



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 9, 1990

Dear Colleague,

I enclose the minutes of the 15th IUPAC Commission V.8 meeting which took place at the University of Lund, Lund, Sweden during the 35th IUPAC General Assembly August 10-13, 1989. In addition, there are attached summary minutes of the Subcommittee meetings.

The next (16th) meeting of the IUPAC Commission V.8 will be held on July 30-31, 1990, just prior to the 4th International Symposium on Solubility Phenomena, August 1-3, 1990 at the Rensselaer Polytechnic Institute, Troy, New York, U.S.A., 12180-3590. Your participation both at the meeting and the Symposium is urgently requested.

I look forward to seeing you in Troy this year and offer my belated wish to you for a happy New Year.

Sincerely,

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Secretary

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Minutes of the 15th Commission V-8

meeting held at

University of Lund, Lund, Sweden

during the 35th

IUPAC General Assembly

August 10-13, 1989

Section I. DISCUSSIONS OF THE FULL COMMISSION

A. List of Attendees

H. Akaiwa (Japan), R. Battino (USA), H. U. Borgstedt (FRG), K. R. Bullock (USA), H. L. Clever (USA), G. Coffy (France), M. T. S Cohen-Adad (France), R. Cohen-Adad (France), J. J. Counieux (France), T. P. Dirkse (USA), R. Duhlev (Bulgaria), J. Eysseltova (CSSR), V. Filippov (USSR), P. G. T. Fogg (UK), H. Gamsjäger (Austria), F. W. Getzen (USA), L. H. Gevantman (USA), H. Grünbauer (Holland), C. Guminski (Poland), H. Gryzlova (USSR), G. T. Hefter (Australia), J. B. Jensen (Denmark), N. Kebir-Ariguib (Tunisia), S. Krause (USA), K. Lambert (UK), J. W. Lorimer (Canada), A. Maczynski (Poland), Z. Maczynska (Poland), A. Mather (Canada), T. Mioduski (Poland), H. Miyamoto (Japan), A. D. de Namor (UK), M. Salomon (USA), J. Sangster (Canada), D. Shaw (USA), A. Skrzecz (Poland), B. H. Takman (USA), R. P. T. Tomkins (USA), V. Valyashko (USSR), J. Vanderdeelen (Belgium), E. Wilhelm (Austria), C. L. Young (Australia).

B. Approval of Minutes and Agenda

The Chairman called the meeting to order at 9:15 AM. The minutes of the 14th meeting were approved as was the agenda of the 15th meeting. A general welcome was extended to the attendees by the Chairman.

C. Report of Chairman/Editor-in-Chief

1. Contract and Manuscript Preparation

The Chairman announced the successful conclusion of the IUPAC/Pergamon Press contract in January 31, 1989, calling for Pergamon to publish the Commission's output until 1992 with an option for annual renewals. Copies of the final contract are in the hands of titular members and subcommittee chairman. The two singular changes to be noted are the lowering of price per volume and the uniformity of price across countries. Consistent with these changes were the new responsibilities for the submission of properly prepared

manuscripts. The Chairman stressed the need for document preparation to conform to the Commission guidelines, both basic and supplement. Units and symbols are to be followed as displayed in the IUPAC Green Book. A new committee, the Interdivisional Committee on Nomenclature and Symbols (IDCNS) will scrutinize all documents for conformance with IUPAC symbols and nomenclature and will prove troublesome if such procedures are not followed. Another need to prepare clean and complete manuscripts is that attention be given to reviewers' comments. Indications were that internal reviews were working well, but the need continued to exist for good external review. After some discussion on how to approach this problem, the conclusion reached was that editorial board members could be used. Other items related to manuscript preparation included a need for a 200-word summary that both described the contents of the volume and yet was promotional in nature. Finally, the Chairman presented a flow plan for document submission by the volume editors and subcommittee chairmen which reflected the complications in the process. Upon further discussion, it was decided that this description was not adequate, and G. Hefter was assigned the task of rewriting the instructions which, when accepted, will replace page 4 of the guidelines. A copy of the changes is attached.

