preparation which employ the original format of separate boxes for Components, Original Measurements, Variables, etc. are acceptable. New manuscripts can use the format proposed by Adam Skrzecz (see the minutes to the 21st meeting held at the University of Surrey, 5-7 August 1995). For reference, attached at the end of these instructions is a page reproduced from Volume 66 of the Solubility Data Series. All manuscripts can be prepared on letter size paper, 8.5 x 11-in (21.6 x 27.9 cm) or on A4 paper (21.0 x 29.7-cm).

Important notes on manuscript preparation: (1) Do not place a line border around the outside of the page or any vertical lines within the body of the data page (see example attached at the end of these instructions). (2) If there are numerous equations (mathematical) please use the word processor's equation format options.

Number all pages in single sequence beginning with the title and abstract page.
The **Title** should be concise but informative enough to facilitate information retrieval. The **Abstract** should be self-contained (contain no footnotes). It should be adequate as an index (giving all subjects, major and minor, about which new information is given), and as a summary (giving the conclusions and all results of general interest in the article). "Part I," or simply "I," will not be included as part of the title of an article unless Part II has already been submitted for publication. Part III, IV,..., etc., are likewise unacceptable unless the prior parts have already been accepted or have appeared in this Journal, and are properly identified in the references.

Author's names should preferably be written in a standard form for all publications to facilitate indexing and avoid ambiguities.

Equations should be neatly typed, punctuated, and aligned to bring out their structure, and numbered on the right. Mathematical operation signs indicating continuity of the expressions should be placed at the left of the second and succeeding lines.

Notation must be legible, clear, compact, and consistent with IUPAC recommendations as given in ***Quantities, Units and Symbols in Physical Chemistry*, 2nd ed.** (The Green Book) or in other official IUPAC recommendations. A few necessary symbols or terms not defined in IUPAC publications can be used; these are described fully in the

Introduction to the Solubility Data Series: Solubility of Solids (Liquids, Gases as appropriate) in Liquids, which is published with each issue of the series.

Superscripts are normally set directly over subscripts; authors should note where readability or the meaning requires a special order. If there is any possibility of confusion, indicate superscripts by a black penciled ~ underneath the superscript and subscripts by a black penciled ' over the subscript.

References and footnotes are treated alike. They must be numbered consecutively in order of first appearance in the text and should be given in a separate double-spaced list at the end of the text material. Reference should be made to the full list of authors rather than to first author followed by an abbreviation such as et al. References within tables should be designated by lowercase Roman letter superscripts and given at the end of the table. The number of a grant or contract is meaningless to our readers and should be omitted unless its inclusion is required by the agency that supports the research.

Tables (with Arabic numerals in the order of their appearance) should be used for all but the simplest tabular material; they should have captions that make the tables intelligible without references to the text. The structure should be clear, with simple column headings giving all units. Unaltered computer output and notation are generally unacceptable.

Note that use of tabs to align tables is not acceptable since this creates problems for the publisher in processing tabular materials. Tables should always be prepared by using the "insert table" function of your specific word processor: i.e., place the numeric data in the tables inside the word processor's table format

Illustrations: Illustrations published in JPCRD are either scanned by AIP using a digital scanner or received electronically from the author, and integrated with the text of the article, creating completely electronic pages. To receive optimal quality, we strongly encourage you to send electronic graphics files rather than laser output. (Note: if you are submitting electronic graphics files, you are still required to send PUBLICATION QUALITY hardcopies of the figures to the Editorial Office. Adherence to electronic submission instructions is important.

