



# *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)

**January 26, 1994**

**Dear Colleague:**

I enclose the minutes of the Commission V.8 meeting which took place at the IUPAC General Assembly in Lisbon on August 6-8, 1993.

If you have any particular items for the agenda for the meeting in Buenos Aires, Argentina, on August 20 and 21, 1994, please send them to me for consideration.

**Best regards.**

**Sincerely,**

*Reginald P. T. Tomkins*

**Reginald P. T. Tomkins  
Secretary**

**RPTT:ns**

*Chairman:* Dr. M. SALOMON  
US Army Electronics Research and  
Development Laboratories,  
Mail Stop SLCET-PR,  
Fort Monmouth,  
New Jersey 07703-5000, USA  
TEL: +1 (908) 544 2832 (days), +1 (908) 747 2745 (evenings)  
FAX: +1 (908) 741 0277 (home)

*Secretary:* Prof. R. P. T. TOMKINS  
Department of Chemical Engineering,  
Chemistry and Environmental Sciences,  
New Jersey Institute of Technology,  
University Heights,  
Newark,  
New Jersey 07102, USA  
TEL: +1 (201) 596 5656  
FAX: +1 (201) 802 1946

MINUTES OF THE 19TH ANNUAL COMMISSION V.8 MEETING

HELD AT THE 37TH GENERAL ASSEMBLY

LISBON UNIVERSITY, LISBON, PORTUGAL

ON

AUGUST 6-8, 1993

SECTION I. DISCUSSIONS OF THE FULL COMMISSION

A. List of Attendees

C. BALAREW, (BULGARIA)	J. W. LORIMER, (CANADA)
A. BYLICKI, (POLAND)	Z. MACZYNSKA, (POLAND)
B. R. CHURAGULOV, (RUSSIA)	A. MACZYNSKI, (POLAND)
H. L. CLEVER, (USA)	C. MAGALHAES, (PORTUGAL)
M. Th. SAUGIER-COHEN ADAD, (FRANCE)	H. MIYAMOTO, (JAPAN)
R. COHEN-ADAD, (FRANCE)	V. MYASOEDOVA, (RUSSIA)
A. F. DANIL DE NAMOR, (UK)	V. PLATIKANOVA, (BULGARIA)
R. DUHLEV, (UK)	P. RUOSTESUO, (FINLAND)
J. EYSSELTOVA, (CZECH REPUBLIC)	M. SALOMON, (USA)
M. FERRIOL, (FRANCE)	J. SANGSTER, (CANADA)
P. G. T. FOGG, (UK)	V. SAZONOV, (RUSSIA)
H. GAMSJÄGER, (AUSTRIA)	P. SCHARLIN, (FINLAND)
F. W. GETZEN, (USA)	D. G. SHAW, (USA)
H. J. M. GRÜNBAUER, (THE NETHERLANDS)	A. SKRZECZ, (POLAND)
E. GRYZLOVA, (RUSSIA)	E. SZCZEPANIEC-CIECIAK, (POLAND)
A. GOTO, (JAPAN)	R. P. T. TOMKINS, (USA)
C. GUMINSKI, (POLAND)	V. M. VALYASHKO, (RUSSIA)
R. I. HAINES, (CANADA)	E. WILHELM, (AUSTRIA)
W. HAYDUK, (CANADA)	R. G. WISSINGER, (USA)
G. T. HEFTER, (AUSTRALIA)	C. L. YOUNG, (AUSTRALIA)
J. B. JENSEN, (DENMARK)	
N. KBIR-ARIGUIB, (TUNISIA)	
S. KRAUSE, (USA)	

## 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 18th Commission meeting held in Moscow, Russia were approved and the agenda (copy attached) for the present meeting was approved.

## C. Tributes and Condolences

Professor V. M. Valyashko paid tribute to Professor Ivan Nikonovich Lepeshkov (Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences) who passed away in January 1993. Professor Lepeshkov was the first Russian scientist to participate in the Commission V.8 project. A volume on the solubilities of alkali metal perchlorates will be dedicated to his memory.

Professor R. P. T. Tomkins reported the death of Ruth Dirkse, the wife of Dr. Ted Dirkse, a longtime and very active contributor to the Solubility Data Commission. A message was sent to Ted Dirkse expressing the feelings of the Commission.

