



# 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 22, 1993

Dear Colleagues:

I enclose the minutes of the 18th IUPAC Commission V.8 meeting which took place at the Hotel "Uzkoe" of the Academy of Sciences, Moscow, Russia, July 6-7, 1992. In addition, there are attached summary minutes of the subcommittee meetings.

I have also attached two other documents which you will probably find useful.

- an updated list of contributors to Commission V.8, including addresses and related communication information.
- an updated listing of the solubility data series which includes published volumes and volumes in preparation. This was prepared by Dr. Lorimer.

Please let me know if there are any errors or changes needed in the address list. Also I would appreciate your keeping this copy in a safe place as it is fairly costly to send all this information to 120 people in different countries.

The next (19th) meeting of the IUPAC Commission V.8 will take place during the 37th IUPAC General Assembly in Lisbon, Portugal on August 6-8, 1993. Your participation is urgently requested.

I look forward to seeing you in Lisbon later this year. Best wishes.

Sincerely,

*Reginald P. T. Tomkins*  
Reginald P.T. Tomkins  
Secretary

RPTT/gal  
Enclosures

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MINUTES OF THE 18TH COMMISSION V.8 MEETING

HELD AT THE HOTEL "UZKOE" OF

THE ACADEMY OF SCIENCES, MOSCOW, RUSSIA

ON

JULY 6-7, 1992

SECTION I. DISCUSSIONS OF THE FULL COMMISSION

A. List of Attendees

C. Balarew (Bulgaria)	G. A. Krestov (Russia)
O. Chiavone-Filho (Denmark)	J. W. Lorimer (Canada)
B. R. Churagulov (Russia)	A. Maczynski (Poland)
H. L. Clever (USA)	M. Magalhaes (Portugal)
R. Cohen-Adad (France)	A. Mather (Canada)
J. J. Counioux (France)	H. Miyamoto (Japan)
A. F. Danil de Namor (UK)	Y. Miyano (Japan)
I. A. Dibrov (Russia)	V. Myasoedova (Russia)
G. Dragan (Romania)	H. Ohtaki (Japan)
J. Eysseltova (Czechoslovakia)	F. Perez (Spain)
P. G. T. Fogg (UK)	R. Popescu (Romania)
H. Gamsjager (Austria)	M. Salomon (USA)
M. Gaune-Escard (France)	J. Sangster (Canada)
F. W. Getzen (USA)	M. T. Saugier-Cohen Adad (France)
S. Gradinov (Bulgaria)	K. Sawada (Japan)
E. Gryzlova (Russia)	V. Sazonov (Russia)
C. Guminski (Poland)	P. Scharlin (Finland)
W. Hayduk (Canada)	D. Shaw (USA)
G. T. Hefter (Australia)	A. Skrzecz (Poland)
R. Herrera (USA)	A. Slobodov (Russia)
J. B. Jensen (Denmark)	R. P. T. Tomkins (USA)
I. L. Khodakovsky (Russia)	W. Voigt (Germany)
E. Konigsberger (Austria)	A. Vorob'ev (Russia)
S. Krause (USA)	Y. Yampol'skii (Russia)

## B. Approval of Minutes and Agenda

Mark Salomon, the Chairman of Commission V.8 called the meeting to order. Attendees were asked to identify themselves and their affiliation. The minutes of the 17th Commission meeting held in Hamburg, Germany were approved. The agenda for the present meeting was also approved subject to the inclusion of a discussion on the prioritizing of SDS volumes and the adoption of common software for the production of the volumes.

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

### 1. Termination of Publishing Contract with Pergamon Press

It was announced that Pergamon Press has decided to discontinue publication of the SDS Series effective at the end of 1992 and therefore the Commission would have to actively recruit a suitable replacement in order to continue publication of their work. The chair reviewed the status of published volumes as well as volumes which are currently in final stages of preparation.

### 2. Activities within IUPAC

There still exists a strong desire amongst the leadership at IUPAC to reduce both the number of commissions and the number of members within the various commissions. Also there is a recommendation to establish more interactions between the commissions. There is also a move to have IUPAC become involved with "global" needs and that the membership should give serious consideration to the prioritization of published volumes and projects. It has been suggested that some outside consultants should be appointed to assist with this action. Outside experts from industry and editors of scientific journals would be particularly appropriate.

It was also reported that the Union was now taking a much more aggressive approach relative to database activities. The Commission on Chemical Databases has expressed an interest in continuing their collaborations with Commission V.8 and possible funding was mentioned. The Chairperson felt that Commission V.8 has reached a point where it can produce a working database on solubility data and some firm commitment as to whether this activity should be strongly pursued, should be made at this meeting.