2. Finances

The operating budget of the Commission continues low. For that reason, not all members asking for financial support could be aided in coming to Lund.

Dr. Rumen Duhlev was introduced as the recipient of support from the Franzosini Fund. It was decided that perhaps the ground rules governing the use of the funds could be broadened at the Chairman's discretion.

A report on income from royalties on all of the volumes was given by L. H. Gevantman. It would appear that there is a decrease in series sales and that the more recent volumes are not selling well. It also seems that the cost of preparing a volume has risen on the average by \$1,000.

3. Analytical Division Reorganization Affecting Commission V.8

The Chairman reported on the meeting which took place at the Division level in which proposed changes in Division makeup of commissions would have reduced the autonomy of Commission V.8. After a long discussion in which arguments against the plan were delivered primarily by the officers of V.8, the Division decided not to adopt the proposed changes and opted instead to create a new commission. Subsequent indications were that this plan would be approved by the Union Council.

D. Guides to Commission's Future Work

F. Getzen presented the results of the Task Group on Setting the Commission's Future Work Philosophy. It consisted of a survey of member opinions to six questions regarding Commission activities and future planning. The overall response to 152 inquiries was greater than 30 percent. Although some range of opinion was reflected in the responses, the general conclusions summed up in the report were as follows:

The comments made and the ideas proposed relative to the work and purpose of the Solubility Data Commission were overwhelmingly positive. One can assume that observations and comments were based upon knowledge and experience considering the fact that those who replied to the survey have been directly involved with various aspects of Solubility Data volume preparation and publication, some for many years.

Regarding the specific issues addressed in the survey, the following summaries are made:

1. Future of the Solubility Data Series. The overwhelming opinion was expressed that the series should remain open-ended to accommodate newly generated solubility data and emerging fields of interest. However, concerns related to the recruitment of compilers, evaluators, and authors and to the future rate of volume production (which may decrease in time) were expressed.

2. Focused Volume Preparation. Positive support was expressed for the production of special topic volumes. In a broad sense, such volumes might be appropriate as update and combined topic volumes, and they might be useful for reducing the amount of unused material in the hands of the Commission.

3. Fate of Unused (Unassigned) Material. A consensus appeared that the Commission should find definite ways to use the unassigned material (data sheets, evaluations, etc.) either by publication in combined, or special, topic volumes or by storage in accessible computer files for public use. At least the material should be cataloged and publicized within the commission (for constructive use) as quickly as possible. Also, it should be reviewed on a periodic basis.

4. Updating Published Volumes. There was good agreement that updating should be done after some period of years (10-12). These update volumes might include several systems, in order to satisfy the volume page requirements, or they might be placed in a different format from regular volumes in the series.

5. Electronic Publication. There was considerable support for expanded efforts in "electronic publishing." The phrase suggested to most repliers the use of computers to organize and edit the material (data sheets, evaluations, tables, graphs, etc.) for publication and the use of high quality printers such as laser printers for "camera-ready copy" production. Many, for legitimate reasons (lack of facilities, lack of experience), express reservations on this point. Still, the overall response was positive. It appears that the Commission should support, as much as possible, those who might wish to exploit this area without obstructing the initiatives of those who are not able to do so.

The question of the development of a searchable database was addressed by many and the idea was supported with some reservations. The concerns focused on possible costs of development, expertise within the Commission, and diluting the efforts of the Commission members (priorities). A strong recommendation was made that the Commission coordinate its efforts with others (in IUPAC) working along similar lines.

6. Volume Publicity. There was general agreement among a reasonable sample that the Commission and its members and associates, individually, should provide meaningful assistance to the publisher of the Solubility Data Series. However, there also appeared some feeling of resignation concerning the realities of volume sales of this type of publication. The question of the price per volume arose in a few cases, but not many.

During the discussion period that followed, it was agreed that sponsorship of symposia by the Commission should also be strongly endorsed. The overall conclusion of the report supports the unanimity of opinion by Commission members to ongoing Commission activities and their dedication to their continuance.