## D. Report of the Chairman (M. Salomon)

### 1. Activities within IUPAC

Dr. Salomon reported that IUPAC will emphasize project-oriented problems in the future as opposed to field-oriented scientific work. Two limited lifetime (LLTC) Commissions (2-4 years) had been established in the Analytical Chemistry Division, one involving chromatography and other analytical separations and the other on environmental analytical chemistry. The Chairman also reported that due to the restructuring, the number of Titular members in Commission V.8 would be reduced by one. The reduction to Six Titular members created a problem for present and future membership planning and funding which was temporarily solved by the agreement of two current Titular members (Fogg and Hayduk) to step down for the next two years. This adjustment also required changes in the associate membership which is listed in Section N.

Dr. Salomon then referred to the 1992 Critical Assessment by the Vice-President, Professor H. A. Staab. The Vice-President viewed the solubility data compilations in terms of rather narrow and specialized ranges of organic and inorganic systems and found it difficult to see how priorities were ranked. He felt that the work needed coordinating according to importance and timeliness. Professor Staab also expressed surprise that the data were still prepared for printed publication rather than placing a greater emphasis on a computer database. He did give strong support for the proposed book on "Experimental Determinations of Solubilities".

Dr. Salomon raised the issue of the enforcement of using an external reviewer for all new Proposal Initiation Forms (PIFS). It is being suggested that the Commission chairperson should propose a reviewer who is outside IUPAC activities. Questions were raised by members of the Commission as to what type of instructions should be prepared for the Reviewers. Professor Marcus, the external assessor for Commission V.8, recommended that the Commission should prepare the instructions. There was a general consensus that the selection of external reviewers would present difficulties. Also, it was noted

that the use of external reviewers would delay the submission date of the PIF. Instead of the end of September, it is being suggested that the revised deadline for submission of a PIF be extended to December 1.

The Chairman then reviewed the status of the Commission Projects. An updated list is attached to these minutes.

There are good possibilities of outside support for the volumes on Lead Sulfate (Bullock and Lorimer) and CO<sub>2</sub> (Scharlin et al). Dr. Salomon then addressed the issue of solicitation of external funds to assist with the preparation of an SDS volume. Industrial support for IUPAC projects requires prior approval from the National Adhering Organization of the particular country involved. Members of the Commission were encouraged to seek possible support from corporations and other agencies. This approach was particularly important with the reduction of other sources of funding.

Dr. Salomon next reviewed the funding for traveling to Commission meetings. In the past, Pergamon Press had contributed \$3000 per year to subsidize travel of participants. We cannot count on such support from a new publisher. The modest budget provided by IUPAC is used exclusively to support travel. Every attempt is made to distribute these limited funds in an equitable way. Mention was made of the ICSU grant which was used to provide some support for the text of the book, "Experimental Determination of Solubilities". The bottom line is that the availability of travel funds is becoming more limited.

#### The Franzosini Award

Interest income from the Franzosini Award Fund was used to assist Dr. Michel Ferriol (Universite Claude Bernard, Lyon) to attend the meeting. Due to a rapid drop in interest rates, the funds available for future awards will be limited to around USD \$250 (i.e. about half of the interest previously generated at the higher interest rates prior to 1993).

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

##### 1. Search for a New Publisher for the SDS Volumes

Dr. Lorimer reported that a large number of publishers had been approached concerning publication of the SDS volumes. Several offers were received but apart from Oxford University Press, they did not meet the requirements, particularly with regard to the Commission having editorial control of the volumes.

Dr. Lorimer indicated that the offer from Oxford University Press possessed many attractive features but he was not in a position to spell out any details as the chairperson of the Commission and the Editor-in-Chief were still involved with negotiations over details with Oxford University Press, including financial matters. OUP wishes to publish the series as an occasional journal in a hard cover, with four issues per year (The Commission proposes 4-6), an arrangement which has attractive features, but also problematic ones, especially a limitation to a total of 1,184 pages per four issues. Dr. Lorimer indicated that every effort would be made to draw up a much simpler contract than the previous one with

Pergamon Press. ( Note: The second draft of the contract was received on 12 December, 1993 and appears to be acceptable for signing after correction of a few minor errors. The restriction to 1,184 pages per year, and 264 to 328 pages per volume, stands. )

Dr. Lorimer then reported on recent completed volumes (volumes 48, 49, 52, 53, 58).