Note that all figures are numbered sequentially throughout the entire manuscript.
Please adhere to the following guidelines when preparing your illustrations for submission:

While the publisher will scan figures, it is preferable that all graphics be submitted as electronic files. See below for preparation of illustrations and figures:

Sizing illustrations, Electronic Graphics Files and Hardcopy.
- **Prepare hardcopy illustrations in the final published size, not over-sized or undersized.** Size your illustrations accordingly. Submit each illustration at the final size in which it will appear in the journal. The standard is 8.573 cm maximum width for one column. This is especially important for screened or shaded illustrations; reduction

of screened/shaded originals during the digitizing process introduces an unacceptable moiré pattern.
- **Ensure a minimum of 8-point type size and 1-point line width within illustrations.** Ensure that line weights will be **0.5 points** or greater in the final published size. **Line weights below 0.5 points will reproduce poorly.** Avoid inconsistencies in lettering within individual figures, and from one figure to the next. Lettering and symbols cannot be handwritten. Avoid small open symbols that tend to fill in if any reduction is necessary.

Preparation of Hardcopy Illustrations for Scanning
- **Number figures in the order in which they appear in text.**
- **Place only one figure per page including all parts.** Place all parts of the same figure on one sheet of white bond paper, spaced 1/4 in (0.635 cm) apart, using a glue stick or wax on the back of the illustration and leaving a 2 in (5.08 cm) bottom margin. Label all figure parts with (a), (b), etc. Make sure each figure is straight on the page. Photocopies of artwork are not acceptable.
- **Do not use correction fluid or tape on illustrations.** The scanner is extremely sensitive and reproduces all flaws (e.g., correction fluid, tape, smudges, dust). Do not write on the back of the figure because it will be picked up by the scanner.
- **Authors' laser-generated graphics are acceptable only if the lettering and lines are dark enough, and thick enough, to reproduce clearly,** especially if reduction is required. Maximum black-white contrast is necessary. Choose a laser printer with the highest dot-per-inch (dpi) available (i.e., the highest resolution possible). Remember that fine lines in laser-generated graphics tend to disappear upon reduction, even if the oversized original looks acceptable.
- **Submit continuous-tone photographs in final published size on white glossy or matte paper.** Avoid glossy paper stock that is off-white, ivory, or colored because contrast within the illustration will be lost in reproduction. Print the photograph with more contrast than is desired in the final printed journal page. Avoid dull, textured paper stock, which will cause illustrations to lose contrast and detail when reproduced.

Preparation of Electronic Graphics Files
- We recommend that all halftone art (screened art), shaded figures, and combinations (line art 1 halftone) be submitted electronically. Computer-generated illustrations output to desktop laser printers produce a screen. These figures are most problematic in the scanning process, because scanning screened output produces an unacceptable moiré pattern.
- **Acceptable formats:** Graphics must be submitted as PostScript, EPS (using either Arial or Times Roman fonts), TIFF (lzw compressed), GIF or JPEG. Do not send application files, e.g., Corel Draw, SigmaPlot, etc.
- **Settings:** Set the graphic for **600 dpi** resolution for line art, **264 dpi** for halftones (noncompressed), and **600 dpi** for combinations (line art 1 halftone). Save the files to grayscale (B/W), not color.
- Make sure there is only ONE figure per file. Each figure file should include all parts of the figure. For example, if Figure 1 contains three parts (a, b, c), then all of the parts should be combined in a single file for Figure 1.
- You are still required to send hardcopies of all figures to the Editorial Office, along with a hardcopy of the manuscript.

Compuscripts: AIP is accepting author-prepared computer files for use in production. If you have used REVTeX, LaTeX, Microsoft Word or WordPerfect to compose your manuscript, AIP may be able to use your file to produce author proofs. AIP uses translation software to convert REVTeX, LaTeX, MS Word or WordPerfect files into Xyvision composition files for production.

Checklist: Use this checklist to avoid the most common mechanical errors in submitted manuscripts.

1. The manuscript should be double-spaced.
2. Number all pages in sequence.
3. Type title, abstract, and key words on a separate first page.
4. Number tables, figures, and references starting with 1.
5. Use IUPAC-recommended quantities, units and symbols properly, including use of italics for physical quantities, Roman type for units, and quantity calculus (algebra of quantity) in table headings and labels for graphs.
6. Submit (a) one clear copy with clear copies of figures and (b) the original figures. An electronic version of all figures is highly recommended:
7. The original figures must be clear line drawings or high-contrast, identified by figure number.

