



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

Minutes of the 26<sup>th</sup> Annual Meeting (20<sup>th</sup> of SDC)  
to be held in conjunction with the 9<sup>th</sup> ISSP  
at Grand Palais des Congrès, Hammamet, Tunisia  
July, ~~2001~~ 2000

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

1. **Welcome of participants**

David Shaw, Chairman of Commission V.8., called the meeting to order and welcomed the participants.

**Obituary**

Professor Shaw paid tributes to the late Professors Alessandro D'Aprano and T. Mioduski.

**Introduction of participants**

Attendees were asked to identify themselves and their affiliation. The Chairman welcomed in particular Vladimir Zbranek, who received the "Franzosini Award 2000".

2. **Approval of Minutes of the 25<sup>th</sup> Meeting (10<sup>th</sup> of SDC) held at Freie Universität Berlin, Berlin, Germany, August 8 - 10, 1999**

The Berlin Minutes were approved.

3. **Other Items for Agenda**

The attendees were informed that Peter Fogg was not able to participate in this meeting, because he had to undergo a coronary triple bypass operation. The commission V.8 wished him a speedy recovery.

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 colleagues presently contributing to the activities of Com. V.8 disagree with the members listed in the IUPAC Handbook 2000-2001. An effort will be made to improve the situation before the next edition appears. Contributors to the Commission's activities are requested to provide their text on discs when they want to communicate it via the minutes.

## 5. Chairman's Report for 1999-2000 - D. Shaw

Solubility Data Commission V.8

Activity Report 1999-2000

Prepared by D. Shaw, Chair

June 2000

In the past year the Solubility Data Commission (SDC) has actively continued to pursue its goals of compiling and evaluating published solubility data and fostering international research interest in topics related to chemical solubility.

### I. Volume Preparation for the Solubility Data Series.

During the second year (July 1999-June 2000) of our agreement for publication of the Solubility Data Series (SDS) in the Journal of Physical and Chemical Reference Data two volumes have appeared. These are:

Volume 70, *Gasses in Glassy Polymers*; Y. Yampol'skii et al., editors

Volume 71, *Nitromethane with Water or Organic Solvents*, V. Sazonov et al., editors

In the next year (July 2000-June 2001) we expect to submit at least four volumes. Work in advanced stages of preparation includes the following volumes:

- (1) Nitromethanes-ternary systems (V. Sazonov, editor).
- (2) Metal formates (T. Dirkse and C. Balereu, editors).
- (3) Actinides (J. Hala, editor)
- (4) Noble gas update (L. Clever, editor)
- (5) Ethyne (P. Fogg, editor)

### II. Solubility Database.

An agreement has been concluded between the SDC and the US National Institute of Standards and Technology (NIST) for electronic dissemination of evaluated solubility data. The agreement calls for the completion of a pilot project under which evaluated data from four previously published volumes of the SDS (Volumes 20, 60, 67, and 68; all of which concern solubility of halocarbons with water) will be adapted for distribution over the world wide web as paper of NIST's ChemistryWebBook. The pilot project was chosen because the volumes deal with systems of commercial and environmental importance and present a range of preparation dates. From the experience gained with this project, we expect to move on to the incorporation of additional material into electronic formats in cooperation with NIST.

### III. Symposia.

The SDC organizes a series of scientific meetings, the International Symposia on Solubility Phenomena (ISSP) with IUPAC sponsorship. These meetings provide

opportunities for presentation of original research and the discussion of topics related to solubility. These meetings, held in even numbered years, also provide venues for participants in the work of the SDC to meet and discuss the progress of Commission projects. The Ninth ISSP will be held in Hammamet, Tunisia, 25-28 July 2000. The Tenth ISSP is tentatively scheduled for Varna, Bulgaria in August 2002.

In the fall of 1999 the Commission submitted a proposal to plan and hold a workshop to address applications of solubility to the improvement of the environment. We proposed that the workshop be held in conjunction with the 10<sup>th</sup> International Symposium on Solubility Phenomena in the summer of 2002 in Varna, Bulgaria. This proposal was recently approved and planning is underway.