### Subscriptions and Sales of Volumes

It was noted that volumes up to Vol. 58 had been advertised by Pergamon Press. A problem exists concerning a mechanism for the transfer of subscription money from Pergamon Press to the new publisher. There is a case where an organization has paid subscriptions to include Vol. 117. It was also suggested that a breakdown of corporate, university and other types of subscriptions would be useful. This should be discussed with the new publisher. In addition the demand for reprints and the number of print runs will also need to be discussed. With regard to sales of volumes it appeared that there was a trend towards an increase in individual sales compared to subscriptions. For example:

<u>Vol</u>	<u>Subscriptions</u>	<u>Individual Sales</u>	<u>Total</u>
48	92	101	193
51	92	102	194
52	92	132	224

### Evaluation of Commission V.8 by Vice-President of Union

In his capacity as a Co-opted Member of the Executive Committee of the Analytical Chemistry Division, Dr. Lorimer made some remarks concerning the report of Professor Staab. He felt that more coordination and planning was needed particularly in trying to advance priority volumes. He also felt that Prof. Staab's suggestion to move towards a database approach could be difficult to implement over a short term.

### F. *Experimental Determination of Solubilities (G. Hefter)*

The contents of the book are as previously accepted by the Commission but the rapidly approaching deadline for completion of the text required the following changes:

\*The chapter on thermodynamics will now be authored by Professor R. Cohen-Adad (previous author was J.J. Counioux).

\*The chapter on solubilities in super critical fluids is now co-authored by Dr. Karel Aim from Prague (joining Professor M. Fermiglia from Trieste).

\*The chapter on the solubilities of gases in metals is now co-authored by Professor Y. Sakamoto of Nagasaki University (joining Dr. F. Lewis from Belfast).

\*The chapter on solubilities at high temperatures and pressures is now co-authored by B. Churagulov and K. Kravchuk both from Moscow State University and Professor A. Mather (joining Professor Valyashko from Moscow).

\*The chapter on solubilities of gases in polymers is now co-authored by Professor Y. Yampolski from Moscow (joining Dr. R. Paterson from Glasgow).

Only relatively minor changes to authorships, titles and organization are expected from hereon.

2. Since the last meeting of the Commission in Moscow in 1992, first draft chapters have been received from:

*Lewis and Sakamoto	"Gases in Solids"
*Szczeplaniec-Ciecak	"Cryogenic Liquids"
*Valyashko et al.	"High Temperatures & Pressures"
*Yampolski and Paterson	"Gases in Polymers"

Good progress has also been reported by several other contributors who have submitted some preliminary material to the editors. Regrettably, a number of contributions remain outstanding although all authors report some progress.

Contributors who are further towards completion (i.e. at the second draft stage) have been asked to wait until the editors have all first draft contributions to hand.

3. The critical need at the present time, apart from the outstanding contributions, is for some funds from the Commission/ICSU to enable C. L. Young and G. T. Hefter to get together in Australia later this year to edit the material to hand. This will be essential if we are to achieve IUPAC's deadline for completing the project by the 1995 IUPAC General Assembly.

#### G. Working Group on Macrocyclic Supramolecular Chemistry (A.F. Danil de Namor)

Dr. Angela F. Danil de Namor, Chairman of the Working Party involving a new initiative on Macrocyclic Chemistry outlined a plan for a horizontal project with Commission V.6. Dr. Danil de Namor will coordinate the joint (horizontal) project. Commission V.8 will be responsible for the compilation and critical evaluation of solubility data for one volume, while Commission V.6 will produce a volume on thermodynamic data.

It was also reported that Professor D. G. Tuck (Commission V.6, Equilibrium Data) has agreed to collaborate on this project as an Horizontal Program. As soon as details are worked out, an official proposal must be submitted to the Union for their approval.

Dr. Namor also recommended the preparation of a textbook on "Thermodynamic Aspects of Macrocyclic Chemistry". It was also suggested that the new initiative on Macrocyclic Chemistry by

Commission V.8 should be a topic for the Second International Symposium on Macrocyclic Chemistry for the Design of New Materials to be held in Buenos Aires, Argentina in August, 1994.

#### H. Solubility Database (M. Salomon)

During the Commission meeting several discussions were held on possible new approaches to a previously proposed establishment of a solubility Database. Dr. Ken Marsh (Thermodynamics Research Center) indicated that he was interested in working with IUPAC in the preparation of a suitable database. The IUPAC Committee on Chemical Databases (CCDB), chaired by Steve Heller met with the Commission and discussed possible approaches with the Commission and indicated that they would consider a well-documented proposal.