Components

(1) Ammonium dihydrogenphosphate; $NH_4H_2PO_4$; [7722-76-1]
(2) Methionine; $C_5H_{11}NO_2S$; [59-51-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Amilova, B. M. Beglov, B. S. Zakirov, Kh. Kucharov, Zh. Neorg. Khim. **30**, 1342-3 (1985).

Variables:

Temperature and composition.

Prepared By:

J. Eysseltová

Experimental Data

Crystallization temperatures in the $NH_4H_2PO_4$–methionine–H_2O system

$NH_4H_2PO_4$		methionine		H_2O		Solid
$100w_1$	m_1/mol kg^{-1} [a]	$100w_1$	m_1/mol kg^{-1} [a]	$100w_1$	t/°C	phases[b]
33.7	4.47	0.8	0.08	65.5	41.6	A+B
32.5	4.19	0	0	67.5	33.0	A+C
31.1	3.96	0.7	0.07	68.2	34.6	A+C
30.6	3.88	0.9	0.09	68.5	35.0	A+B+C
25.7	3.06	1.2	0.11	73.1	24.6	B+C
18.7	2.03	1.4	0.12	79.9	4.2	B+C
18.0	1.91	0	0	82.0	4.3	C+D
17.9	1.91	0.8	0.07	81.3	−4.4	C+D
17.8	1.92	1.5	0.12	80.7	−4.5	B+C+D
16.8	1.79	1.5	0.12	81.7	−4.2	B+D
9.8	0.96	1.6	0.12	88.6	−2.2	B+D
0	0	1.7	0.12	98.3	−0.1	B+D

[a]The mol/kg H_2O values were calculated by the compiler.
[b]The solid phases are: A = β-$NH_4H_2PO_4$; B = methionine; C = α-$NH_4H_2PO_4$; D = ice.

Auxiliary Information

Method / Apparatus / Procedure:

A visual polythermic method was used.[1]

Source and Purity of Materials:

Pure methionine and reagent grade $NH_4H_2PO_4$ were recrystallized before being used.

Estimated Error:

No information is given.

References:

[1]A. G. Bergman, N.P. Luzhnaya, Fiziko-Khimicheskiye Osnovy Izucheniya i Ispol'zovaniya Solyanykh Mestorozhdeniy Khlorid-Sul'fatnogo Tipa, Moscow IAN SSSR (1951).

Components

(1) Ammonium dihydrogenphosphate; $NH_4H_2PO_4$; [7722-76-1]
(2) Triethylamine hydrochloride; $C_6H_{16}ClN$; [554-68-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

1. S. A. Mazunin, O. E. Sosnina, A. A. Volkov, T. L. Danina, Termicheskiy Analiz I. Fazovye Ravnovesiya, Perm, 79-88 (1985).
2. O. E. Sosnina, A. A. Volkov, Uch. Zap. Perm Gos. Univ., Ser. Khim. **289**, 20-5 (1973).

Variables:

Composition at 20 and 60 °C.

Prepared By:

L. V. Chernykh and J. Eysseltová

Experimental Data

Solubility isotherms in the $NH_4H_2PO_4$ – $(C_2H_5)_3N$·HCl – H_2O system

$NH_4H_2PO_4$		$(C_2H_5)_3N$·HCl		H_2O	Refract.	Solid
$100w_1$	m_1/mol kg^{-1} [a]	$100w_1$	m_1/mol kg^{-1} [a]	$100w_1$	index[b]	phase[c]
			temp = 20 °C			
27.2[d]	3.25	—	—	72.8	1.3700	A
17.6[e]	2.19	12.4	1.33	70.0		A
15.1[d]	1.82	12.7	1.33	72.2	1.3775	A
8.8	1.2	27.4	3.24	63.8	1.3905	A
6.5	0.97	35.0	4.51	58.5	1.3995	A
2.6	0.42	43.8	6.16	53.6	1.4115	A
1.2[e]	0.24	55.2	9.54	43.6		A+B
—	—	57.2	10.1	42.8	1.4295	B
			temp = 60 °C			
—	—	64.0	13.4	36.0		B
3.3	0.80	61.0	12.9	35.7		B
4.1	1.0	60.2	12.7	35.7		A+B
5.5	1.1	52.5	9.42	42.0		A
9.8	1.7	40.7	6.19	49.5		A
13.0	2.11	33.5	4.72	53.5		A
19.0	2.95	25.1	3.38	55.9		A
30.3	4.69	13.5	1.81	56.2		A
38.4	6.07	6.6	0.90	55.09		A
45.2	7.17	—	—	54.8		A