#### IV. Planning for the Future.

The SDC has engaged in extensive discussions of its future plans in light of the reorganization of IUPAC scheduled for 2001. The Commission recognizes six goals:

1. to compile and evaluate solubility data for systems of recognized importance,
2. to update compilations and evaluations for previously published systems as appropriate,
3. to publish volumes of compiled and evaluated data ,
- 4 to integrate evaluated data into an established an professionally managed database,
5. to organize International Symposia on Solubility Phenomena in even numbered years.

The Commission submitted a proposal for the creation of a new Commission to pursue these goals after 2001. While that proposal was received with positive comments and is still pending, it has been made clear that action will not be taken until sometime after 2001. Thus, the Commission expects to operate as one or more Task Groups to pursue our goals in the period following the next General Assembly when all existing Commissions are disbanded. A group of projects consistent with the Task Group structure will be proposed in time for consideration at the 2001 General Assembly.

#### 6. Editor-in-Chief's Report for 1999-2000 - M. Salomon

##### 1. General comments of the Editor-in-Chief

Starting with Volume Number 66, The Solubility Data Series (SDS) is published in special issues of the Journal of Physical and Chemical Reference Data (JPCRD). The Series is being published under the title of the IUPAC-NIST Solubility Data Series. The JPCRD is a bimonthly journal with the objective of providing critically evaluated physical and chemical property data, fully documented as to the original sources and the criteria used for evaluation. The articles published in JPCRD are the result of work by data centers and data projects sponsored by the Standard Reference Data Program in the division of Measurement Services in the NIST Technology Services Laboratory.

The EIC and David Shaw would like to acknowledge the guidance of Dr. John Rumble

and Dr. Malcolm Chase in publishing the SDS in JPCRD.

## 2. Volumes published or in course of publication

For details on the JPCRD (publisher, subscriptions, etc.), please refer to the Commission's home page on the internet. Briefly, NIST has agreed to publish four SDS volumes per year in JPCRD, and in fact 5 volumes have already been published :

- Volume 66 J. Eysseltová and T.P. Dirkse, *Ammonium Phosphates*.  
JPCRD, **27 (5)**, 1289 (1998).
- Volume 67 A.L. Horvath, F.W. Getzen and Z. Maczynska, *Halogenated Ethanes and Ethenes with Water*.  
JPCRD, **28 (2)**, 395 (1999).
- Volume 68 A.L. Horvath and F.W. Getzen, *Halogenated Aliphatic Hydrocarbons C<sub>3</sub> - C<sub>14</sub> Ethenes with Water*.  
JPCRD, **28 (3)**, 649 (1999).
- Volume 69 A. Skrzecz, D. Shaw and A. Maczynski, *Ternary Alcohol-Hydrocarbon-Water Systems*.  
JPCRD, **28 (4)**, 983 (1999).
- Volume 70 Yu. P. Yampol'skii, R. Paterson and P.G.T. Fogg, *Gases in Glassy Polymers*.  
JPCRD, **28 (5)**, 1255 (1999).

Two more completed volumes are now at the publisher (JPCRD) which will be published in 2000. The two volumes are:

*Binary Nitromethane Systems*, V. Sazonov, G.T. Hefter and K.N. Marsh, eds.

*Nitromethane with Water or Organic Solvents: Ternary and Quaternary Systems*, V. Sazonov, G.T. Hefter, eds.

The agreement reached with NIST also requires that all volumes prepared by Commission V.8 members be submitted electronically. This is an important requirement as it relates to ease of publication of the SDS as well as for future use in electronic dissemination of the SDS via the Internet. Finally, there are a number of new formatting procedures to be followed in preparing manuscripts for JPCRD, and details can be looked up in the Minutes of Berlin 1999. The respective copies are available on request by the Secretary of Com.V.8.

## **7. Database agreement**

NIST Standard Reference Data and The IUPAC Solubility Project  
John Rumble, Jr., NIST, [john.rumble@nist.gov](mailto:john.rumble@nist.gov)

### NIST Standard Reference Data Program

To make critically evaluated reference data available to scientists, engineers, and the general public.