The Solubility Data Commission adopted the goal of developing standard ASCII file formats for the electronic storage of 1) compiled and 2) evaluated solubility data. These formats are appropriate for two uses:

1. Internal use by the SDC for storage, retrieval, revision and exchange of data and for the automated production of paper camera-ready-copy;
2. Marketing by the Union for external use as a searchable database when combined with third party search and visualization software.

To reach this goal the Chair appointed a Working Party (F. Getzen, A. Maczynski, D. Shaw (Chair), and A. Skrzecz, and charges the Party with the following tasks:

1. Develop and document file structures for compilations and evaluations of solubility data which are suitable for the above stated uses;
2. Prepare approximately 100 sample records (to be specified by the Chair of the SDC) which demonstrate a range of system types (gas, liquid, solid, binary, multicomponent, low and high pressure; etc.);
3. Develop a recommended plan of action for creating an externally marketable database. This plan is for submission to the Union through the CCDB and may include proposals and cost estimates for encoding of data in published volumes and volumes in preparation.

The Commission's target timetable for this work is

Working Party Draft Report to SDC, June 1994  
Comments to Working Party, August 1994  
Revised Report to SDC Chair, November 1994  
Report transmitted to CCDB, January 1995

#### I. Report on Fifth International Symposium on Solubility Phenomena

Professor V. Valyashko reported on a successful fifth International Symposium on Solubility Phenomena, which was held in Moscow, Russia from July 8-10, 1992.

The Symposium consisted of seven main sessions:

- \*Phase Equilibria and Equations of State
- \*Thermodynamics of Molten Salts
- \*Nonaqueous, Mixed and Gaseous Systems
- \*Complex Solution Chemistry and Electrolyte Equilibria
- \*Application of Solubility Data to Technology
- \*Pollutant Solubilities, Natural Waters and Environmental Chemistry
- \*Solubility Phenomena in Polymer Systems

There were fifteen plenary and invited lectures, twenty five oral presentations and about 150 poster presentations. A total of 150 people participated in the conference, of which 62 were from outside of Russia.

**J. Status Report on Sixth International Symposium on Solubility Phenomena and the Second International Symposium on Macrocyclic Ligands for the Design of New Materials**

Dr. Angela Danil de Namor outlined the current status of the Sixth International Symposium on Solubility Phenomena to be held in Buenos Aires from August 22-26, 1994.

The first circular announcing the Conference has been mailed to prospective participants. Sessions are planned for the following topics:

- \*Solution Thermodynamics
- \*New Solubility Data
- \*Supramolecular Systems
- \*Pollutant Solubilities and Environmental Chemistry
- \*Solubilities of Polymers, Micelles and Pharmaceuticals
- \*Molten Systems

Some plenary lecturers have been identified.

The Symposium will be held in a hotel in the Center of Buenos Aires. It is planned to devote the middle day (Wednesday) of the Conference to an organized tour. The Symposium will be sponsored by



the Faculty of Exact and Natural Sciences of the University of Buenos Aires, Argentina and the University of Surrey, U.K.

Dr. Namor indicated that funding is being sought from the European Community and several industrial corporations to assist with travel for participants.

Dr. Namor also reported that the Second International Symposium on Macrocyclic Ligands for the Design of New Materials will be held after the Solubility Symposium from August 29-September 1, 1994 in Buenos Aires. This conference will also have sessions on collaboration between Latin American countries and other countries relative to scientific research and chemical education.

#### **K.    The Seventh International Symposium on Solubility Phenomena**

The Commission accepted an invitation from Professor Gamsjager to hold the Seventh International Symposium on Solubility Phenomena at the University of Leoben, Austria. Dr. Gamsjager reported that the director of the University had agreed to host the Conference. The University is situated about three hours from Vienna and it was suggested that the Symposium be held between the beginning to the middle of August, 1996.

