



INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
Analytical Chemistry Division
SOLUBILITY DATA COMMISSION (V.8)

Minutes of the 24th Annual Meeting (18th of SDC)

Held at Bandai Civic Hall, Niigata, Japan
August 3 – 4, 1998

The List of Attendees with complete addresses, telephone and fax numbers together with e-mail addresses is attached to these minutes.

1. Introduction of participants

David Shaw, Chairman of Commission V.8 called the meeting to order and welcomed the participants. Attendees were asked to identify themselves and their affiliation.

2. Approval of Minutes of the 23rd Meeting held at the University of Geneva, Geneva, Switzerland, in conjunction with the 39th IUPAC General Assembly.

The Geneva-Minutes were approved.

3. Other Items for Agenda

None

4. Announcements by Secretary

The Secretary requests the participants to fill in the attendance list the actual postal and E-mail addresses, fax and phone numbers. The Commission members are requested to inform the Secretary about their periods of service on IUPAC-bodies. Contributions to the Commission's activities should be stored and handed out on discs so as to hopefully speed up the production of Minutes.

5. Chairman's Report for 1997-1998

Publication

Since the last meeting of Commission V.8 (Solubility Data) during the 39th General Assembly of IUPAC held in Geneva in August 1997, a formal agreement for continued publication of the Solubility Data Series (SDS) through the year 2001 has been concluded with the Journal of Physical and Chemical Reference Data (JPCRD). JPCRD is a well respected journal jointly published by the American Institute of Physics, the American Chemical Society and the U. S. National Institute for Standards and Technology (NIST). Volumes of the SDS will appear as extended articles in JPCRD in a format very similar to our prior volumes and be available to regular subscribers to JPCRD, to subscribers to the SDS and for individual purchase. In addition there is considerable interest at NIST in developing an electronic data base to make solubility data compiled and evaluated by our Commission available over the Internet. This possibility will receive serious and detailed discussion in the coming year leading, it is hoped, to a formal proposal for consideration by the Commission in one year's time. The financial arrangement of our

publication agreement provides a modest improvement over our previous contract with Oxford University Press. This will allow some coverage of the costs incurred by the Subcommittee Chairs and the Editor-in-Chief.

The Union

Reorganization of IUPAC continues to be a topic under active consideration at many levels. The Executive Committee has accepted the report of the Strategic Implementation and Development Committee. This report proposes extensive changes which, if implemented, would take place after 2001. Regardless of the exact form of any changes which are implemented, it is our task to bring forward proposals for projects which respond to important needs and to complete those projects in realistic time frames.

In January 1998 a two day meeting of representatives (Chairman or Secretary) of each of the eight commissions in the Analytical Chemistry Division (ACD) together with the Chairman and Secretary of the Division was held in Idstein, Germany. The principal focus of this meeting was to formulate a consensus position relative to a new structure for the ACD within the Union. The meeting was valuable because a consensus quickly emerged around the concept of responding to the world-wide needs of the chemical community and society with projects which reflect the knowledge and viewpoints of analytical chemists. The meeting was also valuable because it brought together representatives of all of a division's commissions outside the pressures of a General Assembly.

Current Activities

As part of our new publication agreement for the Solubility Data Series, a tentative list of volumes to be published during the first two years of the contract was submitted. This list includes :

1. Halogenated Ethanes and Ethenes with Water (Horvath and Getzen)
2. Ternary Alcohol-Hydrocarbon-Water Systems (Skrzecz, Maczynski, and Shaw)
3. Ammonium Phosphates (Eysseltova and Dirkse)
4. IA and IIA Azides, Cyanides and Thiocyanides (Hala and Salomon)
5. Alkaline Earth Metal Carbonates (Lorimer et al.)
6. Alkali Metal and Ammonium Perchlorates (Chan et al.)
7. Gaseous Alkynes (Fogg)
8. Gases in Polymers (Yampol'skii and Patterson)

The list was prepared based on the Chairman's and Editor-in-Chief's best judgment of volumes nearing completion. However, the list is tentative. Substitutions will be made as necessary and it may be possible to increase to total number of volumes published.

An Internet web site (<http://www.unileoben.ac.at/~eschedor/welcome.html>) for the Commission was prepared by M Salomon. This site contains a variety of information about the activities of the Commission and is generating awareness of and interest in our work by the chemical and scientific community. Of particular use to participants is an up-to date list of email addresses for individuals involved in the Commission's work.