E. Task Group on Duties of Commission Officers: Official and Semi-Official

A final version of the report outlining the duties of those holding either official or unofficial positions within Commission V.8 was presented by R. Battino. This report had been presented but not approved at the 13th meeting of the Commission. The Commission gave its endorsement to the report and adopted its provisions as its official stance on official responsibilities.

F. Report of the Database Automation Task Group

R. P. T. Tomkins presented the outcome of a one-year review of the adoption of the Maczynski "Floppy Book" format to the production of an automated data. The report was favorable and recommended that a first attempt should focus on well-evaluated systems, high user interest, and being user-friendly by reducing the information to an essence. A copy of the final report is available upon request from R. P. T. Tomkins. Subsequent to a meeting with the IUPAC Chemical Database Committee, whose preliminary response was positive to the sample format, the Database Automation Task Group was disestablished and a new "Task Group on Implementation of Automated Databases" was established under the chairmanship of A. Maczynski. Assuming final approval and funding by the IUPAC Chemical Database Committee, Maczynski and his group are to produce a diskette containing the solubility of $C_1 - C_{36}$ hydrocarbons in water. Guidance for final format and other aspects of this task will be relayed to Maczynski as they become known.

G. Status of Fourth and Fifth Symposia on Solubility Phenomena

Prior to hearing about the 4th and 5th Symposia, A. D. de Namor was asked to review the results of the 3rd Symposium, which she chaired. She noted that the Symposium was successful. The Plenary Lectures were published in IUPAC Pure and Applied Chemistry and many others in the Journal of the the Chemical Society, Faraday I. Some \$2,500 remains for transfer to support future meetings. She cautioned that to maintain strict control over papers for scientific quality, authors must be present at the meeting to present either oral or poster presentations and that certain vagaries regarding authors' needs for presentation should be clarified by the authors well prior to the meeting.

S. Krause then described plans for the 4th Symposium on Solubility Phenomena. It will take place August 1-3, 1990, following the Commission meeting at Rensselaer Polytechnic Institute, Troy, New York, USA. The first circular has engendered approximately 180 replies from 26 countries. There will be eight plenary lectures including a memorial lecture to A. S. Kertes. A second circular will be issued in December 1989.

The 5th Symposium, originally slated for Leningrad in 1992, has been shifted to the N. S. Kurnakov Institute of General and Inorganic Chemistry in Moscow. V. Valyashko cordially extended the invitation on behalf of the USSR Academy of Sciences and promised a firm date (July-August) by summer of 1990. He also promised to look into arranging a trip to Leningrad for those attendees who wished to visit that city.

H. Recruiting

The Chairman viewed recruiting as a continuing problem. After some discussion the Commission membership was urged to continue seeking new contributors. A suggestion for a paid translator was voted down.

I. Suggestion by G. Hefter to issue a Volume Documenting the Experimental Determination of Solubilities

Individual chapters by chosen experts would cover all of the Commission's activities. Although some overlap exists with a book being authored by R. Cohen-Adad, the Commission established a working group to develop the idea further and report back at its meeting in 1990. The task group consists of G. Hefter, C. Young, and J. J. Counioux.

J. Meeting with the Pergamon Representative

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K. Lambert, a senior publishing manager of Pergamon Press, reviewed a number of issues that need further explanation. The question of gratis copies was explained as an internal Pergamon error, and Lambert assured the Commission that such copies were and will in the future be held to a minimum. A gratis copy for Russia was added as a possibility. The use of laser printers for camera-ready copy was endorsed by Lambert as the most desirable, but dot matrix printer output would be acceptable provided the product was clear and readable. Lambert cautioned volume editors to number their manuscript pages in the lower right corner in pencil. Finally, he reviewed the status of the present number of manuscripts with Pergamon (3) and urged the Commission to meet its quota of six. He emphasized the need for the Commission to be realistic in its prediction of volumes for 1990 and suggested that it was now time for such a submission. He indicated his willingness to discuss any problem that might arise in future. His address is Mr. Keith Lambert, Senior Publishing Manager, Engineering and Material Sciences, Headington Hill Hall, Oxford OX3 OBW, UK. His telephone is (0865) 64881, Telex 83177, and Fax 0865-60285.