Mark Salomon then reviewed the somewhat controversial issue of the listings in the Blue Book. The policy of IUPAC to reduce the number of members listed in the Blue Book is one of economics. The new policy is that the Commission is not allowed to have a National Representative from a country which also has a representative as a member of that same Commission.

Several requests had been made to the Union to make an exception for Commission V.8 and include all selected National Representatives in the Blue Book. After the requests were denied all the unlisted National Representatives were placed on the appropriate sub-committees so that they gained some visibility for their considerable efforts.

Next the Chair reviewed the status of Computer Equipment purchases that have been made over several years for some members of the Commission. Pergamon has requested the return of all such equipment. The Commission is currently negotiating with Pergamon on the possibility of selling the equipment to the users at a reduced fee, converting the purchase into a gift or other possible actions to minimize any complications. It was pointed out that most of this equipment is now obsolete.

It was reported that under recent changes to statutes and By-Laws and starting with effect from the 1993 General Assembly the officers of the Commission will remain in office until 31 December of the year in which the period of office is due to terminate. All periods of office will begin on 1 January following the General Assembly.

Income from the Franzosini Award Fund was employed to bring Stephen Gradinov to the meeting.

### **Common Word Processing Software for Production of CRC**

The Commission is exploring the use of common word processing software for production of CRC (Camera Ready Copy) and for submitting draft manuscripts for review. Also to be explored at a later date with the new publisher is the possibility of submitting all manuscripts on floppy disks for direct production of the volumes. Based on a survey taken at the meeting in Moscow, the most common software packages are Word Perfect 5.1 and Microsoft Word. Other, but less common software programs, which are being used are LATEX for PC, Lotus Manuscript, Wordstar, Pagemaker and T3. It is concluded that access to Word Perfect and Microsoft Word would greatly facilitate the submission of draft materials.

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

A brief history of the relationship between Pergamon Press and the Solubility Data Commission was presented culminating in the termination of the contract effective, December 31, 1992. The main reason for the end of the relationship was due to the drop in the number of subscriptions to the SDS Series.

Dr. Lorimer reported that a new contract was drafted at the end of 1991 with the latest contract used for the Pergamon renewal being used as a model. The new contract was written in a general form and included details of the some 117 volumes including those already published.

Lorimer indicated that the new contract together with a covering letter was sent to several potential publishers. They included Blackwell Scientific Publishers Ltd, World Scientific Publications, John Wiley, Lewis Publishers, Ellis Horwood and The Thermodynamics Research Center (K. Marsh). It was noted that Blackwell Scientific was not interested in pursuing the offer due to the low potential size of the market and World Scientific has indicated a problem with advanced payments, although this point was open to negotiation. No replies had been received from the other publishing companies at the date of the Moscow meeting.

After the Commission meeting in Moscow, several other Publishing houses were contacted. They include Captus Press, Marcel Dekker, CRC Press, Kluwer Academic Publishers, Plenum Publishing Company, VCH and Taylor and Francis. The sale of three hundred copies was cited as a viable number for publication and with this target number in mind Mr. Gujral (IUPAC) was requested to compile the sales numbers on recent volumes. This information is obviously very important to a potential publisher. Also Commission members were again encouraged to try to have their libraries subscribe to the series.

Lorimer then reported on the Sales of volumes for the past year (Volumes 45/46 and 47). There were 92 subscriptions to each of the volumes. In addition there were 103 individual sales for volume 45/46 (Gases in Molten Salts, Tomkins and Bansal eds) and 148 individual sales copies for Volume 47 (Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems), R. Cohen-Adad and Lorimer, eds).

Lorimer then turned to the status of the production of on-going volumes. The following is a summary of this item

- \* Volume 48 (Alcohols and Hydrocarbons, Shaw, Skrzecz, Maczynski, eds) and Volume 49 (Esters with Water, Part I: Esters 2-C to 6-C, Getzen, Hefter, Maczynski, eds) have both been sent to the publishers.
- \* Volume 50 (Esters with Water. Part II: Esters 7-C to 32-C, Getzen, Hefter, Maczynski, eds): Volume 51 (Alkaline Earth Metal Hydroxides in Water and Aqueous Solutions, Lambert, Clever, eds) and Volume 52 (Carbon Dioxide in Non-aqueous Solvents at Pressures under 200 k Pa, Fogg ed) are all at the publishers awaiting production.
- \* Six more Volumes (53-57) and the Cumulative Index for Volumes 39-57 will be completed before the end of the 1992 calendar year.