This year a dual award from the Franzosini Fund was made to Lan-Chi Tran-Ho (nominated by H Gamsjaeger) and Kiril Loza (nominated by Y Yampol'skii). This award, made possible by a bequest from the estate of Prof P Franzosini, helps to support the travel expenses of younger colleagues in attending meetings of Commission V.8.

The Commission continues to organize International Symposia on Solubility Phenomena (ISSP) which are held in even numbered years in conjunction with meetings of the Commission. The 9th ISSP is scheduled for 2000 in Tunisia under the organization of N Kbir-Ariguib, M Guane-Escard and H Gamsjaeger.

Progress continues on two volumes outside the Solubility Data Series. These volumes deal with solubilities of gases in aerosols (P Fogg, editor) and the experimental determination of solubility (G Hefter and C Young, editors).

Work continues on the organization of a sub-series of volumes for the Solubility Data Series on the solubility of salts in seawater. The organizers (J Lorimer, R Cohen-Adad, and C Balarew) are considering a proposal through IUPAC to ICSU for support of this effort and the organization of a symposium during the IUPAC Congress to be held in conjunction with the General Assembly in Brisbane, Australia in 2001. Another possible symposium topic, "Medical Applications of Solubility Data", has been proposed by E Königsberger.

6. Editor-in-Chief's Report for 1997-1998

Sales

Unfortunately, no sales figures are available. Volumes 1-53 of the SDS were published by Pergamon Press, and according to the terms of the original publishing contract, Pergamon was to continue to sales of volumes for 10 years after termination of the contract. It was standard practice to submit yearly sales figures to the IUPAC Secretariat, but since the end of the agreement in 1993, no sales figures or unsold stock at Pergamon are available.

Volumes 54-65 of the SDS were published by OUP (1994-1996) who transferred all stock to Dawsons which is a backstock agent in Folkestone, UK. OUP sales figures and numbers of volumes transferred to Dawsons are unknown.

The *IUPAC-NIST Solubility Data Series* will be offered to subscribers both in hard copy and electronic versions of the *Journal of Physical and Chemical Reference Data* (see 6d below). All subscribers to *JPCRD* will receive the SDS volumes as part of their normal subscriptions to The Journal, and reprints of individual volumes will be made available. What has not yet been decided are the prices and whether the SDS will be offered as a separate subscription to only SDS-JPCRD issues. We hope to place this information on the web as soon as possible. The American Chemical Society handles all requests for subscriptions and reprints.

6b. Production Schedule. Under the new publishing agreement with NIST, the series will be called the *IUPAC-NIST Solubility Data Series*. There will be four volumes published per year, and from June-July 1998, the following volumes were submitted to NIST (these will be numbered 66-68).

Vol 66: *Ammonium Phosphates* (Eysseltová, Dirkse)

Vol 67: *Halogenated Ethanes and Ethenes with Water* (Horvath, Getzen)

Vol 68: *Halogenated Aliphatic Hydrocarbons C₃ - C₁₄ with Water* (Horvath, Getzen).

Volumes to be submitted in August and September 1998:

Vol 69: *Gases in Polymers* (Patterson, Yampol'skii, Fogg) - August.

Vol 70: *Ternary Systems Alcohol - Hydrocarbons-Water* (Skrzecz, Maczynski, Shaw) - September

6c. Completed Volumes. Volumes very near to completion (draft hard copy and, in some cases electronic versions available at this time). Some completed (draft - under review) volumes are listed below, and more complete information will be made available by the Subcommittee Chairs in Niigata.

Transition metals, Lanthanides and Ammonium Halates (Miyamoto, Haines). Draft volume in hand, but considerable editing/revisions are required. Diagrams in particular need to be redone, and Bob Haines has sent me the data pages as WordPerfect files. To be discussed within subcommittee.

Polycyclic Aromatic Hydrocarbons: Binary & Ternary Nonaqueous Systems (additional data) (Acree). The crc of this volume is with Marie-Therese and Bill could produce the WordPerfect 5.1 files upon request.

Alkali metal and Ammonium Perchlorates, Part II: K, Rb, Cs and Ammonium Perchlorates (Chan, Khoo, Gryzlova & Cohen-Adad).