[a]The mol/kg H_2O values were calculated by the compilers.
[b]The refractive indices are given in source paper[2] only.
[c]The solid phases are: A = $NH_4H_2PO_4$; B = $(C_2H_5)_3N$·HCl.
[d]These data are given in source paper[2] only.
[e]These data are given in source paper[1] only.

Auxiliary Information

Method / Apparatus / Procedure:

The refractometric variation of the isothermal method was used. The compilers assume that it was the method described elsewhere.[1] $NH_4H_2PO_4$ was determined by potentiometric titration. The compositon of the solid phase was determined by the Schreinemaker's method.

Source and Purity of Materials:

Reagent grade $NH_4H_2PO_4$ and pure $(C_2H_5)_3N$·HCl were recrystallized before being used.

Estimated Error:

The $NH_4H_2PO_4$ content has a precision of ±0.2%.

References:

[1]E.F. Zhuravlev, A.D. Sheveleva, Zh. Neorg. Khim. **5**, 2630 (1960).

7. Publication agreement and future collaborations with NIST - J. Rumble

NIST Standard Reference Data and The IUPAC Solubility Project
John Rumble, Jr., NIST, john.rumble@nist.gov

NIST Standard Reference Data Program
To make critically evaluated reference data available to scientists, engineers, and the general public

NIST Standard Reference Data Program
- Critical Evaluation of Data
- Areas of Coverage
- Dissemination of Databases and Publications
- NIST and IUPAC

NIST Standard Reference Data Program
- Data users are not experts on how data were generated and do not know the quality of the data as published
- NIST Standard Reference Data Program has subject experts collect and evaluate data and issue them with quality indicators
- NIST Standard Reference Data Program established by Congress in 1968

Critical Evaluation of Data
The Process
- Collect data from published literature
- Review and evaluation by expert scientists
- Design databases and publications to meet users needs
- Disseminate widely to industry, academia, government

How do you evaluate data?
- How well are data documented with respect to their generation?
  - Have all relevant factors been controlled?
  - How has that been demonstrated?
- How do data follow known laws of nature?
- How do data compare to other measurements (calculations) of the same phenomena?

Technical Areas
- Analytical chemistry
- Thermodynamics and thermophysics
- Chemical kinetics
- Atomic and molecular physics
- Ceramic materials
- Crystallographic structure
- Surface analysis
- Alternative refrigerants
- Fundamental constants
- Biotechnology
- Materials degradation

- Fluid properties
- Electronic materials
- Software recognition
- Fire performance of materials
- Statistical reference datasets
- Digital library of mathematical functions

How Data Work Is Done?
- Long term data centers, primarily at NIST
- Short term data projects, often drawing on outside experience
- Joint projects with industrial, national, and international groups
- Coordination to minimize duplication of efforts

Different types of IST SRD Databases
- Online information systems including Internet
- Incorporated directly in analytical instruments
- Self-contained PC packages
- As part of larger commercial software packages
- Files for loading into in-house systems
- Correlation software to predict properties
- Electronic Journal of Physical and Chemical Reference Data (soon)

Journal of Physical and Chemical Reference Data
- First published in 1972
- Now on volume 29
- Joint venture with American Institute of Physics (AIP) and American Chemical Society
- Next year just with AIP
- Malcolm Chase, Editor in Chief
- About 1800 to 2000 pages printed each year
- Only journal to publish complete tables of evaluated data