Example – Chemical Manufacturing

- ♦ Chemical plants transport fluids during chemical production
- ♦ If a liquid turns to gas in a confined space, explosions will occur
- ♦ Plant designers need to have *reliable data* on conditions under which a liquid turns to gas

#### Example - Chemical Analysis

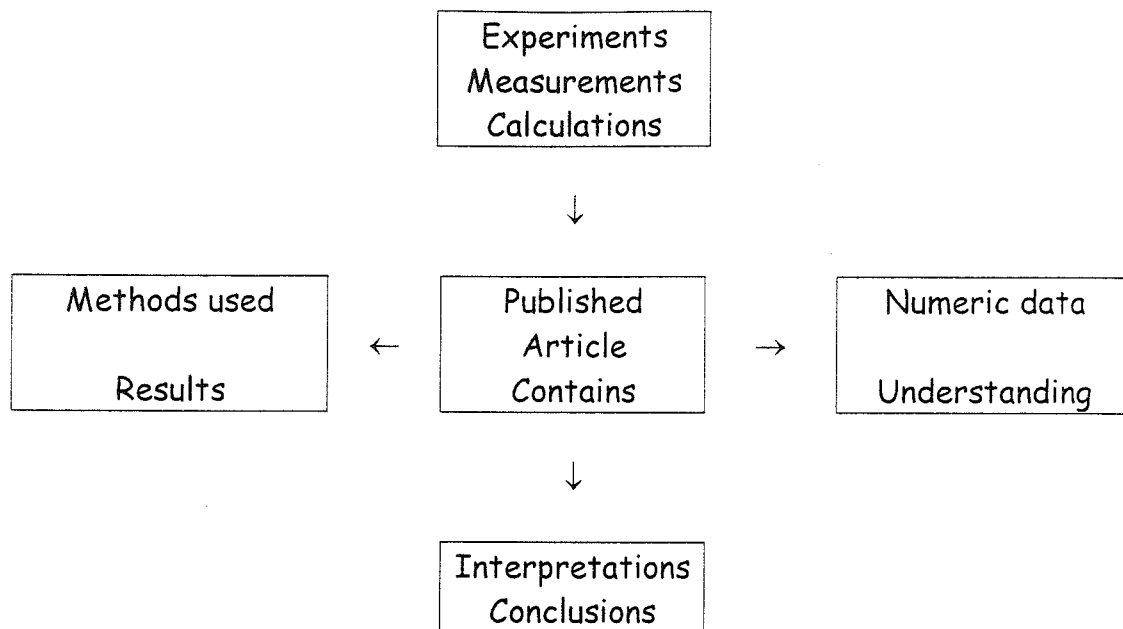
- ♦ People want to identify unknown substances:
  - Police - drugs
  - Environmentalists - air, water, and land pollutants, etc.
- ♦ Accepted Procedure
  - Take unknown substance
  - Make straight-forward measurements
  - Compare results to evaluated database with measurement results for many substances (50,000 to 220,000)
  - Usually can uniquely identify unknown immediately

#### Example - Statistical Datasets

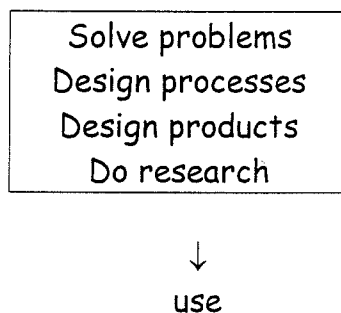
- ♦ People want to establish the reliability of statistical software
- ♦ Usually have many types of statistical procedures
- ♦ Take well document statistical reference data sets as input into software being tested
- ♦ Compare results to well-characterized results as included in dataset

#### NIST Standard Reference Data Program

- ♦ **Critical Evaluation of Data**
- ♦ Areas of Coverage
- ♦ Dissemination of Databases and Publications
- ♦ Final Remarks
- ♦ Data users are not experts on how data were generated and do not know the quality of the data as published
- ♦ NIST Standard Reference Data Program has **subject experts** collect and evaluate data in issue them with quality indicators
- ♦ NIST Standard Reference Data Program established by Congress in 1968



Over 200,000 articles includes in Chemical Abstracts in 1995



Scientific Research

#### NIST and IUPAC

##### Solubility Data Partnership

- Search strategies
- Data on solubility of substance A in substance B
- Do you have solubility data on substance A?
- Do you have solubility data for substances dissolved in solvent B?
  
- No searching on solubility data itself
- Support of multiple units

#### NIST and IUPAC

##### Solubility Data Partnership

Need to work closely together

- System priorities
- Search strategies
- Interface design
- Data quality
- System functionality
- More

#### NIST and IUPAC

##### Solubility Data Partnership

- The beginning of a long partnership
- We look forward to working with IUPAC V.8.

