



# International Union of Pure and Applied Chemistry

A member of the International Council of Scientific Unions

Analytical Chemistry Division: Commission on Solubility Data

December 9, 1985

Dear Colleague:

I enclose the minutes of the Commission V.8 meeting which took place at the IUPAC General Assembly in Lyon, on August 31 to September 3, 1985. In addition, there are attached summary minutes of the subcommittee meetings, financial data, a synopsis of the new Pergamon contract and a proposed agenda for our meeting in 1986.

I have already received a number of suggestions for discussion items under new topics and hereby solicit your suggestions for additional agenda items.

I look forward to your attendance at our Commission's meeting in New Jersey.

Holiday greetings and best regards.

Sincerely,

Lewis H. Gevantman  
Secretary

Enclosures

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Minutes of Commission V.8 Meeting

held during

IUPAC 33rd General Assembly

Lyon, France

August 31-September 3, 1985

Section I. DISCUSSIONS OF THE FULL COMMISSION

A. List of Attendees

H. Akaiwa (Japan), R. Battino (USA), G. Bohnsack (FRG), K. Bullock (USA), R.W. Cargill (UK), C. Y. Chan (Malaysia), H. L. Clever (USA), G. Coffy (France), R. Cohen-Adad (France), M. T. Cohen-Adad (France), J. J. Counieux (France), T. P. Dirkse (USA), J. Eyssaltova (Czechoslovakia), P. Fogg (UK), P. Franzosini (Italy), J. Fritz (USA), J. Fu (China), Z. Galus (Poland), F. W. Getzen (USA), L. H. Gevantman (USA), H. Grunbauer (Netherlands), J. Grzybowski (Poland), C. Guminski (Poland), J. Hala (Czechoslovakia), W. Hayduk (Canada), G. Hefter (Australia), C. Hirayama (USA), J. B. Jensen (Denmark), C. Kalidas (India), R. Kaliszan (Poland), A. S. Kertes (Israel), K. Kimura (Japan), D. Kosanovic (Yugoslavia), I. Lambert (France), K. L. Loening (USA), J. W. Lorimer (Canada), A. Maczynski (Poland), Z. Maczynska (Poland), T. Mioduski (Poland), H. Miyamoto (Japan), A. D. de Namor (UK), S. Otsuka (Japan), R. Piekos (Poland), A. Regosz (Poland), M. Salomon (USA), A. Sebaoun (France), D. G. Shaw (USA), A. Skrzecz (Poland), T. Sokoloski (USA), A. Szafranski (Poland), R. P. T. Tomkins (USA), C. Treiner (France), A. Watanabe (Japan), E. Wilhelm (Austria), B. A. Wolf (FRG), C. Young (Australia).

B. Approval of London Minutes and Lyon Agenda

A correction was noted in page 4 of the minutes in which reference to the polymer solubility effort by Wolf was couched in terms of a feasibility study. This is not the case inasmuch as the full Commission has approved this area of endeavor. Thus, B. A. Wolf has full authority to proceed actively toward producing a volume on polymer solubility. The minutes were then approved unanimously with the above correction.

The agenda was approved unanimously noting some shifts in meeting times which included a conflict with the Analytical Division general meeting.

C. Chairman's Report

The meeting was called to order at 11:30 a.m. by A.S. Kertes. After formally welcoming the attendees and thanking Prof. Cohen-Adad and his able staff for their efforts in making the Commission welcome in Lyon, he announced the elevation of G. A. Yagodin to the position of Minister of Higher Education in the U.S.S.R. Congratulations were sent on behalf of the Commission.

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The Chairman reviewed the events of the past year noting that a publication agreement for the SDS had been signed by IUPAC and Pergamon Press. He pointed out that support of the Commission's work would come from royalties on the sale of volumes. A balance sheet for calendar year 1984 is enclosed as Attachment 1 to describe the financial and sales picture of the SDP as prepared by Pergamon Press.

The Chairman asked the Secretary to read the salient clauses of the agreement to the Commission. A synopsis of these statements is given in Attachment 2.

Some discussion arose concerning the high price Pergamon charged for individual volumes. A resolution by R. Battino was approved to ask IUPAC to urge Pergamon to sell individual volumes at a uniform price - for example, the price in Canada exceeds \$100.00 (U.S.) - and if possible to fix the price at \$35.00 (U.S.) if the individual promises not to resell the volume.

