



International Union of Pure and Applied Chemistry

A member of the International Council of Scientific Unions

Analytical Chemistry Division: Commission on Solubility Data (V.8)

November 27, 1995

Dear Colleague:

I enclose the minutes of the 21st IUPAC Commission V.8 Meeting which took place at the University of Surrey, Guildford, UK, August 5-7, 1995. In addition, there are attached summary minutes of the subcommittee meetings, together with other important information relevant to our activities..

The 22nd meeting of the IUPAC Commission V.8 will take place on July 20-21, 1996 at Montanuniversität, Leoben, Austria.

We look forward to seeing you at the next meeting.

Sincerely,

Reginald P.T. Tomkins

*Reginald P.T. Tomkins
Secretary*

*RPTT/ps
Enclosures*

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MINUTES OF THE 21ST ANNUAL COMMISSION V.8 MEETING

HELD AT THE UNIVERSITY OF SURREY, GUILDFORD, U.K.

ON

AUGUST 5-7, 1995

SECTION I. DISCUSSIONS OF THE FULL COMMISSION

A. LIST OF ATTENDEES:*

H. AKAIWA, (JAPAN)
C. BALAREW, (BULGARIA)
M. BECK, (HUNGARY)
S. CLEGG, (UK)
H.L. CLEVER, (USA)
M-Th. SAUGIER-COHEN ADAD,
(FRANCE)

R. COHEN-ADAD, (FRANCE)
A. F. DANIL DE NAMOR, (UK)
A. D'APRANO, (ITALY)
T. P. DIRKSE, (USA)
J. EYSSELTOVÁ, (CZECH REPUB)
P. G. T. FOGG, (UK)
H. GAMSJÄGER, (AUSTRIA)
F. W. GETZEN, (USA)
A. GOTO, (JAPAN)
E. GRYZLOVA, (RUSSIA)
C. GUMINSKI, (POLAND)
G. HEFTER, (AUSTRALIA)
Y. HORIBE, (JAPAN)
J. B. JENSEN, (DENMARK)

S. JOHNSON, (UK)
N.KBIR-ARIGUIB, (TUNISIA)
N. KOZYREVA, (RUSSIA)
J. W. LORIMER, (CANADA)
C. MACYNSKI, (POLAND)

C. MAGALHÃES, (PORTUGAL)
H. MIYAMOTO, (JAPAN)
V. MYASOEDOVA, (RUSSIA)
M. PALMER, (UK)
M. SALOMON, (USA)
J. SANGSTER, (CANADA)
K. SAWADA, (JAPAN)
P. SCHARLIN, (FINLAND)
D. G. SHAW, (USA)
A. SRZECZ, (POLAND)
Y. TAKEDA, (JAPAN)
R. P. T. TOMKINS, (USA)
V. VALYASHKO, (RUSSIA)
J. VANDERDEELEN, (BELGIUM)
J. S. VELARDE, (UK)
W. VOIGT, (GERMANY)
E. WAGHORNE, (IRELAND)
C. YOUNG, (AUSTRALIA)

****Complete addresses, telephone and fax numbers, together with E-mail addresses are attached to these minutes.***

IN MEMORIAM

The Commission has recently been informed of the untimely death of Dr. J. Birger-Jensen, a long time active member of the Commission. At the time of his death, he was a professor at the Technical University of Denmark. Professor Jensen passed away on October 20, 1995 at the age of 58. Over the past twelve years Birger was a good friend and colleague and his scholarly contributions to the work of the Commission will be sorely missed. The Commission expresses its sincere sympathy to all Dr. Birger-Jensen's family. A memorial notice will be placed in a future issue of Chemistry International.

B. Approval of Minutes and Agenda

Mark Salomon, Chairman of Commission V.8, called the meeting to order. Attendees were asked to identify themselves and their affiliation. The minutes of the 20th Commission meeting held at Buenos Aires, Argentina were approved subject to a minor correction on page 16 (solid-liquid Subcommittee Report). Project NO 33/91 should read Alkali Metal and Project NO TS 12/87 should read Metals in Liquid Alkali Metals. The proposed Agenda (copy attached) for the meeting was approved with the addition of two items in the Editor-in-Chief's report, namely

- article for Chemistry International on Strategy of the SDP
- New Guidelines - printed, or on diskette?

C. Report of the Chairman (M. Salomon)

Dr. Salomon commenced his report by noting the concern within IUPAC that many of the current activities lacked relevance. Projects focusing on societal problems such as the Environment are now favored. In addition, there is concern about the longevity of some of the projects. Commission V.8 has some projects which were initiated ten years ago and unless there are special circumstances, such projects will be eliminated.