A listing of SDS Volumes (Completed and in progress) prepared by Dr. Lorimer is attached as an Appendix.

Lorimer expressed concern over the number of gratis copies of the SDS volumes that were being distributed, despite the fact that in 1987 the Commission had made a recommendation to reduce the number of such copies. For example in 1991 there were 114 gratis copies of volume 35, 95 free copies of Volume 36 and 81 copies of Volume 44.

### **Preliminary Project Formulations**

Lorimer stated that the Analytical Chemistry Division had made the recommendation that PIF's (Project Initiation Forms) should be completed at the even year meetings of the Commission and then submitted to the Analytical Chemistry Division to be reviewed before the odd year meeting of the Commission. Sub-Committee Chairpersons were urged to complete all the necessary PIF forms for newly approved projects or other projects which had not been given a PIF form before the end of the current meeting.

### **Publication of Overall Plan in Chemistry International**

Lorimer discussed the merits of publishing an overall plan of Commission V.8 in Chemistry International. In the past some criticism was made that our Commission did not appear to have such a plan and that volumes were published in a random way. This was certainly not the case and it was felt that the plan prepared by L. Clever for the Sub-Committee on Gas Solubilities could be used as a model for an overall plan. It would also serve as a vehicle for giving priorities to projects. Ideas for this type of plan were solicited from members of the Commission.

### **Review of Manuscripts**

Lorimer led a discussion on the possibility of upgrading the Review process for the publications of the Commission. For the most part the reviewing of manuscripts was undertaken by members of the Commission as a large percentage of the experts in the field were active members of the Commission. However, it was felt that editors of the volumes should be encouraged to suggest possible external reviewers. The problem of the large size of the manuscripts was recognized and the possibility of sending the introductory material, together with the critical evaluations was suggested as a compromise.

Also it was suggested that a list of qualified external reviewers should be compiled. Maybe as an incentive the publishers could provide another technical book of the reviewer's choice. It was generally felt that the review process needed some refining. A recommendation was made that Dr. Lorimer prepare some guidelines on the Review Process.

#### **E. Book on "Experimental Determination of Solubilities"**

G. Hefter presented an update on the status of the proposed text

- \* The contents of the book remain as previously accepted by the Commission with only a few minor adjustments.
- \* Contributors have now been arranged for all the major areas of solubility determination which were outstanding at Hamburg. The new contributors include  
Fred Lewis - Gases in Metals  
Jorgen Cristofferson - Kinetics of Solubility  
Elzbieta Szczepaniec-Cieciak - Cryogenic Liquids  
Vladimir Valyashko - High Pressures & Temperatures  
Russel Paterson - Gases in Polymers
- \* Approximately half of the prospective chapters have been received in first draft form and commented on. Firm commitments from contributors have been obtained for most of the other sections.
- \* A number of chapters are now in second draft form. The projected size of the book is 250-300 pages.
- \* The Commission was successful in obtaining \$3000 from ICSU Special Project funds which are being used to assist in production of the book and also help some of the contributors to attend the Commission meetings.
- \* A PIP form was prepared as the proposed text represents a new project.

#### **F. Database Project**

At the Commission meeting in Hamburg in 1991 A. Maczynski presented a demonstration of his latest version of the database (approved in principle by Commission V.8) to members of the Committee on Chemical Data Bases (CCDB). At that time the CCDB requested a number of minor changes to the draft database as well as a copy of the source code for the database program (written in C++ by Maczynski and Skrzecz). Maczynski indicated that the requested information was sent to S. Heller (Chairperson, CCDB) but no response had been received.

At the Commission meeting in Moscow Dr. Maczynski presented a new proposal which had not been discussed by the Commission. He offered to produce a modified database which involved access of original numerical data via the database at the Thermodynamics Research Center at Texas A&M, USA. This did not meet with the Commission's approval and after extensive debate on the issue Dr. Maczynski agreed to produce a complete database on the

alcohol-hydrocarbon Systems in the original format worked out at the Hamburg meeting. This database will contain all experimental values and critically evaluated recommended values. Maczynski promised to send a copy of the completed database to the Chairman of the commission before the end of 1992 so that it could be distributed to members of the working group on Databases and some other members of the Commission for evaluation. The revised version would then be sent to CCDB before the Lisbon meeting with the plan to achieve a recommendation at that meeting.