6d. New Publishing Policy. The *IUPAC-NIST Solubility Data Series* will initially be published in separate issues of the *JPCRD*. This journal is a NIST-ACS-AIP joint venture, and electronic versions of all submissions to *JPCRD* are standard practice. NIST has requested that all submissions to *JPCRD* be in both hard copy and electronic. A toolkit for assistance in preparation of manuscript is available at

<http://www.aip.org/epub/compuscripts.info.html>

Standard word processing programs such as Word, WordPerfect, WordPro and LaTeX are easily handled by the publishers.

6e. Introduction to the SDS. The status of all introductory materials to the *IUPAC-NIST SDS* has not yet been agreed upon. The introductions to each subseries (gas/liq, liq/liq and solid/liq) published in volumes 1 to 65 may or may not be published in all volumes subsequent to and including volume 66. These introductions have been submitted with volumes 66-69, but whether or not they will be included in the printed *JPCRD* issue has not been fully discussed with the publishers. Other options exist, e.g. publishing these introductions once in standard *JPCRD* issues and providing reference to each in appropriate *JPCRD*-SDS issues or providing reference to each at Commission V.8's web site (see below).

6f. Home Page of Commission V.8. Updated in July, Commission V.8's web site offers considerable information to visitors on history of the SDP, contributors, ISSP meetings, the publisher, past and future publications, links to related sites and examples of compilations and critical evaluations from previously published volumes. This information can be found at

<http://www.unileoben.ac.at/~eschedor/welcome.html>

We welcome your comments and suggestions for revisions and/or inclusion of additional information. Please contact D. Shaw, H. Gamsjäger or M. Salomon for suggestions.

7. Status Report on Book on Experimental Methods for the Determination of Solubilities

To speed up the publication of this book:

1. Reg Tomkins was appointed as co-editor,
2. Colin Young and Glenn Hefter should be informed until 1 September if there are any objections,
3. Glenn Hefter should be asked to provide a list of manuscripts already submitted,
4. Peter Fogg and Reg Tomkins should sort out the publisher (Wiley, NIST as a second action).

8. Solubility Data Base Project

NIST is very interested in Kehiaians material. For Berlin a proposal should be prepared to make data of past SDS projects available in electronic form. To achieve this, support is needed.

9. Horizontal programs

Solubility of Gases in Aerosols

Commission V.8 and VI.2 (Commission on Atmospheric Chemistry)

For the completion of the book "Solubility of Gases in Aerosols" Peter Fogg needs competent help, if he is not able to recruit contributors the project has to be discontinued.

10. Project: Solubilities of Salts in Seawater

Preparation of Proposal for Submission to ICSU

IUPAC Commission V.8 - Oceanic Salts Project

The group met on 4 August, 1998 at 1600 h in Bandai Civic Hall, Niigata. Present were: C. Balarew (Chair), R. Cohen-Adad, J. Eysselevà, N. Kbir-Ariguib, J. Lorimer (Secretary), M.-Th. Saugier-Cohen Adad, V. Valyashko, W. Voigt and C. Magalhães (by invitation).

Agenda and Report

1. Participants and update of Purpose and Goals - see Appendixes 1, 2.
2. Division of work and status of compilations - see Appendix 3.
3. Volumes planned for 1999 - By the end of 1999, it is planned to:
 - finish all compilations of binary and ternary systems.
 - finish evaluations of $\text{MgCl}_2 - \text{H}_2\text{O}$, $\text{CaCl}_2 - \text{H}_2\text{O}$.
4. Status of data base of relevant publications

Both W. Voigt (about 300 entries) and J. Lorimer (about 400 entries) have Papyrus files of references that have been converted from lists in other data base formats. These files need extensive editing, which is being carried out. When editing is complete, the files will be merged to exclude overlapping entries. W. Voigt hopes to be able to provide FTP access to his data base by 1 October, 1998.

5. Format for data sheets.

J. Lorimer presented sample data sheets prepared by a word processing program in the new format, i.e., with horizontal boxes only. It was agreed that all new compilations should be prepared in this form. An attempt will be made to convert older compilations to the new format. Preparation of data sheets may be done: (a) using any common word processing software (Word 7.0, 8.0 or WordPerfect 5.1, 6, 7 8 are preferred); (b) using the Skrzecz automatic data entry software.