Regarding the membership of the Commission, Dr. Salomon announced that the number of Titular Members has been reduced from six to five in order to accommodate Titular Membership in special IUPAC projects. Dr. Salomon also indicated that voting rights were now extended to Associate Members as well as Titular Members.

Next, Dr. Salomon reported that a new assessor has been appointed to review the work of Commission V.8. He is Professor R. Van Grieken, University of Antwerp, Belgium and is a member of the Division Committee.

Professor Van Grieken, in his assessment for the work of the Commission for the period 1994-1995 felt that the overall output of the Commission was very good even though the membership was about 60. He did note the minimal progress made with some of the listed volumes.

Dr. Salomon then reviewed the Status of the Commission Projects. Essentially, the current status is reflected in both the minutes of the meeting in Buenos Aires and the

Sub-Committee reports which are appended to the minutes of this meeting and also highlighted in the Editor-in-Chief's report. (see later)

The Chairman then led a discussion on the use of E-Mail for draft and CRC materials. Contributors were encouraged to make more extensive use of E-Mail for submitting draft materials to volume editors. The turn-around time for comments and suggestions on draft materials is much faster and less expensive than the use of traditional methods of communication. Where possible, manuscripts should be sent via INTERNET with coded attachments. Copies of BINHEX coding software are available from Dr. Salomon. The use of MIME to transmit either word processing or graphics files was another possible method. The final outcome of the discussion was that the use of E-Mail should be left to the individuals and was not adopted as a policy as yet.

Dr. Salomon then discussed a recommendation on the use of standard word processing programs for the preparation of the SDS volumes. Common word processing programs such as Microsoft Word 2.0 or higher, and Word Perfect 5.x or higher were recommended. Dr. Salomon indicated several advantages of implementing this requirement viz:

- easier to review manuscripts as only floppy discs need be mailed
- it would speed up and restore efficiency in the reviewing process
- it could be added to an archive of all data and volumes for future reprinting and/or integration into some form of database.

During the course of discussions, it was recommended that if standard word processing programs were to be used, it was important to provide implicit instructions on their use in order to avoid time wasting in decoding.

It was pointed out that Oxford University Press has the capability of handling a variety of software packages but for the time being, their preference was to receive a hard copy for the CRC.

The Commission entertained a proposal from Andrzej Maczynski and Adam Skrzecz, who in conjunction with David Shaw, have perfected a fairly simple method for archiving data as ASCII files (floppy book format) which can be used in a variety of ways. One use is to produce data sheets directly from the archived data, and Adam Skrzecz promised to make the program available to members of the Commission by October 1995. The Commission agreed that this method was attractive and would like to phase it in to supersede all previous computer-based methods. In addition to the archival route, a proposed major modification of the format of the data sheets will result in a further compression of the material and easier editing. This modification consists of replacing the present two-column boxes with single-column boxes. The Commission approved use of this new format, realizing that it would be phased in over a period of time, particularly as there exist numerous data sheets which have been produced in camera-ready form using the old lay sheet method. This revised format was subsequently approved by Oxford University Press, and the new format is preferred whenever an entire volume can be produced using it.

Dr. Salomon then addressed the topic of possible funding for the projects. Currently funding for our activities is very limited. The Commission did receive ICSU support for the preparation of the textbook on experimental methods. Topics involving issues of the environment, health sciences and agriculture were areas for consideration by such agencies as UNESCO. Interdisciplinary projects are given priority. Members were encouraged to continue efforts in seeking funding especially in collaboration with industry.

The Franzosini Award

Dr. Salomon announced that the recipient of the award for 1995 was Mr. Jose Sueros Velarde, a student working under the direction of Dr. Angela Danil De Namor in the Thermochemistry Laboratory at the University of Surrey at Guildford. Mr. Velarde is originally from Peru. The Commission offered its congratulations to Mr. Velarde.

D. Report of the Editor-in-Chief (J. W. Lorimer)

Status of Volumes

Professor Lorimer first reported on the volumes which were published/submitted by Oxford University Press(OUP) in 1995 (Volumes 58-61). He also outlined the production schedule for volumes 62-65 and noted tentative titles for volumes 66-68. This information is summarized in detail as an Appendix.

Payment Policies for Volumes

Professor Lorimer reiterated the payment policies for volumes viz: a payment of GBP 1000 (USD 1500) per volume arranged by the Chairman in consultation with the Volume Editors.