#### 8. Volumes for next year's SDS proposals, D. Shaw and M. Salomon

A review of volumes in course of publication in JPCRD is presented below.

Volume 73 Chr.Balarew and T.P.Dirkse, *Metal Formates*.

JPCRD, in course of publication.

Volume 74 J.Hála, *Actinide Carbonates and Carbon-Containing Compounds*.

JPCRD, in course of publication.

Volume 75 H.U.Borgstedt and C. Guminski, *Non-Metals in Liquid Alkali Metals*,

JPCRD, in course of publication.

Before the General Assembly in Brisbane we need the projects which will be finished in the near future. After the GA 2001 we will have projects of a larger scope instead of individual volumes. Subcommittees should focus on the upcoming projects and decide what can be completed in the course of two years.

9. Status Report on the Textbook " The Experimental Determination of Solubilities"  
by R.P.T. Tomkins

### PUBLISHER

John Wiley has agreed to publish the textbook and currently a contract is being prepared. Details are being worked out between Dr. David Shaw (Commission Chair), Dr. John Jost (IUPAC Secretariat) and Ms. Murray (Assist to Martin Rothlingsberg, Editor, John Wiley).

### STATUS OF CHAPTERS

CHAPTER	AUTHOR	STATUS
Preface	Hefter	Submitted; needs minor changes
Introduction	Lorimer	Not submitted
1.1 Thermodynamics	Lorimer/Cohen-Adad	At least $\frac{3}{4}$ of first draft submitted, reviewed by Tomkins, Knox, Gray(Exxon)
1.2 Kinetics	Christoffersen	Received; Reviewed by Tomkins, Nancollas and Hefter
2.1 Low Pr. gases	Clever/Battino	2 <sup>nd</sup> draft received Reviewed by Tomkins and Hefter (earlier)
2.2 High Pr. gases	Aim	not submitted
2.3 Gases in polymers	Yampolski/Paterson	Reviewed-rewritten by Tomkins for English style; sent to S. Krause for review
2.4 Gases in Molten Salts	Tomkins	-2 <sup>nd</sup> draft submitted -Hefter needs to make final comments
2.5 Gases in Solid Metals	Lewis/Sakamoto	- no major changes needed - reviewed by Hefter and Tomkins
3. Liquids	Hefter	1 <sup>st</sup> draft not received
4.1 Solids in Liquids	Cohen-Adad / Cohen-Adad	2 <sup>nd</sup> copy submitted reviewed by Lorimer; Reviewed by Tomkins and Hefter (earlier)
4.2 Sparingly Soluble Solids in Liquids	Gamsjäger/Königsberger	3 <sup>rd</sup> revision needed after Lorimer comments
4.3 Aqueous Systems at high temps & pr.	Valyashko/Kravchuk	1 <sup>st</sup> draft reviewed; major revisions made by J.Lorimer; 2 <sup>nd</sup> draft sent to Tomkins



4.4 Solids in molten and solid metals	Borgstedt/Guminski	Minor changes needed
4.5 Solids in solids	Sangster	Minor changes needed; Reviewed by Hefter and Tomkins
5.1 Solids/liquids in supercritical fluids	Fermeglia	First draft submitted
5.2 Solids/liquids in cryogenic liquids	Szczepaniec-Cieciak	several drafts submitted
5.3 Polymers in liquids	Krause	Minor revisions needed

#### OTHER COMMENTS

1. All contributors will need to add references to incorporate the period 1990-2000.
2. Manuscript should be completed by December 31, 2000.

#### 10. Project: Solubilities of Salts in Seawater - J. Lorimer

Prof. Lorimer reported at the General Assembly in Berlin that he met with Dr. David Turner, the IUPAC representative on SCOR, during the General Assembly, and assured him that: (a) the proposal of the Oceanic Salts Working Group for cooperation with SCOR was still valid in the form presented previously (minutes of Commission V.8, Niigata, 1998); (b) the Working Group would continue with their activities even if there is no involvement with SCOR, but that cooperation with SCOR would seem to be a desirable project involving both IUPAC and ICSU committees. Dr. Turner reported that the proposal of the Oceanic Salts Working Group is on the agenda for the meeting of the SCOR Executive in India in October 1999. He also indicated that he would try to talk with individual members of the SCOR Executive before their meeting.