Journal of Physical and Chemical Reference Data
Plans for an electronic Journal
- In 2000, full text online
- In 2001 , electronic database, searchable by substance and property
- Will then reduce size of full text online articles, links to databases for figures and graphs
- Printed Journal will continue as long as demand exists
- After three years, data will be available in other NIST online systems

NIST and IUPAC V.8
- Several components to partnership
  - Publication of SDS
  - Grants to support manuscript preparation
  - Building a online system of all still valid solubility data
  - CD-ROM is possible if demand exists
- Will include strong identification with IUPAC

- NIST online systems have, a wide variety of data, with 10000s users per month
- Online Handbooks of the Future

JPCRD and SDS
- Solubility Data Series a welcomed partnership
- Transition period should end in 12-18 months
- Will review guidelines in detail later today in smaller groups
- Flexibility with understanding is key
- Look forward to long relationship

JPCRD and SDS
- Goal to have all electronic manuscripts
- Figures and graphs should be electronic to reduce costs
- Must conform to JPCRD and IUPAC styles
- Prefer Word, WordPerfect, others are acceptable
- Keep reformatting to minimum
- Page borders, should not be included

NIST and IUPAC
A great partnership serving the chemistry and chemical engineering communities

8. **Status Report on Book on Experimental Methods for the Determination of Solubilities - R. Tomkins**

INTRODUCTION

A textbook entitled: THE EXPERIMENTAL DETERMINATION OF SOLUBILITIES was initiated in 1990 by G. Hefter and C Young. The purpose of the textbook was to present a broad coverage of the different methods used for determining solubilities of gases, liquids and solids. Although the focus was on experimental aspects, sufficient theoretical background was given where appropriate.

Various contributors who were experts in the field, were solicited. However, because of altered circumstances, the failure of some to meet deadlines or the Editors' requirements, a number of changes in personnel have occurred. The list of those who are currently participating in the project is given below together with their topics.

Preface Hefter

Introduction (Lorimer)

Chapter 1 Fundamentals of Solubility
1.1 Thermodynamics of Solubility (Lorimer and R. Cohen-Adad)
1.2 Kinetics of Dissolution and Precipitation (Christoffersen)

Chapter 2 Gases
2.1 Low pressure gases in liquids (Clever/Battino)
2.2 High pressure gases in liquids (Aim)
2.3 Gases in polymers (Yampolski/Paterson)
2.4 Gases in molten salts and molten metals (Tomkins)
2.5 Gases in solid metals (Lewis/Sakamoto)

Chapter 3 Liquids (Hefter)

Chapter 4 Solids
4.1 Solids in liquids (P. Cohen-Adad/M.-T. Cohen-Adad)
4.2 Sparingly soluble solids in liquids (Gamsjaeger/Koenigsberger)
4.3 Aqueous Systems at high temperatures and pressures (Valyashko/Churagulov/Kravchuk/Mather)
4.4 Solids in molten and solid metals (Borgstedt/Guminski)
4.5 Solids in solids (Sangster)

Chapter 5 Special Systems

5.1 Solids and liquids in supercritical fluids (Aim/Fermeglia)
5.2 Solids and liquids in cryogenic liquids (Szczepaniec-Cieciak)
5.3 Polymers in liquids (Krause)

During the period 1990-1993 first drafts of most chapters were received.

Hefter and Young reviewed the draft chapters and sent their comments back to the contributors for further revision. In most cases second drafts were submitted but because of competing demands for the Editors' time and various other reasons little further progress was made.

Due to the lack of progress and the need to complete the text in a timely fashion, R-Tomkins was asked by the Commission to assist with future editorial aspects.

During the period 1998 to the present, Tomkins has been involved in gathering all the material that was available. This was achieved by contacting all the contributors and currently except for chapters 1.2, 2.2 and 3 all the material has been assembled without any further editing.