K. Meeting with Analytical Division Officers

G. Nancollas and G. den Boeff visited the Commission for a review of activities now ongoing in the Analytical Division and how they might affect the Commission's work. They emphasized the use of proper units and symbols as discussed earlier in the minutes under the Chairman's report. They endorsed the need for subject matter in future volumes that related to the solution of acknowledged national and global problems. They also endorsed the Commission's activities in the construction of an automated numerical database.

L. Time and Place of the Next Meeting

The next meeting of Commission V.8 (16th) will be held on July 30-31, 1990, just prior to the 4th International Symposium on Solubility Phenomena, August 1-3, 1990, at the Rensselaer Polytechnic Institute, Troy, NY 12180-3590, USA.

M. Adjournment

The meeting was adjourned August 13, 1989 at 4:30 PM.

Section II. REPORTS ON RELATED COMMISSION ACTIVITIES

A. Reports by National Representatives

Belgium - J. Vanderleelen

Three levels of activity were pursued: first, introducing and promoting the Commission's activities to other Belgian scientific organizations; second, a report was delivered to the Comité National Belge de Chimie proposing an industrial solubility data project on phospholipids; third, completion of a first draft on a volume on earth alkaline metal carbonates.

China - Fu Jufu

Eight scientists within China were contacted with proposals to join the Commission's work. Each declined because of previous commitments. Several data sheets were completed as contributions from the Chinese literature to ongoing Commission projects, and articles from the Chinese literature were sent on request.

Czechoslovakia - J. Hala

One new contributor has been recruited and is working on the solubility of polymers. A publication slated for the CCS Bulletin regarding future goals of the Commission is also being planned.

Denmark - J. B. Jensen

Collaborative efforts with USSR scientists have resulted in mutual visits and further progress on Commission projects. There is continued effort on recruitment.

India - C. Kalidas

Six Indian scientists continue to contribute to the work of the Commission. Lack of adequate funding and resources continue to retard the recruitment of new contributors. However, some scientists and one institution (Central Salt and Marine Chemicals Research Institute - Bhavnagar) have expressed interest in the project.

Japan - H. Akaiwa

Difficulty in finding young scientists as contributors to the Commission's work hampers progress in Japan. Nevertheless, three scientists remain as active compilers.

Law! Malaya - K. H. Khoo

Two volumes are in progress, one of which has reached completion. Active collaboration with other country scientists has spurred these efforts.

The Netherlands - H. J. M. Grunbauer

Recruitment of new contributors to the Commission's work continues. An article describing the goals of the solubility data project is planned for publication in the KNCB (Royal Dutch Chemical Society).

Poland - A. Bylicki

Sixteen scientists throughout Poland continue their contributions to Commission projects. Two new projects are being initiated. The work in Poland continues to be of great importance to the Commission's program.

United Kingdom - M. R. Masson

Although no progress is reported, the suggestion to involve national representatives in a more specific way bears noting. This has been done in other instances.

United States - K. R. Bullock

Considerable activity on Commission projects continues in the United States. A request that contributors submit some mention of their work annually to the national representative is considered useful.

Union of Soviet Socialist Republics - V. M. Valyashko

The scientific effort in the USSR has grown with over 20 Soviet scientists taking part in the Commission's work. Thirteen volumes are in various stages of completion. Two new efforts on molten salts are being initiated. Some difficulty is being experienced with finding English speaking coeditors.

The Soviet Union has kindly offered to host the 5th International Symposium on Solubility Phenomena in Moscow, 1992, at the N. S. Kurnakov Institute of General and Inorganic Chemistry.

B. Reports by Subcommittee Chairmen

Each subcommittee met as indicated in the agenda. Progress was assessed. A synoptic view on the status of volume production, publication, and related activities for each is attached. Further details may be obtained from the individual chairmen.

Attachment