6. Statement of relation of the Tunisian and EC projects to this project.

See Appendix 4 for a brief description of these projects. These projects use the same data base and the same compilations as the IUPAC project. However, they do not involve preparation of data sheets, and do not involve the detailed evaluations of the IUPAC project.

7. Relevance of work of Nancy Weare (USA).

W. Voigt pointed out that Dr Weare (California) has recently submitted for publication a large work of evaluation on some of the systems of interest to the Oceanic Salts Project. While her model is useful, her data are incomplete, and thus her work does not conflict directly with the aims of this Project. It was suggested that she be invited to the 9th ISSP in Tunisia.

(Note: Plenary and Invited Lecturers have already been identified for the 9th ISSP, so she would only be eligible to present a regular paper or poster. Najia may have comments on this.)

8. Relations with SCOR (Scientific Committee on Ocean Research - an ICSU committee)

A proposal was made last year to SCOR for limited financial support. No reply was received until just before this meeting. This reply, from David Turner (Göteborg University, Sweden and IUPAC Representative on SCOR) is as follows:

"The SCOR proceedings from the 1996 General Meeting include the following paragraph on the Oceanic Salts project:

"This Commission (i.e. V.8) sought the support of SCOR for a project on the Solubility of Oceanic Salts. The General Meeting agreed that, while the group wanted financial support from SCOR, there did not seem to be any possibility of substantial SCOR involvement in the project. The Chair of the project (Jack Lorimer, Canada) [I told them I was the Secretary!! - JWL], should be asked to submit a more formal proposal to SCOR, setting out the scientific justification for it, the total budget and the amount sought from SCOR, a time schedule, plans for reporting progress to SCOR and publication plans, including details of how SCOR's sponsorship would be acknowledged."

"I must admit that I forgot to forward you a copy of this (these proceedings do not come out until 6-12 months after the meetings, so the sense of urgency has often evaporated by publication date).

"Clearly, a direct approach to SCOR would have to follow the guidelines set out above. SCOR's key criteria are (i) that the project contributes to SCOR's own scientific interests, and (ii) that SCOR scientists are able to participate in and/or influence the project. I think that the choice between an approach direct to SCOR, or an application to ICSU, depends on the extent to which you feel that SCOR's requirements could be accommodated. I will be attending the SCOR General Meeting in Amsterdam in November of this year, and will of course be pleased to present a proposal on your behalf. I have now been officially appointed as the IUPAC representative to SCOR, so any proposal should be submitted through me.

"Let me know how you wish to proceed. In the meantime, I will find out when a written proposal should be submitted in order to be included with the meeting papers."

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It was remarked that the previous submission to SCOR included exactly those items that are listed above, with the exception of: (1) direct evidence of the relevance to SCOR's specific interests; (2) acknowledgement of SCOR's contributions (a minor point); (3) involvement of SCOR scientists.

Discussion of a possible role for SCOR was inconclusive. J. Lorimer is to explore if using SCOR scientists as external referees would constitute sufficient involvement.

Previously, SCOR wanted inclusion of the minor constituents of sea water (fluorides, bromides, carbonates in particular) as part of the study. At best, this would appear to be only possible after compilation and evaluation of the main salts were complete.

Appendix 1:

Participants in IUPAC Commission V.8 - Oceanic Salts Project

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Appendix 2:
**IUPAC Commission V.8 (Solubility Data): Oceanic Salts Project
Proposal to SCOR**

1 Scientific Justification of the Project

In 1933, d'Ans published a comprehensive bibliography and compilation of primary data for solubilities of oceanic salts. He also made what we consider to be preliminary evaluations of these data. No comprehensive update to the bibliography or to the compilations has been made, despite the importance of the data in constructing models of seawater and brackish water, in planning industrial crystallization and extraction processes, and in the solution of environmental problems in oceanic and brackish environments, in mining of salt deposits, and in interactions between the oceans and the atmosphere. While many partial models of seawater have been reported in the literature, these make use of only limited sets of data. Thus the overall goal of a detailed theoretical description of solutions of oceanic salts, based on a complete set of carefully-evaluated data over wide ranges of temperature and pressure, does not exist at present. Methods for treatment of the thermodynamic properties of aqueous systems (including sea water) are well advanced, and these will form the basis of improved methods of achieving this description.

