



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)

December 16, 1994

Dear Colleague:

I enclose the minutes of the 20th IUPAC Commission V.8 meeting which took place at the Hotel Bauen, Buenos Aires, Argentina, August 20-21, 1994. In addition, there are attached summary minutes of the subcommittee meetings.

The 21st meeting of the IUPAC Commission V.8 will take place during the 38th IUPAC General Assembly at the University of Surrey, Guildford, U.K. on August 5-7, 1995. Your participation is urgently requested.

We look forward to seeing you at the next meeting.

Sincerely,

Reginald P. T. Tomkins

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Secretary

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Enclosures

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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 19th Commission meeting held at Lisbon University, Portugal were approved. Professor Gamsjäger noted that the Seventh International Symposium on Solubility Phenomena will be held from July 22-26, 1996 instead of in August as previously announced in item "K" of the minutes. Also on p.4 of the List of Current Programs 12/87 is not a Revised Title as indicated.

C. Report of the Chairman (M. Salomon)

1. The Franzosini Award

Dr. Salomon announced that the recipient of the award for 1994 was Dr. Erich Königsberger (Montan Universität, Leoben, Austria). This award assisted Dr. Königsberger in attending the meeting in Buenos Aires. Recommendations for the 1995 award should be sent to Dr. Salomon.

2. Activities within IUPAC

Dr. Salomon reported that after deliberations on restructuring, the number of Titular Members on Commission V.8 was now reduced to six and there was a possibility of a further reduction. This action would definitely create problems in the future as the travel budget for such a large Commission is already strained to the limit.

The general idea of the restructuring was to create a pool of Titular Members with four members being allocated to each division so that Limited Lifetime Commissions (LLTC) could be established to work on topical problems. It is proposed that such special Commission projects would last from 2-4 years. Professor A. Hulanicki (Chairman, Analytical Chemistry Division) favored the creation of a LLT Commission on Macrocyclic Ligands in Cooperation with the Commission on Equilibrium Data (V.6). Some members of Commission V.8 suggested the possibility of creating a new Commission for this particular area of Macrocyclic Chemistry instead of a joint project. However, this approach did not gain universal agreement with the membership. It was also pointed out that the Commission should try to avoid diluting its main effort.

Dr. Salomon then led a discussion related to the visibility of the work of Commission V.8 both within and outside IUPAC. It was felt that our work is not well understood by IUPAC. It was agreed that we need to prepare some background information on the SDS which outlines the objectives, the accomplishments and focuses on important applications of the work and also includes a general overall plan of action. We need some coverage in magazines such as Chemical and Engineering News (the weekly ACS publication) and Chemistry International and other publications published by Chemical Societies in various countries. A committee formed from the Sub Committee Chairpersons will prepare relevant information by December 31, 1994. Professor Lorimer agreed to serve as the editor for the material. Input from any members of the Commission

is encouraged. The information obtained would also be used for potential contributors to the project as well as for the consumers. Dr. Danil De Namor felt that the Commission should have a slick presentation available with overhead transparencies or slides for use at conferences, etc.

Dr. Salomon then reviewed the financial state of the Commission. A loss of income from both the union and the previous publishers of the Series, Pergamon Press (USD3000 per year) has meant a reduction in the overall budget for the Commission with the main impact being on assistance for travel to meetings. It was recommended that where possible funds should be solicited from industrial corporations but it was important to avoid soliciting the IUPAC Company Associates (see Appendix to Minutes). In all cases where funding was being requested from private industry, Commission members were urged to inform their National Adhering Organizations (e.g. Royal Society, U.K.) It was noted that Dr. Kathryn Bullock was currently involved in exploring possible support from ILZRO for the volume on Lead Sulfate. The membership also expressed a preference that financial support from private industry should be given directly to universities rather than through IUPAC.