The Chairman expressed his satisfaction with the outcome of the 1st International Symposium on Solubility Phenomena. The meeting attracted about 75 attendees with balanced distribution from North America and the rest of the world.

A review of the IUPAC's position concerning computerized solubility data indicated that it intended to set up a permanent committee to deal with all automated data projects. The Commission was joined by Dr. S. R. Heller who would serve as Coordinator for the IUPAC Committee on Chemical Data Bases and the Commissions. Heller fielded questions on how Commission V.8 should proceed in developing a formal project under IUPAC. His recommendations were referred to R. P. T. Tomkins and the Task Group on Automated Solubility Data which would meet and devise a procedural plan.

D. Status of IUPAC-Pergamon Press Contract

This item was covered in the Chairman's remarks. He added that he was pleased with the contract and that the contract provided flexibility due to its clauses allowing for annual renegotiation.

E. Data Automation

R. P. T. Tomkins reviewed the history of the Task Group and, in particular, the development of a position paper and the events of a meeting held with Pergamon Press representatives in the Washington, D.C. area in early May, 1985. The latter had resulted in having H. L. Clever and J. W. Lorimer send data sheets recorded on diskette to Pergamon for reproduction. To date, no response has been received from Pergamon. Following discussion on the pros and cons of dealing with Pergamon, Kertes summarized by charging the Task Group to deliberate on:

1) The need to provide camera-ready copy to Pergamon and how best to accomplish this task expeditiously. The Commission wished to retain as much flexibility in accomplishing this task as would be possible.

2) The Task Group should recommend how best to distribute among Commission members the Pergamon payment of \$6,000 (U.S.)

The Task Group met to consider these points and recommended that a pilot project aimed at extracting the critically evaluated data for entry into a database be proposed to IUPAC. The work would be performed at Emory University under H. L. Clever's direction. An estimated cost of approximately \$15,000 (U.S.) was envisaged. R. P. T. Tomkins was assigned the task of preparing the proposal for submission to IUPAC.

In addition, the Task Group recommended that the \$6,000 (U.S.) be used to purchase printers of high quality for those individuals who could usefully serve as preparers of camera-ready copy. The spending plan would give highest preference to a laser printer at Emory with others being recommended considering need and cost. A. S. Kertes was given the spending authority to disburse these funds on written recommendation from the Task Group Chairman.

#### F. Status of the Solubility Data Center

H. L. Clever continues to operate the Solubility Data Center at Emory University in Atlanta, Georgia, U.S.A. He sees the operation continuing for another 5-6 years. He has some gas solubility data and solid (metal salts) data stored in a file. Questions on support for the operation of the Center resulted in suggestions for soliciting industry and also preparing a flyer which would be distributed at the next solubility symposium. Clever will prepare a flyer.

#### G. Report on 1986 Solubility Symposium

M. Salomon described the progress to date. The first circular attracted 115 responses. Six plenary lectures were planned. A second circular would soon be issued. Sponsorship and funding support for the Symposium was being requested from professional societies (IUPAC has approved), U.S. Government agencies, and industry. The timing of the meeting is again planned to adjoin meetings dealing with calorimetry and thermochemistry. In all, the planning for this meeting is proceeding satisfactorily.

#### H. Volume Updates; New Data, Errata

R. Battino indicated that errata and new gas data were being held at the Solubility Data Center. He recommended that other subcommittees adopt similar schemes. He estimates approximately 380 pages are available for an update volume on gas solubility. Escalation of new data presents a problem in keeping up with the literature. The Commission considered the need for publishing updates vs. new topics and opted for a continued emphasis on publishing volumes on new topics.

#### I. Status of the Cumulative Index

C. L. Young described the format of the cumulative index (Volume 19) and the indexing system employed. This volume should issue in October. He indicated that Volumes 1-24 are now recorded on floppy disk. He asked that all editors sending manuscripts for indexing use their national

postal service rather than freight shippers and mark the package either "PRINTED MATERIAL" or "TYPESCRIPT" to avoid loss and delay in reaching him.