The d'Ans bibliography contains data on only the major components of sea water: NaCl, KCl, MgCl_2 , CaCl_2 , Na_2SO_4 , K_2SO_4 , MgSO_4 , CaSO_4 in binary, ternary, quaternary systems. Compilation and evaluation of data for these is the current aim of the Oceanic Salts Project sponsored by IUPAC Commission V.8 (Solubility Data). The d'Ans bibliography contains only sparse references to pressure dependence of solubilities, a subject on which much data has appeared since 1933.

The minor constituents of sea water are not included in current projects simply because of the very large amount of literature that must be compiled for the major components alone. There are two exceptions; the alkaline earth carbonates, which are the subject of another current IUPAC project (Vanderdeelen, Lorimer; see Appendix 1 for current contributors) and preliminary work on sodium and potassium carbonates (Krumgalz). We consider data on the carbonates to be of particular importance because of their role as sinks for atmospheric CO_2 and their consequent use in global climate models. Other minor constituents that we consider to be of importance include the bromides and fluorides.

The question of the minor constituents (including carbonates) is one for which we should like to have the involvement of SCOR scientists. The carbonates present particular problems because of the ionization equilibria in solution that are used in all models in addition to ion interaction terms.

2 Specific Goals of the Current Project

2.1 Compilations. To produce up-to-date compilations of data (with bibliography), constructed in the format of the IUPAC Solubility Data Series (SDS).

(a) One aspect of current work involves compilation of a computerized bibliographic database with associated reprints of all relevant publications as an ongoing process. This is well advanced, with about 400 entries from several contributors who have extensive files of reprints.

(b) The latest methods for producing compilations in the SDS are being used. Data (compilation) sheets may be prepared in the new SDS format using any common word processing software (Word 7.0, 8.0; Word Perfect 5.1, 6, 7, 8 are preferred).

2.2 Publication. To publish compiled data both in printed form (via the IUPAC Solubility Data Series) and possibly in the form of a computerized on-line database.

The IUPAC Solubility Data Series is now being published as special issues of the Journal of Physics and Chemistry Reference Data (JPCRD), published jointly by NIST, ACS and AIP. The first volume with the new publisher is in production. Plans for electronic distribution of the compilations and/or critical evaluations are under discussion.

2.3 Critical Evaluation. To devise and document appropriate methods for critical evaluation of the data, and to publish these, again via the IUPAC Solubility Data Series. These methods will include methods for describing paragenesis of systems, for example, compositions of solid and solution phases during the evaporite sequence in removal of water from sea water.

Ordinarily, a volume of the SDS contains compilations and evaluations for a relatively small number of chemically-related salts; e.g., SDS Vol. 47: Alkali Metal and Ammonium Chlorides in Water and Heavy Water: Binary Systems, R. Cohen-Adad and J.W. Lorimer, eds. (1991). However, the complexity of oceanic salt systems makes this approach difficult. For example, data on the solubility of potassium chloride in the absence of other salts are found mixed in with data for ternary and higher systems. Thus, to avoid compiling the same paper more than once, we have decided to base compilations on systems of increasing complexity for purposes of publication. Evaluations can then proceed on the same basis, but data for evaluation of, for example, the solubility of KCl in absence of other salts, will be drawn from across the whole range of compiled data, as appropriate.

2.4 Duration of Project. It is estimated that the current project will require at least five more years for completion, i.e., by 2003. By the end of 1999, it is planned to:

- finish all compilations of all binary and ternary systems.
- finish evaluations of $\text{MgCl}_2 - \text{H}_2\text{O}$, $\text{CaCl}_2 - \text{H}_2\text{O}$.

3 Specific Goals of the Contributions of SCOR Scientists: an Extended Oceanic Salts Project

3.1 Background

Several submissions have been made to SCOR, the latest via Dr. David Turner (IUPAC Representative to SCOR). The latest detailed reply from Dr Turner is as follows.

"The SCOR proceedings from the 1996 General Meeting include the following paragraph on the Oceanic Salts project:

"This Commission (i.e. V.8) sought the support of SCOR for a project on the Solubility of Oceanic Salts. The General Meeting agreed that, while the group wanted financial support from SCOR, there did not seem to be any possibility of substantial SCOR involvement in the project. The Chair of the project (Jack Lorimer, Canada) [actually Secretary - please note] should be asked to submit a more formal proposal to SCOR, setting out the scientific justification for it, the total budget and the amount sought from SCOR, a time schedule, plans for reporting progress to SCOR and publication plans, including details of how SCOR's sponsorship would be acknowledged."