Review of Financial Obligations of Oxford University Press (OUP) and IUPAC

Although the new publishing agreement with Oxford University Press (OUP) was fully discussed by Prof. Lorimer at several Commission meetings during the negotiation phase and subsequent to signing of a contract, numerous colleagues appear to be uncertain about important details of this new contract. The main features of this contract are reviewed in the Editor-in-Chief's report below. To clarify the financial arrangements, the following details are provided. When Pergamon Press terminated the publishing contract with IUPAC, all agreements regarding separate payments for typing fees, compilation fees, evaluation fees, honoraria, etc. were also terminated. The new publishing contract with Oxford University Press provides fees for contributors (see below), but makes no distinction between types of contributions (typing, compiling, indexing, etc.). Upon termination of this contract, the liability for any monetary advances made by Pergamon towards fees for volumes in preparation was transferred to IUPAC: i.e. any advanced payments made by Pergamon were charged to IUPAC. Thus IUPAC must deduct these advances from any income provided by the new publisher. The new contract with OUP is simply based on a profit/loss arrangement. Under this new contract, IUPAC is guaranteed payment of GBP 1000 upon receipt of each volume by the publisher. These funds are sent directly to the IUPAC Secretariat, and IUPAC agreed to make all of these funds available to the authors based on the number of pages produced by each author. If OUP makes a loss, IUPAC will be expected to make up 50% of the loss, and if OUP makes a profit, then these profits are shared amongst all (OUP, IUPAC, authors). Since there is little information available at this time on profits from future sales, we must wait until this information becomes available before it can be decided how these profits can be equitably shared. An annotated CLAIM FORM is attached for information purposes.

Proposal to initiate a project (PIP) forms

Requests for PIP forms should be sent to the Commission Chairman. Also note that Dr. Salomon has a template for microsoft word which can be sent to anyone who needs to prepare a PIP form.

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

1. New Contract with Oxford University Press

Prof. Lorimer reported that the new contract with Oxford University Press (OUP) for the publication of the SDS volumes was signed on February 24, 1994. The contract is valid for a period of 2 years.

The main features of the contract were as follows:

- The series would be published as a journal with four issues per year. The volumes would look physically the same as earlier ones.
- A limit of 1484 pages was set for the 4 volumes (an average of 371 pages/volume). This size limit included title pages, indices, etc. OUP agreed to accept volumes as small as 192 pages or as large as 496 pages.
- Prof. Lorimer strongly recommended that the 371 pages should be established as the working limit. If a particular volume exceeded this limit, a special agreement would have to be made as another volume for that year would have to be smaller. NOTE: The four volumes published in 1994 comprise a total of almost exactly 1484 pages.
- Fifteen gratis copies of each volume would be provided (these include the editors' copies).
- OUP agreed to pay a GBP1000 (~ USD1500) compilation fee per volume in advance. Subsequent payments would be dependent upon sales of the volumes in years 2 & 3 etc. The question of how to divide these monies needs addressing.
- Subscription prices for 4 volumes were set at GBP265 (USD375) for 1994 and 1995. Retail price was set at GBP75 (USD115) per volume for 1994 and GBP80 (USD120) for 1995. A 25% reduction was available for IUPAC members.
- In order to accomplish the publication of 4 volumes per year, the following production schedule was recommended for delivery dates of the CRC of each volume to Oxford University Press:

January 12
April 12
July 14
October 16

The volumes should be delivered to the IUPAC Secretariat at least two weeks before these dates. Oxford University Press indicated that bound copies of each volume would be available six weeks after receiving the final copy of the manuscript.

- The following volumes have been published in 1994:
 - vol. 54. Polycyclic Aromatic Hydrocarbons in Pure and Binary Solvents. W.E. Acree, Jr., ed.
 - vol. 55. Actinide Nitrates. S. Siekierski, S.L. Phillips, J.D. Navratil, eds.
 - vol. 56. Alcohols with Hydrocarbons. D. Shaw, A. Skrzecz, J.W. Lorimer, A. Maczynski, eds.
 - vol. 57. Ethene. W. Hayduk, ed.

- The income from the volumes will be the result of sales. Details are still being negotiated. This is a departure from the previous contract with Pergamon Press.
- OUP will provide marketing questionnaires for each volume. Information gained from these questionnaires would be used for generating publicity materials. Prof. Lorimer requested a list of the next five volumes as soon as possible to aid in special publicity efforts.

2. Revisions to Preparation of Volumes

Prof. Lorimer reported that he had revised all the Introductory Materials for the volumes on Gas/Liquid, Solid/Liquid and Liquid/Liquid. A reduction of all the front matter to ten pages had been achieved. Also, the foreword has been eliminated. All the volumes will have some common material and in addition specific sections will be included for each of the three areas.