The following represents the current status of the text:

Preface	Hefter	Submitted
Introduction	Lorimer	Not submitted
1.1 Thermodynamics	Lorimer/Cohen-Adad	¾ of first draft submitted, no review
1.2 Kinetics	Christoffersen	Not submitted Promised for March 1, 2000

2.1 Low Pr. gases	Clever/Battino	2nd draft submitted -basically complete
2.2 High Pr. gases	Aim	not submitted
2.3 Gases in polymers	Yampolski/Paterson	Reviewed- minor comments
2.4 Gases in Molten Salts	Tomkins	-2' draft submitted -minor revisions needed
2.5 Gases in Solid Metals	Lewis/Sakamoto	-no major changes needed
3. Liquids	Hefter	Promised for April 1, 2000
4.1 Solids in Liquids	Cohen-Adad/Cohen-Adad	2' copy submitted- reviewed by Lorimer
4.2 Sparingly Soluble Solids in Liquids	Gamsjäger/Königsberger	3' revision needed after Lorimer comments
4.3 Aqueous Systems at high temps & pr.	Valyashko/Kravchuk	1st draft reviewed
4.4 Solids in molten and solid metals	Borgstedt/Guminski	Minor changes needed
4.5 Solids in solids	Sangster	no changes needed
5.1 Solids/liquids in supercritical fluids	Fermeglia	First draft submitted
5.2 Solids/liquids in cryogenic liquids	Szczeparnec-Cieciak	several drafts submitted
5.3 Polymers in liquids	Krause	Minor revisions needed

UPDATE

1. Dr. Christoffersen (Denmark) has agreed to send in the chapter on "Kinetics of Dissolution and Precipitation by March 1, 2000.

2. Dr. Glenn Hefter has committed to have his first draft on Liquid Solubilities by April 1, 2000.

3. Dr. Aim has been invited to write the chapter on "High Pressure Gases in Liquids" but no correspondence has been received to date.

4. Professor Lorimer has submitted a section on Physico-Chemical Quantities and Units for the Chapter on Thermodynamics of Solubility.

5. R. P. T. Tomkins in collaboration with G. Hefter, J. Lorimer and D. Shaw has sent a proposal for the publication of the text to Wiley.

6. R. P. T. Tomkins and G. Hefter have agreed to work on the final editorial action needed to complete the manuscript. G. Hefter has a copy of the latest draft of the manuscript which was delivered to him in Berlin.

7. All authors will need to update their manuscripts to reflect the literature between 1990-2000.

8. The manuscript should be completed by September 2000.

9. **Chemicals in the Atmosphere - Solubilities in Aqueous Media - P. Fogg**

This project originated from contacts between members of the Solubility Data Commission and Prof. Warneck of the Atmospheric Chemistry Commission at the IUPAC General Assembly in Hamburg (1991) and Lisbon (1993) when ways in which the two commissions could co-operate were discussed. At a meeting of the Solubility Data Commission in Buenos Aires in 1994 it was agreed that the Solubility Data Commission should proceed with a project involving the solubility of gases in aerosols.

The help was enlisted of Dr Simon Clegg of the School of Environment Sciences, University of East Anglia. A draft proposal defining the scope of a project involving the presentation of data with a description of the theoretical and experimental background was prepared by Dr Peter Fogg, Chairman of the Subcommittee on Gas Solubilities. This proposal was presented to a joint meeting with the Atmospheric Chemistry Commission during the IUPAC General Assembly in Guildford (1995). It was agreed that Simon Clegg should take editorial responsibility for the project with Peter Fogg having a managerial role. It was agreed that the project should be submitted to IUPAC by the Solubility Data Commission with the title Chemicals in the Atmosphere - solubilities in aqueous media.

Simon Clegg recruited various atmospheric chemists to help with the project and the original details were elaborated following interchanges of emails. In 1996 Peter Fogg submitted the proposal to IUPAC for approval . The condition for approval was that the project should lead to a publication and that a contract for publication should be agreed.