#### J. Nomenclature

K. Loening described his interactions with Commission members as generally satisfactory. R. Piekos raised a question on the use of systematic names. When using other than Chemical Abstract names, Loening urged that clarity and flexibility be exercised by the author. Following further discussion dealing with nomenclature, a standard format for reporting the Commission's output was proposed by Loening. He will send his proposal to Lorimer and Gevantman for review. They, in turn, will draft a reply for Kertes' signature.

Lorimer, upon his request, was replaced by R. Cohen-Adad to represent the Commission on the Analytical Nomenclature Commission. He was asked to give special attention to the incorporation of physicochemical symbols, terms and qualities relating to solubility into the analytical chemistry glossary.

#### K. New Topics

The topic dealing with new approaches to the compilation and publication of solubility data volumes was tabled for discussion at the next Commission meeting.

#### L. General Division and Union Topics of Importance

The Commission was visited by F. Pellerin, G. den Boef and G. H. Nancollas who is the incoming president of the Analytical Division. Pellerin commented on a need for updated terms of reference by Commissions but adding that Commission V.8's was satisfactory. He also commented on the next two-year budget which is considered in three parts; administrative, routine projects, and special projects. Nancollas expanded on the treatment of special projects noting that a special project proposal of 100-200 words was acceptable. He considered data base activities to be fit subjects for special project funding. Funding levels were not specified and would depend upon the overall budget of the Division.

The Commission was next visited by P. D. Gujral who is the Managing Editor of the Solubility Data Series. He felt that, in the future, Pergamon would limit volume publication to four. He also suggested that the Union ask Pergamon to publish a cumulative index within 6 months of the termination of the contract. He was asked to urge Pergamon to speed up payments to various editors and contributors.

The new editor of "Chemistry International", Michael Freemantle, was introduced to the Commission. His duties as editor, IUPAC Information Officer, and the newly developed scheme for affiliate members, were described. He wants to increase interest in C. I. with emphasis on affiliate member interaction. He encouraged the submission of newsworthy items from the Commission dealing with its activities. He invited the Commission to submit a 3000 word contribution, to appear in C.I., describing the industrially important aspects of the S.D.P.

R.P.T. Tomkins was asked to author and sign the article for the Commission. Freemantle was asked to consider sending C.I. to people other than titular and associate members and national representatives.

M. Election of Members

R. Cohen-Adad was elected as the seventh titular member. A. Maczinski, J. J. Counioux, M. T. Cohen-Adad, C. Y. Chan, G. Hefter were elected as associate members.

N. Time and Place of Next Meeting

The next meeting of Commission V.8 will be held on August 9-11, 1986 at the New Jersey Institute of Technology, Newark, New Jersey, U.S.A. It will be followed by the 2nd International Symposium on Solubility Phenomena which will run August 12-15, 1986 at the same site.

O. Adjournment

The Commission meeting was adjourned at 4:54 p.m. on September 3, 1985.

Section II. REPORTS ON RELATED COMMISSION ACTIVITIES

A. Reports by National Representatives

1. H. Akaiwa - Japan

Six Japanese contributors are actively at work compiling data sheets all intended for the solid solubilities area. Three Japanese colleagues are working in the area of gas-liquid solubility. General satisfaction was expressed with the work being done in Japan.

2. J. Fu - China

The work of the Commission is highly regarded in China. Some work of interest to the Commission has started and attempts to place other Chinese members on the Commission will continue. Dr. Fu suggested the Commission consider other topics such as interfacial tension.

3. J. Hala - Czechoslovakia

Some disappointment with his country's participation in the Commission's work was expressed. Only he and J. Eysseltova are active. He will continue efforts to recruit more people.

4. C. Kalidas - India

The activity in India continues at about the same level of two to three people. He mentioned some difficulties in obtaining Russian literature translations.

5. J. B. Jensen - Denmark

An article published in the Danish Chemical Society has generated some interest in the Commission's work. He has not as yet gotten any new people but plans to continue his efforts to do so.

6. B. A. Wolf - Federal Republic of Germany

Dr. Wolf reported on his continued efforts to recruit contributors in Germany.

B. Reports by Subcommittee Chairmen

The subcommittees met on two of the four days devoted to Commission matters. D. G. Shaw was acting Chairman for the Liquid/Liquid Subcommittee. Progress on the work of compilers, evaluators and editors was assessed. A synoptic review of the report given by each Subcommittee is attached. Fuller details in the form of a report may be obtained from each Subcommittee Chairman.