

Back in 1972, the idea of collecting and evaluating solubility data emerged from a commission of the IUPAC Analytical Chemistry Division. The planning, coordination, implementation, and realization of the project took many turns over the years, but the project always survived and as of today it has bloomed into 79 volumes spanning more than 25 000 pages. As an early player in this endeavor, and author of three of the first four volumes in the series, Larry Clever has now prepared a historical review of the project, including appendixes listing all the meetings of the group, all events and key records of the International Symposia of Solubility Phenomena, all members of the Commission V.8 from its inception in 1979 until 1999, and complete detailed references of the 79 published volumes of the Solubility Data Series. The excerpts below are extracted from the original review, which is available online at <[www.iupac.org/publications/ci/2004/2603/4\\_clever.html](http://www.iupac.org/publications/ci/2004/2603/4_clever.html)>.

## The IUPAC Solubility Data Project: A Brief History

by Larry Clever

**A**ll scientists have a need to refer to handbooks. Some find their needs met by one comprehensive handbook, others may need to refer to many. Some handbook tables give evaluations and there is normally little question about their reliability. Other tables present an experimental quantity such as atomic mass, melting point, boiling point, vapor pressure, or solubility, and in these tables the reliability and the source of the numbers is often not addressed.

The problem with many handbooks is that often only one value is given, usually without error limits, without literature citation, and without mention of other data that were not used. And most handbooks make little or no effort to provide a complete literature survey or to evaluate in a systematic way the data they present.

Although some people may have wished for a handbook that presented *all* available experimental data on a given property, an *evaluation* of these data, and, where possible, a table of tentative or recommended data, such a handbook was never available. To do so is time-consuming and financially unrewarding. However,

for more than 25 years the Solubility Data Project has been successfully pursuing this elusive goal.

### Project Organization

In 1972, A. Stevan Kertes (The Hebrew University, Israel), proposed that the IUPAC Commission V.6, Equilibrium Data, of which he was a member, start a project on collecting and evaluating solubility data. Publications were envisaged in which all reliable data would be presented as they appeared in the original literature. In addition, experts would evaluate the data and, where appropriate, tables, figures, or fitted equations of tentative or recommended data would be prepared and presented for the use of the scientific community. Fortunately, the idea had the strong support of Commission V.6 Chair George Nancollas (SUNY Buffalo, USA) and of the IUPAC Executive Secretary Maurice (Mo) Williams. Without their support, the presence of strong opposition meant that the idea would have likely gone no further.

In 1973, a working party—appointed by the commission to consider further the idea of a solubility data project—authorized Kertes to set up a group independent of Commission V.6. In the fall of 1974, a group of recognized experts in the field of solubility was invited to meet with Kertes at McGill University in Montreal, Canada for what was the first Solubility Data Project meeting. (The complete attendance list can be found in the online version of this article.)

The following issues, first discussed in Montreal, were to come up at almost every Solubility Data Project meeting:

- guidelines for data sheets and evaluations
- evaluation methods and the preparation of useful evaluations
- recruitment of compilers, evaluators, and editors
- computers, databases, and electronic publication

At the meeting, a tentative format for collecting and evaluating solubility data was decided upon. Several attendees took on the task of preparing sample compilations and the evaluation of a single system in their areas of expertise. It was also decided that detailed guidelines for the compilation and evaluation of data should be developed.

*... most handbooks  
make little or no effort  
... to evaluate in a  
systematic way the  
data they present.*

*Participants at the Workshop on Solubility Phenomena: Applications for Environmental Improvement, organized during the 10th ISSP Varna, Bulgaria, in July 2002 (see diagram): 1. Jack Lorimer (CDN), 2. Earle Waghorne (IRL), 3. Kiyoshi Sawada (J), 4. Reginald Tomkins (USA), 5. Jim Sangster (CDN), 6. Alan Mather (CDN), 7. Mark Salomon (USA), 8. Andrzej Maczynski (PL), 9. David Shaw (USA), 10. Dana Knox (USA), 11. Valerii Sazonov (RUS), 12. Jan Vanderdeelen (B), 13. Cezary Guminski (PL), 14. Ryo Miyamoto, 15. Roger Cohen-Adad (F), 16. Justin Salminen (FIN), 17. Pirketta Scharlin (FIN), 18. Clara Magalhaes (P), 19. Hitoshi Ohtaki (J), 20. Vesselina Platikanova (BG), 21. Stefka Tepavitcharova (BG), 22. Adam Skrzecz (PL), 23. Christo Balarew (BG), 24. Wolfgang Voigt (D), 25. Marie-Therese Cohen-Adad (F), 26. Heinz Gamsjäger (A), 27. Jitka Eyseltova (CZ), 28. Ken Marsh (NZ), 29. Hiroshi Miyamoto (J), 30. Vladimir Valyashko (RUS)*



The IUPAC General Assembly met in Madrid, Spain in 1975. Commission V.6 invited observers interested in the solubility project to attend. Larry Clever, Colin Young, and Alan Clifford accepted the invitation and attended the meeting. Plans for the project moved ahead quite rapidly. The Solubility Data Project was made a Subcommittee of Commission V.6. Finally, in 1979 at the IUPAC General Assembly in Davos, Switzerland, the Solubility Data Subcommittee became a full commission (Commission V.8 of the Analytical Chemistry Division).