#### **L.    Proposal for Establishing a Scientific and Technological Network for Solubility Studies**

Professor C. Balarew reported on the project on the Pan-European Scientific and Technological Network on Solubility Studies. The aim of the project is to promote and re-establish scientific contacts between EC countries (Denmark, France, Germany, Spain, UK) and Eastern Europe (Bulgaria, Czech Republic, Poland, Rumania and Russia). The project was submitted to the EC Commission of Science and Technologies in August 1992 and was, unfortunately, not among those placed on the final selection list of the Community action for Cooperation in Science and Technology with Central and Eastern Europe.

Helpful suggestions for possible support were made by Professor E. Wilhelm (Vienna), Professor M.T. Cohen-Adad (Lyon) and Dr. Angela Danil de Namor (Guildford). The IUPAC Solubility Data Commission fully supports the proposed projects and any further attempts for its resubmission to the EC. After considering the referee's comments, it was recommended that other funding agencies should also be approached.

#### **M.    New Business**

Dr. J. Birger-Jensen was nominated as the Commission V.8 representative for the revision of the Orange Book.

#### **N.    Membership of Commission V.8**

Dr. Salomon announced the membership and changes in offices for the period commencing January 1, 1996. These recommendations were voted on at a special meeting of the current Titular members of Commission V-8 for the period 1993-1995.

Chairperson	M. Salomon (Titular Member)
Secretary	R. P. T. Tomkins (Titular Member)
Editor-in-Chief	J. W. Lorimer
Chairperson Elect	D. G. Shaw (Commencing after next General Assembly)
Secretary Elect	H. Gamsjäger (Commencing after next General Assembly)

Titular Members

J. Eysseltova  
 F. Getzen  
 E. Hefter  
 A. Maczynski  
 M. Salomon  
 R. Tomkins

Associate Members

C. Balarew  
 M. T. Saugier-Cohen Adad  
 A. F. Danil de Namor  
 H. Gamsjäger  
 H. J. M. Grünbauer  
 C. Kalidas  
 S. Krause  
 A. E. Mather  
 H. Miyamoto  
 P. Scharlin  
 V. M. Valyashko  
 J. Vanderdeelen

National Representatives

J. B. Jensen (Denmark)  
 M. C. J. Magalhaes (Portugal)  
 K. Sawada (Japan)  
 R. Scrosati (Italy)  
 E. W. Waghorne (Ireland)  
 E. Wihelm (Austria)

O. 20th ANNUAL COMMISSION V.8 MEETING

The 20th Annual Commission V.8 meeting will be held on August 20 and 21, 1994 in Buenos Aires, Argentina immediately preceding the Sixth International Symposium on Solubility Phenomena.

SECTION II. REPORTS ON RELATED COMMISSION ACTIVITIES

A. REPORTS BY NATIONAL REPRESENTATIVES

AUSTRIA - E. WILHELM

Professor Wilhelm, the Austrian representative expressed concern on the lack of financial support for Austrian scientists to participate in Commission meetings and/or the General Assembly. In addition,

he felt that the relevant Austrian organizations were not acknowledging the importance of the various IUPAC activities and in particular, activities associated with data compilation and evaluation.

#### **DENMARK - J. B. JENSEN**

The Danish representative reported that Professor Valyashko (Russia) visited the Department of Physical Chemistry (Technical University of Denmark, Lyngby) for two weeks for detailed discussions on critical evaluations of solubility data.

#### **FINLAND - P. SCHARLIN**

The Finish representative devoted most of the time during the past year to advancing the SDS volume on carbon dioxide. She indicated that she had been unsuccessful in recruiting new Finish scientists to the project. She also pointed out the difficulty in obtaining funding for travel to meetings and stressed the need for a special invitation letter for use in soliciting funds.

#### **B. ADDITIONAL REPORTS FROM MEMBERS COUNTRIES**

##### **RUSSIA - B.R. CHURAGULOV**

Professor Churagulov gave an update on the status of some thirteen SDS volumes. Further details of volumes involving Russian scientists can be found in the Appendix.

#### **C. REPORTS BY SUB-COMMITTEE CHAIRPERSONS**

Each subcommittee met as indicated in the agenda. Using the reports submitted by each subcommittee chairperson, an official projects list (current programs 1993) was prepared and is appended to these minutes. Further details may be obtained by corresponding with the individual subcommittee chairpersons.

##### **Sub-Committee Chairpersons**

\*Gas Solubilities H. L. Clever (this position will now be assumed by P.Fogg)

\*Liquid - Liquid Solubilities - F. Getzen

\*Solid Solubilities - M. Th. Saugier-Cohen Adad