### **G. Report on Fifth International Symposium on Solubility Phenomena**

V. M. Valyashko gave a brief report on the 5th International Symposium on Solubility Phenomena to be held July 8-10, 1992 in Moscow, Russia. He indicated that 150 Russian scientists had registered for the Symposium and he anticipated that approximately 100 would attend. 60 participants had registered from other countries. Seven Plenary Lectures and Seven invited Lectures will cover subjects ranging from Environmental Chemistry, Polymer Solubilities, Molten Salt Thermodynamics, Theoretical Thermodynamics, Phase Equilibrium and Chemical Databases.

### **H. Plans for The Sixth International Symposium on Solubility Phenomena**

Dr. Angela Danil De Namor indicated that plans were moving ahead for the 6th International Symposium on Solubility Phenomena to be held in Buenos Aires, Argentina. She reported that she had been in contact with Dr. Fernandez-Prini (Argentina) and he has agreed to be the contact person in assisting with the organization of the Symposium. The Argentinian Chemical Society has agreed to collaborate. Dr. Namor would work through the European Community Commission on Science and Technology to secure funding for the conference. A tentative date for the Symposium was suggested as the third week in August, 1995. It should also be noted that Professor H. Gamsjager extended an invitation to hold the 7th ISSP in Leoben, Austria. This invitation will be discussed at the next Commission meeting in Lisbon.

### **I. New Business**

#### **1. Macrocyclic Supramolecular Chemistry as it Relates to Commission V.8 Activities**

Dr. Danil De Namor discussed the growing interest in macrocyclic supramolecular chemistry and recommended that this area could be a separate topic for attention of the Commission. After some discussion on the merits of establishing these "new" electrolytes as a priority area a working group consisting of M. Salomon, A. Danil De Namor, J. Lorimer, R. Tomkins and E. Waghorne was formed to further explore the suggestion. The goal would be to produce a volume of solubilities of Macrocyclic Ligands which would include an evaluation of the thermodynamic data that have been published. Also it was suggested that the topic Macrocyclic Chemistry would be highlighted at the 6th International Symposium on Solubility Phenomena. Also this could be a possible joint project with the Physical Chemistry Division or with Commission V.6 (Equilibrium Data).

#### **2. Cooperation in Science & Technology with Central and Eastern European Countries**

Professor Christo Balarew (Bulgaria) informed the Commission of a proposal for the establishment of a Pan European Scientific & Technological Network for Solubility Studies. Members of Commission V.8 all agreed that this is an excellent proposal and concluded that the Commission should strongly recommend support for this initiative.

The proposal aims to establish firm associations between a number of laboratories from central and eastern European countries with the objective of creating a network to solve both

theoretical and practical problems which involve solubilities. Most of the laboratories suggested for this network are well known and have worked with Commission V.8 on small and independent projects on compiling and critically evaluating solubility data. The need for a close association of laboratories cooperating on new studies relevant to modern problems has long been recognized by Commission V.8, but the establishment of such a network is not within the Commission's charter. The European Communities Commission on Science & Technology has the means to create such a network, and Commission V.8 strongly recommends support of this proposed network.

#### **J. Time & Place of Next Meeting**

The next Commission meeting (19th) will be held during the 37th IUPAC General Assembly in Lisbon, Portugal from August 6-8, 1993.

#### **K. Adjournment**

The meeting was adjourned at 16:30, July 7, 1992.



## SECTION II. REPORTS ON RELATED COMMISSION ACTIVITIES

### A. Reports by National Representatives

#### **Denmark - J. B. Jensen**

The Danish representative reported that with financial support from the Danish National Research Council Professor Valyashko (Russia) will visit the Technical University of Denmark during August, 1992. Discussions will take place on possible new SDS initiatives. It was also reported that two graduate students at the Technical University are currently engaged in the measurements of Solubilities of Tungsten & Molybdenum Compounds.

#### **Finland - P. Scharlin**

The Finish Representative has devoted most of her attention to advancing the volume on carbon dioxide and continues to try to recruit other scientists to the project.

### B. Additional Reports from Member Countries

#### **Japan - K. Sawada, H. Miyamoto**

Kiyoshi Sawada and Hiroshi Miyamoto reported on the progress of volumes on Halates, Alkaline Earth Metal Carbonates and Divalent Metal Carbonates

#### **Russia - B.R. Churagulov**

Professor Churagulov gave an update on progress of SDS volumes currently in progress by Russian Scientists. A total of 13 volumes were detailed.

### C. Reports by Chairpersons

Each subcommittee met as indicated in the agenda. Progress was assessed. An annotated review on the status of volume publication and related activities is attached. Further details may be obtained from individual chairpersons. It was also suggested that the procedure used by Professor H. L. Clever for the Gas Solubility Subcommittee of Soliciting information prior to the meeting was useful in facilitating discussion of progress to the whole Commission.