Sales of Volumes

The Editor-in-Chief then summarized the sales figures for 1994 indicating that there were only 53 subscriptions. Melinda Palmer (OUP) gave a breakdown of these subscriptions as follows: 5 (UK), 15 (Europe), 16 (USA), 10 (Japan), 7 (Rest of World).

For 1995, Ms. Palmer indicated that to date there were 26 subscriptions (3 (UK), 4 (Europe), 11 (USA), 5 (Japan), 3 (Rest of World). Individual sales for 1994 were as follows:

Vol 54	33
Vol 55	33
Vol 56	33
Vol 57	16
Vol 58	1

Oxford University Press reported an overall loss of GBP 1442 for 1994. Subscription prices for 1996 will be GBP 280, an increase from GBP 265 but for 1 volume will remain the same at GBP 80.

Publicity

Expressing concern over the reduction in the number of subscriptions, Professor Lorimer led a general discussion on publicity of the SDS and related activities. Steve Johnson and Melinda Palmer (OUP) made valuable contributions to the discussions. Ms. Palmer indicated that about 5000 copies of the SDS brochure were mailed to IUPAC members, heads of chemistry departments and selected people from Publishers' lists. In addition to this about 80,000 individuals world-wide received announcements about the series. The mailing coverage appears to be very good. Commission members were urged to talk to their own institutions concerning a subscription.

Publicity in Magazines and Journals

Professor Lorimer discussed an article (appended to the minutes) to be submitted to Chemistry International entitled: "The IUPAC Solubility Data Project: Strategies and Coverage". (A slightly amended version was submitted to CI in October, 1995).

It was also noted that several Commission members and others had published short articles in magazines on the SDS activities including reports on the International Conference on Solubility Phenomena. These included an article by Pirketta Scharlin (Finland) in *Kemia-Kemi*, a contribution by Jitka Eysseltova (Czech Republic) in a Czech

Republic Chemical Society Journal and an article by Alan Barton (Australia), a former Commission member in the Journal of Chemical Education. There has also been a full research paper on the SDS authored by Roger Cohen-Adad, Jack Lorimer, Sid Phillips and Mark Salomon; See the appended report of the Editor-in-Chief.

Dr. De Namor stressed the importance of including the publication of Plenary and Invited Lectures from the Solubility Phenomena Symposia in Pure and Applied Chemistry as an additional method of promoting the work of the Commission.

Procedures for Submission and Publication of Manuscripts

Professor Lorimer next discussed revised procedures for submission of manuscripts. The text containing details of the procedures is attached as an Appendix to these minutes, together with a flow chart. These revised procedures reflect current practice, adherence to IUPAC recommendations, and aim to create a greater uniformity of appearance.

E. Solubility Data Base Project (D. Shaw)

Professor Shaw first reviewed the events of the last two years concerning the Electronic Data Archive. Draft guidelines for the preparation for compilation and evaluation records for the archive were prepared by the working party consisting of F. Getzen, A. Maczynski, D. Shaw (Chair) and A. Skrzecz. These guidelines were attached as an Appendix to the minutes of the meeting held in Buenos Aires (1994). Since that time, the set of formats were discussed by several members of the Commission and refined accordingly. It was proposed that the use of the formats be strongly recommended but not required. The guidelines were sent to the Committee on Chemical Data Bases (CCDB) for their review and comments.

Dr. Steve Heller (Chair, CCDB) indicated that the CCDB will be abolished and replaced with an expanded version of the Publications Committee and renamed as the Committee on Printed and Electronic Products. Dr. Heller reported that the CCDB felt that the preliminary proposal of the working group appeared to be sound and stated that there are a variety of options available for a computer-readable form of the data archive.

Several questions were raised in the discussion.

1. There will be a fixed subscription fee for all IUPAC Data Bases through INTERNET and the issue was raised as to whether the availability of a data base would seriously affect the revenue from the printed product.
2. How would back issues be handled and who would pay for the data entry for earlier volumes?

Professor Lorimer recommended that the Commission should approach the newly created Publications Committee to request the transfer of published material to a computer readable form. Also, Professor Lorimer commented on the implementation of putting all new work in archival form. With few exceptions, this was not being done. Most members of the Commission would need explicit instructions and documentation in order to realize this goal. As noted earlier, Adam Skrzecz and Andrzej Maczynski have offered to provide a program for entry into a archival file after October 1, 1995.

The Commission recommended that the working party consider future options and submit a proposal to the new publications committee for financial support for the project.