Prof. Lorimer discussed several strategies for reducing the total number of pages. Some suggestions were as follows:

- Place two compilations on one page.
- Use smaller spacing for references.
- Include two or more systems per page.
- Eliminate compilations for those pages where the data are considered inferior.
- Simplify the continuation pages for critical compilations by avoiding the repetition of the heading boxes.

Prof. Lorimer then led a discussion on the need to produce a more uniform appearance to future volumes. A uniformity of word processing techniques was desirable. A working party was appointed to set up standards for production with the emphasis being on portability. The Committee chaired by J. W. Lorimer consists of F. Getzen, P. Fogg, A. Maczynski, D. Shaw, M. Salomon and A. Skrzecz.

The need for a new version of the Solubility Data Series Guidelines for Compilers, Evaluators and Editors was recommended by several Commission members. The original version was produced twelve years ago with a revision in 1984. There have been significant changes in format, etc. during the last decade and these need to be included in a new version of the Guidelines. It is anticipated that approximately 100 copies (~ 60 pp each) would be needed with the estimated cost being USD4.00. A suggestion was made to put the Guidelines on a diskette. The same working party noted above will initiate work on the revised Guidelines.

E. Solubility Database Project (D. Shaw)

At the meeting in Lisbon a working party consisting of F. Getzen, A. Maczynski, D. Shaw (Chair) and A. Skrzecz was appointed to develop standard ASCII file formats for the electronic storage of compiled & evaluated solubility data.

In June 1994, the working party circulated information about the file formats that have been developed. After receiving comments, draft guidelines containing specific directions for electronic data format have been completed. The material contains about fifty examples. Further

suggestions are needed for refinement. The final draft of the recommendations is scheduled for November 1994. After approval by Dr. Salomon in consultation with other members of the Commission, their recommendations will be submitted to the Committee for Chemical Databases (CCDB) by February 1995 for their consideration at the next General Assembly meeting at the University of Surrey in August 1995. It is expected that the CCDB will suggest possible databases.

In the course of the discussions led by Professor Shaw, it was strongly recommended that all future volumes of the SDS should be accompanied by electronic storage (data archive). There should be a clause in the contract with OUP that they will accept computer based volumes which they can print if required. Also, material from the data archive could be abstracted for future databases.

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

G. Hefter and C. Young were unable to attend the Commission meeting and no information on the progress of the volume was available at that time. However, Dr. Mark Salomon was in contact with G. Hefter immediately after the meeting and the following information on this project is summarized below:

1. Contributions in first draft form have now been received from more than 70% of contributor groups.
2. Authorship and the arrangement of contributions have been further clarified (see Outline in Appendix). Only relatively minor changes are expected in the future.
3. The Editors had an intensive working session over the period 24-30 August 1994 in Perth, Australia.
4. The Editors have contacted all contributor groups with detailed comments on their manuscripts along with a request for revised versions by the end of January 1995.
5. To assist contributors the Editors have produced and distributed a set of Guidelines for Authors (see Appendix).
6. The plan is to have a completed (but not necessarily final form) manuscript by the IUPAC General Assembly at Guildford in 1995.
7. It is anticipated that a decision on a publisher will be made at Guildford.

G. *Horizontal Programs*

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

Dr. Fogg reported on discussions with Professor P. Warneck (Commission VI.4, Atmospheric Chemistry) and confirmed the interest in collaborative efforts between the two Commissions. At the Commission meeting in Buenos Aires it was agreed that preliminary work should be started on a proposed project entitled: "Solubility of Vapors of Liquids Boiling above 298K". The initial effort will be confined to the evaluation of solubilities of vapors in pure water and sea water. A preliminary literature survey will be carried out during the next few months to determine the extent of the data that are available so that the project can be planned in detail. It is expected that most of the relevant data will be in the form of partial vapor pressure measurements on solutions of organic liquids in water. Solubilities of organic vapors of

environmental importance will be given high priority. The status of the proposed project will be discussed at the next Commission meeting at the IUPAC General Assembly in August 1995.

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

Dr. Namor discussed plans for a cooperative project between Commission V.8 and V.6 on Macrocyclic Ligands. One proposed volume will contain solubility and thermodynamic data for all macrocyclic ligands. Solubility data would be the responsibility of Commission V.8 while the equilibrium data such as enthalpies of complexation and heat capacities would be undertaken by Commission V.6. A recommendation was made to prepare a special volume (monograph) outside the normal SDS series. This recommendation was approved. It was suggested that data for 18-crown-6 should be compiled, together with evaluations as an example of a macrocyclic ligand when a large amount of information exists.