The Executive Committee of SCOR never came back to the proposal. Thus it seems to be a waste of time to cooperate with SCOR. It is suggested that Com. V.8 proceeds on its own. Compilation of solubilities of  $\text{Na}_2\text{SO}_4$ ,  $\text{K}_2\text{SO}_4$ ,  $\text{CaCl}_2$  (Jitka Eysseltova) and  $\text{MgCl}_2$  (Wolfgang Voigt) will result in four volumes until 2002.

#### 11. Teaching of undergraduate students: Experimental and theoretical aspects - C. Magalhaes

Clara Magalhaes plans to write a book on teaching solubility phenomena to undergraduates. Colleagues who use simple and illustrative experiments on solubility phenomena in the classroom are requested to communicate with Clara. She will report about her ideas at a conference in Budapest, Hungary.

12. Summary of the Pisa-Workshop (December 1999), Pirketta Scharlin  
1<sup>st</sup> Workshop on Thermochemical, Thermodynamic and Transport Properties of Halogenated Hydrocarbons and Mixtures held under the auspices of the IUPAC, Commission on Thermodynamics

#### OBJECTIVE

to increase the knowledge and understanding of the thermodynamic and transport properties of halogenated organic compounds, especially halogenated aliphatic hydrocarbons, of their mixtures and of mixtures with hydrocarbons.

#### AIMS

- 1) to review available experimental data to identify areas for further studies: thermodynamic data on pure liquids (density, speed of sound, vapour pressure, enthalpy difference, etc.) and for mixtures (density, speed of sound, VLE, LLE, excess properties, etc.), thermochemical data, viscosity and thermal conductivity data for pure fluids and mixtures;
- 2) to consider available methods for thermodynamic modeling, including fundamental EOS for pure fluids and mixtures, innovative mixing rules, model intercomparisons, computer simulations, and model approaches for transport properties of pure fluids and mixtures;
- 3) to select key systems and topics for cooperative research to be carried out for presentation and discussion of the results at future Workshops.

#### SCIENTIFIC PROGRAM

General thermodynamic data:

review and needs

Thermodynamic properties:

models, simulations, and EOS

Precision experimental techniques for pure compounds and mixtures

Phase equilibria, PVT and volumetric properties

Data representation and prediction, and further measurements

Applications of halogenated compounds in organic chemistry

New environment-friendly compounds

Property prediction in near critical region

Applications in medicine

#### What should be our priorities for further research?

(The results of a "Round table" discussion)

Theoretical calculations of the molecular structures of key compounds to improve the representation of their molecular interactions;

initial calculations of intermolecular potentials using *ab initio* methods (GAUSSIAN 99) should be made on HFC's with two carbon atoms;

(suggested key systems:  $\text{HCF}_2\text{CF}_3$  and  $\text{HCF}_2\text{CHF}_2$ )

Measurement of thermodynamic and transport properties of compounds and mixtures where there is an identified data gap and where such data are important for the testing of theoretical models of correlating equations.

It was noted that there is a complete lack of diffusion coefficient data.

Suggested key systems are  $C_6F_{14} + C_6H_{14}$

(plus 2 others, to be agreed).

Measurement of thermodynamic and transport data for technically important HFC binary and ternary mixtures and hydrofluoroethers, for blends of refrigerants with lower alkanes, and for fluorous compounds as media for biphasic catalysis; in medical areas such as liquid ventilation and/or artificial blood substitutes, measurements are required of diffusion coefficients of  $O_2$ ,  $N_2$ ,  $CO_2$ ,  $NO$  in perfluorooctylbromide and in similar compounds with viscosity measurements of the solvents.

Further modeling, for an improved fit to experimental data generally and in particular for the important system of lubricant oils and refrigerants.

(Two or three key systems to be recommended for studying transport properties and phase equilibria measurements.)

With regard to solubility:

what information is available on the solubility of  $O_2$ ,  $N_2$ ,  $CO_2$ ,  $NO$  in liquids which might be considered as blood substitutes or usable in liquid ventilation?

On liquid-liquid solubility for those mixtures which are important in biphasic catalysis? Hence, what additional measurements should be made?