F. Book on Experimental Determination of Solubilities (G. T. Hefter and C. L. Young, Editors)

The following is an update on the progress of the textbook on Experimental Determination of Solubilities:

1. First draft manuscripts have now been received from virtually all contributors.
2. R. Cohen-Adad and J. W. Lorimer have completed a first draft of the Chapter on Thermodynamics of Solubility, and this will be finalized by the end of November, 1995.
3. The Editors had an intensive working meeting in Perth 24-30 August 1994 at which all manuscripts submitted to that date were read and commented on in detail. These comments and various questions, were conveyed, in writing to all contributors. In addition, detailed guidelines for the preparation of "final form" MSS were circulated with a requested deadline for submission of 31 January 1995.
4. About 70% of the contributors have now submitted revised manuscripts.
5. Preliminary discussions with IUPAC representatives have indicated that the book will need to be offered to the IUPAC Publisher Blackwells in the first instance. Representative material was submitted to the IUPAC Publications Committee during the General Assembly. A reasonable time limit will be imposed for acceptance/refusal by Blackwells. Should Blackwells not wish to publish the book other publishers will be sought through the Publications Committee.

G. Status of Horizontal Programs

1. Solubility of Gases in Aerosols (P. G. T. Fogg)

Dr. Fogg reported on the continuing dialog between our Commission and the Commission on Atmospheric Chemistry (VI.4) on a collaborative project on the solubility of vapors and gases in Aqueous Aerosols. A copy of the proposed volume is attached. The main aim of the proposed project is the collection, evaluation and publishing of

solubility data which are relevant to the understanding of chemical processes occurring in clouds and aqueous environmental aerosols. It was agreed that preliminary work should commence immediately as a pilot project.

Several contributors were selected for the project and they are listed in the attached proposal outline. At this time no decision was made as to whether the project should lead to a volume in the SDS Series or to a stand-alone volume. It was agreed that the application for project initiation should be delayed until early 1996.

2. Solubilities and Thermodynamics of Macrocyclic Ligands (A. Danil de Namor)

Dr. Danil de Namor reported on the joint project between Commissions V.6 and V.8 on Macrocyclic Ligands. Dr. Namor will serve as the Project Leader. Rita Delgado (V.6) will coordinate the work on complex equilibria in solution.

It is proposed to clarify the ligands into two groups

- A. Naturally occurring Ionophores
 - 1. Valinomycin group
 - 2. Polyether or carboxylic antibiotics
- B. Synthetic macrocycles
 - 1. Tetraaza macrocycles
 - 2. Crown ethers
 - 3. Cryptands
 - 4. Miscellaneous

The project would be divided into two parts:

- 1. Thermodynamics of solution of Macrocyclic Ligands and Cationic Complexes in Various Solvents
- 2. Thermodynamics of Complexation of Macrocyclic Ligands in different solvents

Dr. De Namor recommended that the initial thrust should focus on the 18-crown-6 ethers plus cations in water and alcohols. There are extensive data published for these systems. A literature search and collection has already been initiated. A decision on the possible inclusion of Ligands with smaller rings will be made at the next Commission meeting in Leoben.

Experts in the area of the evaluation of stability constants need to be recruited. It was also suggested that funds for the project be solicited from the European Commission. The time for completion of the project was estimated as two years. The work will be

published in a single volume using a format similar to that traditionally adopted in the SDS series.

H. Seventh International Symposium on Solubility Phenomena (H. Gamsjäger)

Dr. Gamsjäger reviewed the current Status of the Seventh International Symposium on Solubility Phenomena to be held at Montanuniversität, Leoben, Austria from July 22-25, 1996. The deadline for submission of the First Circular is September 15, 1995. To date, 64 scientists and engineers with 34 accompanying persons have expressed interest in attending the Symposium.

The provisional technical and social program has been organized. The following Topical Areas will highlight the Conference:

- Electrolyte Equilibria and Solution Thermodynamics
- Polymers and Nonelectrolytes
- New Solubility Data and Computational Aspects
- Geochemical, Industrial and Environmental Applications
- Solubility Phenomena and Metallurgy

In addition a general Poster Session will be held.

The following Plenary Lecturers have been identified:

Robert E. Mesmer (Oak Ridge National Laboratory, Tennessee, USA)
Felix Franks (Cambridge, UK)
Rubin Battino (Wright State University, Ohio, USA)
Bernhard Wolf (University of Mainz, Germany)
Ingmar Grenthe (Stockholm, Sweden)
H. C. Helgeson (University of California at Berkeley, USA)
A. D. Pelton (Montreal, Canada)

Invited Lecturers have also been identified. Details of the talks and the Social Program will be available in the Second Circular.