Dr. Turner added:

"Clearly, a direct approach to SCOR would have to follow the guidelines set out above. SCOR's key criteria are (i) that the project contributes to SCOR's own scientific interests, and (ii) that SCOR scientists are able to participate in and/or influence the project. I think that the choice between an approach direct to SCOR, or an application to ICSU, depends on the extent to which you feel that SCOR's requirements could be accommodated. I will be attending the SCOR General Meeting in Amsterdam in November of this year, and will of course be pleased to present a proposal on your behalf. I have now been officially appointed as the IUPAC representative to SCOR, so any proposal should be submitted through me."

The Oceanic Salts working group discussed this reply at its meeting in Japan in August, and since then has been debating on how to proceed in the most effective way. As a result of these discussions, specific goals for the involvement of SCOR are proposed for discussion purposes, with the hope that the proposal will stimulate further communication.

3.2 Specific Goals and Management of the Extended Project

In addition to the specific goals of the current IUPAC project listed in section 2, we propose the following:

3.2.1 Specific interests: SCOR will provide information on the nature of its specific interests.

3.2.2 Recognition of SCOR's contributions (in personnel or financial) is an important but routine matter. Any volume of the SDS contains acknowledgement of contributions of all types.

3.2.3 Involvement of SCOR scientists could be in two areas:

3.2.3.1 All IUPAC projects are refereed externally, and traditionally the referees are not anonymous; the role of the referee, through the Editor-in-Chief of the Solubility Data Series and

volume editors, is an interactive one. Under new IUPAC proposals, proposals will also be refereed. The assistance of SCOR scientists in these tasks would be welcomed.

3.2.3.2 In a more active role, SCOR scientists could assume responsibility for compilation and evaluation of the minor constituents of sea water. The particular constituents are, in the first instance, carbonates (in part), bromides and fluorides of sodium, potassium, magnesium and calcium, and possibly of strontium, barium and radium (where data are available) for completeness.

3.2.4 Project management. IUPAC and SCOR will jointly agree on a project editor who will oversee the progress of both sections of the overall project: major constituents and minor constituents.

3.2.5 Meetings. The IUPAC Solubility Data Commission has usually met annually, in odd years at the IUPAC General Assembly and in even years in conjunction with the International Symposium on Solubility Phenomena. (The ISSP is sponsored by the Commission.) IUPAC is undergoing extensive reorganization at present, and the reorganization will not be complete until about 2003. One possibility is that the Commission will cease to exist in its present form, but we anticipate that IUPAC sponsorship of the Solubility Data Series and the ISSP will continue. However, with changes in the structure of IUPAC, meetings in conjunction with the General Assembly appear unlikely. We envisage, at the moment, continuation of the meeting in conjunction with the ISSP, but any other meetings are most likely to involve specific working groups, of which the Oceanic Salts group would be one. Participating SCOR scientists would, of course, be invited to any relevant meetings.

3.2.6 Duration of the Extended Project. At present, we want to retain the estimated completion date of 2003. However, involvement of SCOR scientists in a new project may require adjustment of this date.

3.3 Budget. Financial assistance for the Project is required in two directions: (a) obtaining reprints of rare or hard-to-get publications and other minor expenses connected with compilations; (b) travel to meetings.

On the basis of current experience, and the number of participants, we estimate USD 5 000 per year for the period 1999-2003 (4 years), for a total of USD 20 000 would greatly facilitate completion of the project within the planned time period.

4. Participants in the Current IUPAC Project

See Appendix 1.

5. Division of Work and Status of Compilations in the Current Project

Details are given in Appendix 3

Appendix 3:

Division of Work and Status of Compilations in the Current Project

Notes:

1. Names listed are those of compilers. The symbol * indicates that compilers for quaternary and higher systems will be chosen through mutual agreement among the compilers of the respective binary and ternary systems.

2. "Complete", in most instances, means that compilations have been made, but data sheets have not been prepared.