The matter was discussed with Dr Mo Williams, then Executive Secretary of IUPAC, who found that Blackwells, the official IUPAC publisher were not interested in the

project. Other possibilities were considered and eventually it was informally accepted by Wiley as a volume in Wiley Series in Solution Chemistry for which Peter Fogg is Series Editor. Mo Williams gave Peter Fogg responsibility for negotiating the details of the contract with Wiley and signing the contract on behalf of IUPAC. It was also agreed that Peter Fogg's name should be on the contract as editor but, in this context, he could delegate editorial responsibility to whomsoever he chose. It was also agreed that œ1000 of advance royalties should be given to contributors on delivery of the manuscript and that this money should be distributed through the Solubility Data Commission. It was also agreed that the manuscript should be completed by May 1998. As the contract was non-standard there was considerable delay before the formal contract was available for signature. The contract was eventually signed in April 1997.

Various contributions to the book were received from the atmospheric chemists who were assisting Simon Clegg but these contributions were insufficient to produce a satisfactory volume for Wiley Series in Solution Chemistry. In late 1997 Peter Fogg became seriously concerned at the apparent lack of progress and began to prepare compilations and evaluations of appropriate data. In January 1998 Simon Clegg found that he could not continue as volume editor because of pressure of other duties. He sent a circular to all collaborators requesting that any further contributions should be sent directly to Peter Fogg who assumed full responsibility for the book.

Dr Fogg has a formal commitment to Wiley for completion of the volume, both as signator of the contract for the book and as Series Editor. Wiley have been willing to extend the deadline for a limited period. Peter Fogg has arranged to co-edit the book with Dr James Sangster who has experience in data collection, presentation and publication. James Sangster has also written one of the volumes already published in Wiley Series in Solution Chemistry.

A useful set of literature references was provided by Prof. Werner Hauthal. These have been supplemented following a detailed survey of the appropriate literature. An extensive data base with details of papers containing relevant data or descriptive material is now available. This is kept up to date by a personal link by Internet with the British Library. Details of papers, and in many cases abstracts, from appropriate journals and conference publications can be downloaded as they are received by the library. Solubility data for almost all of the species agreed by Simon Clegg to be of special interest to atmospheric chemists have now been collected. Data for additional species related to solubility equilibria in the environment will also be included. Progress has been made in the preparation of descriptive chapters. These will be sent by Peter Fogg and James Sangster to appropriate workers in the field for comments and elaboration.

The progress of the project was reported to the IUPAC Atmospheric Chemistry Commission during the IUPAC General Assembly in Berlin (August 1999). This Commission gave full approval and offered help as and when required by Peter Fogg and James Sangster.

10. Project: Solubilities of Salts in Seawater - J. Lorimer

Prof. Lorimer met with Dr. David Turner, the IUPAC representative on SCOR, during the General Assembly, and assured him that: (a) the proposal of the Oceanic Salts Working Group for cooperation with SCOR was still valid in the form presented previously (minutes of Commission V.8, Niigata, 1998); (b) the Working Group would continue with their activities even if there is no involvement with SCOR, but that cooperation with SCOR would seem to be a desirable project involving both IUPAC and ICSU committees. Dr. Turner reported that the proposal of the Oceanic Salts Working Group is on the agenda for the meeting of the SCOR Executive in India in October. He also indicated that he would try to talk with individual members of the SCOR Executive before their meeting.

11. Teaching of undergraduate students: Experimental and theoretical aspects - C. Magalhaes

Clara Magalhaes plans to write a book on teaching solubility phenomena to undergraduates. Colleagues who use simple and illustrative experiments on solubility phenomena in the classroom are requested to communicate with Clara.

12. IUPAC Congress in Brisbane in 2001

Seminar Topic: Medical aspects of solubility

E. Koenigsberger proposed a symposium on medical aspects of solubility to be held at the IUPAC 38th Scientific Congress in Brisbane 2001. Prof. Robert G Gilbert, Co-Chair, Scientific Program, stated that this proposal was not approved and suggested instead a satellite meeting in or around Brisbane. This was considered inpracticable as none of the co-organisers is local. An alternative also suggested by Prof. Gilbert would be to submit papers within theme (c) or (a) subtheme Biomaterials.