### 13. Reports of Subcommittees and Projects

#### 13.1. Subcommittee V.8.1 Gas/Liquid Systems - P. Fogg and P. Scharlin by P.G.T. Fogg

Project descriptions marked with \* have been updated by P. Scharlin on the basis of information obtained in Hammamet, Tunisia (July 23-24, 2000) and in Halifax, Canada (August 6-11, 2000).

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

(data on COS to be included)

A.E. Mather, Editor; H.L. Clever, C.L. Young, Contributors. 230 compilation sheets in draft or camera ready form; 15 evaluation sheets in draft form; estimated length 290 pages:

According to the new agreement with NIST, there is no minimum length for publications in JPCRD. Prof. Mather wants to publish project 9/86 in smaller sections. The systems closest to completion are the lower alkanes (from methane to butane). The figures above refer to these systems. Prof. Mather estimates June 2001 as the completion date for this section.

##### \* 15/89 FLUORIDES OF NOBLE GASES, BORON, NITROGEN, SULFUR, CARBON AND SILICON (other volatile fluorides may be included).

H.L. Clever, Editor; B. Jaselskis, Contributor. Estimated length 400 pages +

14. Report on the 9th ISSP to be held in Hammamet, Tunisia  
July 25 - 28, 2000 by the Official IUPAC Representative to the 9th ISSP,  
J.W. Lorimer.

9th International Symposium on Solubility Phenomena 25-28 July, 2000,  
Hammamet, Tunisia

The seaside resort city of Hammamet, south of Tunis, was the site of the 9th International Symposium on Solubility Phenomena. Welcoming banners in Arabic and English greeted participants at the entrance of the Hotel Sol Azur, where excellent conference facilities were available. The Symposium was co-chaired by Dr. N. Kbir-Ariguib (Institut National de Recherche Scientifique et Technique, INRST) and Prof. R. Chtara (President, Société Chimique Tunisienne, SCT). Joint organizers were IUPAC Commission V.8 (Solubility Data) and the SCT. The Symposium also welcomed the sponsorship of IUPAC and the SCT. Support is also acknowledged from the Faculty of Science of Tunis, High School for Education and Recycling, and INRST.

Ninety-six participants from 22 countries (Austria, Belgium, Bulgaria, Canada, Czech Republic, Egypt, Finland, France, Germany, India, Ireland, Israel, Japan, The Netherlands, Poland, Portugal, Russia, Saudi Arabia, Spain, Sweden, Tunisia and USA) took part. Of the scientific participants, 46 were from Tunisia and 50 from abroad. There were also eight accompanying persons.

The opening ceremonies brought greetings from Prof. Radhouane Chtara and Dr. Najia. Kbir-Ariguib, Symposium co-chairs, David Shaw, Chair of IUPAC Commission V.8, and Jack Lorimer, IUPAC representative.

Plenary lectures were given by Prof. H.A.J. Oonk (The Netherlands), "Solid State Solubility and its Limits", Prof. M.-Th. Cohen-Adad (France), "Phase Equilibria at Very High Temperatures: the Influence of Pressure" and J.-E. Dubois (France, President of CODATA), "New Data Access and Integration: Interdisciplinary Actions of CODATA". Six invited lectures were given by N. Kbir-Ariguib (Tunisia), J. Rumble (USA), W. Voigt (Germany), T. Ogawa (Japan), E. Königsberger (Austria) and M. Gaune-Escard (France). In addition, there were 24 contributed papers and 33 posters. The invited lectures, contributed papers and posters covered the general areas of: solid state solubility and molten salts; thermodynamics and kinetics in solution; biomineralization; fullerenes; nucleation phenomena; applications of co-precipitation phenomena and phase equilibria in separation technology and formulation of thin films; and compilation and evaluation of solubility data. Lectures and contributed papers were given in six sessions, and there was a very half-day poster session. It is planned to publish the plenary and invited lectures in Pure and Applied Chemistry under the editorship of Peter Fogg (UK).

Participants enjoyed an evening reception and a half-day excursion to the site of Carthage and its excellent museum, plus the picturesque seaside village of Sidi Bou Saïd, where the symposium dinner was held. Accompanying persons were well looked after with excursions to the renowned Bardo Museum in Tunis and to the