1. SYSTEMS CONTAINING Na.

1.1 - 1 cation, 1 anion

1.1.1 - NaCl - H₂O

R. Cohen- Adad, J.W. Lorimer - compilations and preliminary evaluations complete (SDS vol. 47)

Chr. Balarew - in progress

1.1.2 - Na₂SO₄ - H₂O

1.2 - 2 cations, 1 anion

1.2.1 - Na, K, Cl/H₂O

M.-T. Saugier-Cohen Adad - almost complete

1.2.2 - Na, Mg, Cl/H₂O

M.-T. Saugier-Cohen Adad

1.2.3 - Na, Ca, Cl/H₂O

J. Eysseltova - complete

1.2.4 - Na, K, SO₄/H₂O

N. Kbir-Arighuib

1.2.5 - Na, Mg, SO₄/H₂O

J.W. Lorimer - complete; old-form data sheets complete; recent papers need to be added.

1.2.6 - Na, Ca, SO₄/H₂O

W. Voigt - in progress

1.3 - 3 cations, 1 anion

1.3.1 - Na, K, Mg, Cl/H₂O*1.3.2 - Na, K, Ca, Cl/H₂O*1.3.3 - Na, Mg, Ca, Cl/H₂O*1.3.4 - Na, K, Mg, SO₄/H₂O*1.3.5 - Na, K, Ca, SO₄/H₂O*1.3.6 - Na, Mg, Ca, SO₄/H₂O*

1.4 - 4 cations, 1 anion

1.4.1 - Na, K, Mg, Ca, Cl/H₂O*1.4.2 - Na, K, Mg, Ca, SO₄/H₂O*

1.5 - 1 cation, 2 anions

1.5.1 - Na, Cl, SO₄/H₂O N. Kbir-Arighuib

1.6 - 2 cations, 2 anions

1.6.1 - Na, K, Cl, SO₄/H₂O*1.6.2 - Na, Mg, Cl, SO₄/H₂O*1.6.3 - Na, Ca, Cl, SO₄/H₂O*

1.7 - 3 cations, 2 anions

1.7.1 - Na, K, Mg, Cl, SO₄/H₂O*1.7.2 - Na, K, Ca, Cl, SO₄/H₂O*1.7.3 - Na, Mg, Ca, Cl, SO₄/H₂O*

1.8 - 4 cations, 2 anions

1.8.1 - Na, K, Mg, Ca, Cl, SO₄/H₂O*

2. SYSTEMS WITHOUT Na

2.1 - 1 cation, 1 anion

2.1.1 - KCl - H₂O

R. Cohen- Adad, J.W. Lorimer - compilations and preliminary evaluations complete (SDS vol. 47)

2.1.2 - K₂SO₄ - H₂O

R. Bouaziz - compilations partly complete

2.1.3 - MgCl₂ - H₂O

W. Voigt - in progress

2.1.4 - Mg SO₄ - H₂O

J.W. Lorimer, N. Kbir-Arighuib - complete; old-form data sheets complete; recent papers need to be added

- | | |
|---|--|
| 2.1.5 - $\text{MgCO}_3 - \text{H}_2\text{O}$ | J. Vanderdeelen - est. completion in 1999 |
| 2.1.6 - $\text{CaF}_2 - \text{H}_2\text{O}$ | SCOR addition |
| 2.1.7 - $\text{CaCl}_2 - \text{H}_2\text{O}$ | W. Voigt - in progress |
| 2.1.8 - $\text{CaCO}_3 - \text{H}_2\text{O}$ | J. Vanderdeelen - est. completion 1999 |
| 2.1.9 - $\text{Ca SO}_4 - \text{H}_2\text{O}$ | J.W. Lorimer, N. Kbir-Arighuib - complete; old-form data sheets complete; recent papers need to be added |
| 2.2 - 2 cations, 1 anion | |
| 2.2.1 - K, Mg, Cl/ H_2O | W. Voigt - complete by end 1999 |
| 2.2.2 - K, Ca, Cl/ H_2O | J. Eysseltova |
| 2.2.3 - Mg, Ca, Cl/ H_2O | J. Eysseltova |
| 2.2.4 - K, Mg, $\text{SO}_4/\text{H}_2\text{O}$ | J.W. Lorimer |
| 2.2.5 - K, Ca, $\text{SO}_4/\text{H}_2\text{O}$ | W. Voigt |
| 2.2.6 - Mg, Ca, $\text{SO}_4/\text{H}_2\text{O}$ | J.W. Lorimer (check for data?) |
| 2.3 - 3 cations, 1 anion | |
| 2.3.1 - K, Mg, Ca, Cl/ H_2O^* | |
| 2.3.2 - K, Mg, Ca, $\text{SO}_4/\text{H}_2\text{O}^*$ | |
| 2.4 - 1 cation, 2 anions | |
| 2.4.1 - K, Cl, $\text{SO}_4/\text{H}_2\text{O}$ | N. Kbir-Arighuib |
| 2.4.2 - Mg, Cl, $\text{SO}_4/\text{H}_2\text{O}$ | J.W. Lorimer, N. Kbir-Arighuib |
| 2.4.3 - Ca, Cl, $\text{SO}_4/\text{H}_2\text{O}$ | J.W. Lorimer |
| 2.5 - 2 cations, 2 anions | |
| 2.5.1 - K, Mg, Cl, $\text{SO}_4/\text{H}_2\text{O}^*$ | |
| 2.5.2 - K, Ca, Cl, $\text{SO}_4/\text{H}_2\text{O}^*$ | |
| 2.5.3 - Mg, Ca, Cl, $\text{SO}_4/\text{H}_2\text{O}^*$ | |
| 2.6 - 3 cations, 2 anions | |
| 2.6.1 - K, Mg, Ca, Cl, $\text{SO}_4/\text{H}_2\text{O}^*$ | |