(a) Materials chemistry for the future
Materials chemistry in confined systems
Supramolecular chemistry
Biomaterials
Spectroscopy, optoelectronics, energy production and storage
Combinatorial methods for novel materials and devices
Novel polymeric and composite materials

(c) Challenges for Drug Discovery and Development in the 21st Century
- joint with AIMECS 01 Target Discovery Libraries and Screens

Molecular Design Molecular Development New Vistas in Therapy

published in journals of high impact externally referred for the work of IUPAC to gain a wide audience.
Therefore, we propose to write a critical review on the thermodynamics of crown ethers (mainly 18-crown-6) and metal cations. Journals to be targeted are : Chem.Rev. or Chem.Soc.Rev., both of which have a high impact factor although the former has the higher.

Background work:

1. Thermodynamics of calixarene chemistry
A. Danil de Namor et al., Chem.Rev., 1998
The work of the commission is quoted at the end, excluding

2. Thermodynamics of cryptands and their metal in complex
A. Danil de Namor and Y. Marcus, Rev.Chem. submitted in October 1999

Description of the volume:

Title: Thermodynamics of crown ethers (18-crown-6) and their metal ion complexes. Contents Part 1
Authors: Prof. Angela F. Danil de Namor, chairman
Prof. Takeda, Prof. Sawada, Dr. M. Salomon, Dr. S. Katsuta, Prof. A. D'Aprano

Content
1. Introduction
2. Solution thermodynamics of crown ethers
   2i. Gibbs Energies of solution. Solubility measurements
   2ii. Enthalpies and entropies of solution
3. Thermodynamics of complexation
   3i. Stability constants of crown ethers and metal cations. Derived standards, Gibbs energies (Takeda, Sawada and Katsuta)
   3ii. Enthalpies and entropies of complexation. Heat capacity measurements.
4. Solution thermodynamics of metal ion complex salts
   4i Gibbs energies of solution
   4ii Enthalpies and entropies of solution
5. Computer modelling studies (M. Salomon and S. d'Aprano)
6. Enthalpies of coordination
7. Final conclusions
8. Future work
9. References

14. Report on the 9th ISSP to be held in Hammamet, Tunisia July 25 - 28, 2000

Complete information on the 9th ISSP is found in the 2nd Circular and on the website (http://www.unileoben.ac.at/~eschedor/meetings.html).

15. **Future International Symposia on Solubility Phenomena**

2002: 10th ISSP, Varna - Bulgaria

A provisional invitation for the 10th ISSP has been made by Christo Balarew. The venue envisaged is Varna (Bulgaria).

Call for Proposals of Future ISSPs

2004: 11th ISSP:

A provisional invitation has been announced by Angela Danil de Namor: Venue - Crakov (Poland).

2006: 12th ISSP:

A provisional invitation has been announced by Clara Magalhaes: Venue - Aveiro (Portugal)

16. **Reports of National Representatives**

No report

16.a Report of the Meeting of Titular Members

For the term 2000/2001 the following colleagues agreed to serve as

Titular Members of Com. V.8:

D.G. Shaw (CC), H. Gamsjaeger (CS), A. Skrzecz, V.M. Valyashko, P. Scharlin

Associate Members of Com V.8:

B.R. Churagulov, J. Eysseltova, J. Vanderdeelen, W. Voigt, Y.P. Yampol'skii, C. Guminski, E. Koenigsberger, C. Magalhaes, K. Sawada, V. Sazonov, M. Gaune-Escard, Ch. Balarew

National Representatives of Com. V.8:

C.B. Melios (Brazil), W. Wang (China), E.W. Waghorne (Ireland), A. Danil de Namor (UK), N. Kbir-Ariguib (Tunisia)

17. **26th Annual Meeting (20th of SDC) to be held in conjunction with the 9th ISSP, Hammamet, Tunisia, July 23-24, 2000**

The meeting of IUPAC Commission on Solubility Data (V.8) will be held on July 23-24, 2000 at Grand Palais des Congrès, Hammamet, Tunisia.

18. **Adjournment**

The meeting was adjourned at 12:05, August 10, 1999.