H. Sixth International Symposium on Solubility Phenomena (A. Danil de Namor)

Dr. Namor reported on the status of the Sixth International Symposium on Solubility Phenomena which was held immediately after the Commission meeting (August 22-26, 1994) at the Hotel Bauen, Buenos Aires, Argentina. Approximately ninety delegates were expected to attend, including twenty-three scientists from Argentina and three from Mexico. The Scientific Program consisted of nine plenary lectures and seven invited lectures. A poster session had twenty-four presentations. There were also twenty-one contributed papers. Sponsorship for the conference had been difficult. The European Union and IUPAC provided a large fraction of the financial support which was used to assist scientists for travel to the conference. Also the Soros Foundation provided support for a number of Russian and Bulgarian colleagues.

I. Second International Symposium on Macrocyclic Ligands for the Design of New Materials (A. Danil de Namor)

Dr. Namor reported on plans for the Second International Symposium on Macrocyclic Ligands for the Design of New Materials which was held after the Sixth International Symposium on Solubility Phenomena on August 29-September 1, 1994. Eighty four delegates attended the symposium with a very good representation from Latin America, including Peru (17), Argentina (15), Chile (4) and Uruguay(2). The Scientific Program consisted of nine plenary lectures, eleven invited lectures and eight contributed papers. A poster session had twenty-four presentations. In addition, there was a Round Table discussion on "Academic and Industrial Links between Latin America and Europe in Research".

J. Future International Symposium on Solubility Phenomena

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

Dr. Gamsjäger reported that the Seventh International Symposium on Solubility Phenomena will be held from July 22-26, 1996 at Montanuniversität, Leoben, Austria. A meeting of the Solubility Data Commission will be held immediately before the Symposium on July 20 & 21, 1996.

Dr. Gamsjäger proposed a conference program which was a balance between established and popular themes together with some new fields such as Solubility and Metallurgy. Drs. P. Fogg and E. Waghorne were appointed as conference editors. The first circular announcing the conference will be ready in November 1994. Some suggestions for Plenary and Invited Lectures have already been made. Additional input is needed.

2. Eighth International Symposium on Solubility Phenomena (1998)

Dr. Salomon indicated that the Commission had received a formal invitation from Professor H. Miyamoto to hold the 8th International Symposium on Solubility Phenomena at Nigata University, Japan.

Dr. Mariã Clara F. Magalhaes also proposed hosting the meeting at the University of Aveiro, Portugal.

The site for the 8th ISSP will be decided at the next Commission meeting in August 1995.

K. National Representative

Dr. Salomon announced that Professor Wenchuan Wang, Beijing University of Chemical Technology had been proposed as a National Representative from China. The Commission accepted the nomination which was subsequently approved by IUPAC.

L. 21st Annual Commission V.8 Meeting

The 21st Annual Commission V.8 meeting will be held on August 5-7, 1995 in conjunction with the 38th IUPAC General Assembly at the University of Surrey, Guildford, U.K.

M. Adjournment

The meeting was adjourned at 5:00 p.m. on August 21, 1994.

SECTION II - REPORTS ON RELATED COMMISSION ACTIVITIES

A. REPORTS BY NATIONAL REPRESENTATIVES

DENMARK - J. B. JENSEN

The Danish representative, a member of the Pan-European Scientific and Technological Network on Solubility Studies contributed to an application for support to the European Union, Commission for Cooperation with Central and Eastern European Countries for a project entitled: "Solubility Studies Connected with Recoveries of Industrial Waste".

As the Commission V.8 representative for revisions to the IUPAC Orange Book, Dr. Jensen has received a copy of the IUPAC Search database from Professor A. Hulanicki.

IRELAND - E. WAGHORNE

Dr. Waghorne contributed an item on the Solubility Data Project to the Irish Chemical News and continues to seek contributors to the project.

PORTUGAL - C. MAGHALHÃES

Dr. Magalhães reported that the recruitment of Portuguese contributors to the project is in progress.

B. REPORTS BY SUB-COMMITTEE CHAIRPERSONS

Each Sub-Committee met as indicated in the agenda. Individual reports are attached. Status reports for the volumes under preparation will be given only for those volumes of authors who are either present at the meeting or have written a progress report to the sub-committee chairperson prior to the meeting.