Appendix 4:

Relevant Research Projects Involving Some Contributors to the IUPAC Project

1. Improvement of industrial crystallization and extraction processes from brines and mining deposits.

Sponsor: Tunisian industry

Participants: R. Cohen-Adad, R. Rokbani, INRST, Tunis

Start date: 1995

End date: 2000-2001

A determination of the crystallization sequence of sea water, brines or mining deposits during evaporation will be performed. It is based on the geometric properties of the isothermal-isobaric sections of the simulating system; the theoretical background of the calculation has already been derived. It will be compared, when possible, to experimental measurements and applied to the derivation of flow charts, including mass balance, for each step of the crystallization process and eventually for recycling processes. In a second stage, a computer-assisted program will be studied and compared to the program actually proposed. The same work will be performed with processes at two different temperatures.

The project has resulted in a thesis by L. Zayani, to be presented at the end of 1998.

2. Evaluation of brines from Chotts and Sebkhas, South Tunisia and Morocco.

Sponsor: none

Participants: R. Cohen-Adad (Lyon), N. Kbir -Ariguib, M. Trabelsi-Ayedi (Tunis), M. El Haddek (Agadir).

Start date: 1995

End date: 2000

These studies, undertaken several years ago in cooperation between Lyon, Tunis and Agadir, have resulted in two published theses, one thesis in preparation, and one book in preparation: "Les Saumures du Sud Tunisien". The objectives are close to the IUPAC project on sea water, and are oriented especially towards the recovery of potassium salts for local industry.

3. Research on solutions to environmental problems.

Sponsor: Copernicus project of the European Community

Participants: C. Balarew (Burgas), R. Cohen-Adad (Lyon), M.-Th. Cohen-Adad (Lyon - coordinator), J. Eysseltová (Prague), S. Petrenko, F. Rull (Valladolid), V. Valyashko (Moscow), W. Voigt (Freiberg).

Start date and end date have to be decided after the proposal has been approved.

These investigations are focussed essentially towards environmental damage in the Black Sea and in Vigo Bay (Spain), but they can be extended to environmental problems in the Gabes Gulf (Tunisia).

11. Teaching of undergraduate students: Experimental and theoretical aspects

Clara Magalhaes proposed to write a booklet on the importance of solubility. The subcommittee chairs were asked to discuss this project with her. Shortly after this Commission meeting Mihaly Beck supported the idea and suggested to prepare a short booklet on the importance of solubility presenting as many experiments as possible. In addition, he is willing to contribute.

12. IUPAC Congress in Brisbane in 2001

Seminar Topic: Solubility of Salts in Seawater

See topic 10.

Seminar Topic: Medical applications of solubility data

Jean-Claude Bollinger, Erich Koenigsberger and Clara Magalhaes will explore the possibility to organize a symposium on "Medical aspects of solubility" at the 38th IUPAC Scientific Congress.

13. Reports of Chairmen of Subcommittees

Subcommittee V.8.1: Gas/Liquid Systems (P. Fogg)

9/86 CARBON DIOXIDE IN NON-AQUEOUS SYSTEMS AT PRESSURES ABOVE 2 BAR

(data on COS to be included)