I. Eighth International Symposium on Solubility Phenomena

Two proposals were received as venues for the Eighth International Symposium on Solubility Phenomena to be held in 1998. They were:

- Niigata University, Niigata, Japan
- University of Aveiro, Portugal

Professor H. Miyamoto presented the proposal on behalf of Niigata University and Dr. M. Magalhães presented a proposal on behalf of the University of Aveiro.

After some discussion the Commission voted to hold the Eighth International Symposium in Niigata University, Japan.

J. Membership of Commission for 1996-1997

Dr. Salomon announced the membership and changes in officers for the period commencing January 1, 1996. These recommendations were voted on at a special meeting of the current Titular members.

Officers

Chairperson	D. Shaw (Titular Member)
Secretary	H. Gamsjäger (Titular Member)
Editor-in-Chief	M. Salomon

Titular Members

P. G. T. Fogg
H. Gamsjäger
M.-Th. Saugier-Cohen Adad
D. Shaw
V. M. Valyashko

Associate Members

A. F. Danil de Namor
H. J. M. Grünbauer
S. Krause
C. Magalhães
A. E. Mather
K. Sawada
P. Scharlin
A. Skrzecz
J. Vanderdeelen
W. Voigt
Yu P. Yampol'skii

National Representatives

J. B. Jensen (Denmark)
R. Scrosati (Italy)

E. W. Waghorne (Ireland)
W. Wang (China)
E. Wilhelm (Austria)

K. Retirement of Commission Member

Professor Walter Hayduk has announced his resignation from the Commission. Professor Hayduk served as a Titular Member and over the years made significant contributions to volumes on Gas Solubilities. The Commission wishes to express its sincere appreciation to Professor Hayduk for his valuable work.

L. Appointments

Dr. Mark Salomon was appointed to a three-year term to serve on the Division Committee of the Analytical Chemistry Division.

Professor Lorimer continues to serve as an elected member of the Bureau and at the General Assembly he was appointed as an Associate Member of the Interdivisional Committee on Nomenclature and Symbols (IDCNS).

M. 22nd Annual Commission V.8 Meeting

The 22nd Annual Commission V.8 meeting will be held on July 20-21, 1996 at Montanuniversität, Leoben, Austria.

N. Next General Assembly Meeting 1997

The next General Assembly meeting will be held at the University of Geneva, Switzerland from August 23-30, 1997.

O. New Business

1. The Membership Lists in the three Sub-Committees needs updating. Those people who have not been active over the last few years should be deleted from the lists. Sub-Committee Chairpersons will contact all members on the current list (see IUPAC Handbook) to ascertain the involvement of all members. In addition sub-committee chairpersons should get an update on progress in January or February of each year so that the external assessor can monitor progress of the Commission's activities.
2. A suggestion was made to examine the possibility of appointing Sub-Committee chairs on a rotating basis. It was decided the newly appointed chairperson will look into this matter.

P. **Adjournment**

The meeting was adjourned at 11:00 a.m. on August 7, 1995.

SECTION II - REPORTS ON RELATED COMMISSION ACTIVITIES

A. REPORTS BY NATIONAL REPRESENTATIVES

DENMARK - J. B. JENSEN

The Danish representative is a member of the Working Party on the "Revision of the Compendium of Analytical Nomenclature". He attended a meeting of the group at the General Assembly at the University of Surrey and will report on progress at the next Commission meeting. Dr. Jensen is preparing a Chapter on "Selected Physico-Chemical Terms used in Chemical Analysis". As a member of "The Pan-European Scientific and Technological Network on Solubility Studies", Professor Jensen contributed to a proposal on "Solubility Studies Connected with Recoveries of Industrial Waste". The proposal was declined but further attempts will be made to solicit funding. In addition, Dr. Jensen continues to work on the SDS volume on Tungstates and Molybdates.

IRELAND - E. WAGHORNE

Dr. Waghorne had nothing specific to report. He continues to try to recruit scientists with interests in the solubility area.

PORTUGAL - C. MAGHALHÃES

Dr. Magalhães has assisted with the translation of the RED Book into Portuguese. She is also active in the Portuguese Chemical Society with particular interest in Nomenclature in Inorganic Chemistry.

B. REPORTS BY SUB-COMMITTEE CHAIRPERSONS

Each Sub-Committee met as indicated in the agenda. Individual reports are attached.

Sub-Committee Chairmen

Gas Solubilities	P. G. T. Fogg
Liquid Solubilities	F. W. Getzen
Solid Solubilities	M.-Th. Saugier-Cohen Adad