In 1999, at the Berlin General Assembly of IUPAC, an extensive reorganization was approved, under which all commissions (with a very few exceptions) were to be replaced by 2001 with working groups for specific projects under the direct control of the appropriate divisions. The plan for the Solubility Data Project was to combine the work of the Solubility Data and Equilibrium Data Commissions into a new subcommittee of the Analytical Chemistry Division called the Subcommittee on Solubility and Equilibrium Data. Thus, the Solubility Data Project has come full circle from subcommittee through commission and back again, albeit with very different terms of reference and very different experience.

The mission of the Subcommittee on Solubility and Equilibrium Data (SSED) is to coordinate projects in the area of compilation and critical evaluation of published experimental data on the chemical solubility of well-defined substances and other equilibrium sys-

tems. The SSED also coordinates the dissemination of evaluated solubility data through traditional (journal) and electronic (Internet-accessible database) means. The SSED works with the Analytical Chemistry Division and the U.S. National Institute of Standards and Technology (NIST, the Solubility Data Series publisher) in the selection of chemical systems for treatment, encourages the formation of Task Groups to perform compilation and evaluation, and assists Task Groups in carrying out their projects.

The initial membership of the SSED consists of H. Gamsjäger (Austria) as chair, P. May (Australia), M. Salomon (USA), P. Scharlin (Finland), D. Shaw (USA), S. Sjöberg (Sweden), and W. Voigt (Germany).

## Publication

In 1978 a contract for the publication of the solubility data volumes was formalized between IUPAC and Pergamon Press. Stevan Kertes insisted on several points in the agreement, which set precedents. First, the agreement called for a page fee to be paid to each compiler and evaluator and for a page-typing fee to be paid to each volume editor. Previously, IUPAC project participants received no payment because it was assumed sufficient that the project was part of their research and enhanced their reputation. Second, these page fees would change in proportion to the UK cost-of-living price index.

Pergamon published the first 53 volumes of the

## The IUPAC Solubility Data Project: A Brief History

*Solubility Data Series* between 1979 and 1992. Due to some disagreements over the price of the volumes and publicity, the commission cancelled the publication agreement with Pergamon at the end of 1988. However, IUPAC and Pergamon agreed on a revised contract (negotiated by Jack Lorimer and Mo Williams) in 1989 that provided even better terms for compilers and evaluators. In 1992, two years after Pergamon Press had been sold to Elsevier Publishing Co., Elsevier decided to drop the series.

Between 1994 and 1996, Oxford University Press (under a contract also negotiated by Lorimer and Williams), published volumes 54 through 65, until that publisher decided to cancel the contract. The *Solubility Data Series* did not have a publisher between 1997–1998. In 1998, Mark Salomon and David Shaw helped forge an agreement between IUPAC and NIST (National Institute of Standards and Technology) that called for publication of the *Solubility Data Series* for at least four years as a part of the *Journal of Physical and Chemical Reference Data*, whereupon the series became known as the *IUPAC-NIST Solubility Data Series*.

### Recruitment

For such an extensive and lengthy project it was necessary to recruit experts in many areas of both theory and practice of solubility. The list of participants in the project is rather difficult to estimate accurately, but certainly has well exceeded 100. Along with Stevan Kertes, Larry Clever and Mark Salomon were very successful in attracting capable people to take part in the project.

One difficult problem with recruitment in the 1980s was to involve the large number of scientists in the then-USSR in the project. Exploratory visits to the USSR under IUPAC auspices were made by Stevan Kertes and by C. Kalidas (India), with promising results. An unexpected problem arose. The copyright agency of the USSR, VAAP, insisted that any payments to contributors from the USSR should be made through and by them. A strong stand by Mo Williams and Jack Lorimer, with negotiations carried out by IUPAC Secretary General Tom S. West, succeeded in retaining IUPAC's right to make payments directly to contributors.

### Committee Leadership

Stevan Kertes took on the responsibilities of both chair of the Solubility Data Commission and editor in

chief of the IUPAC *Solubility Data Series* until 1987. Kertes continued as editor in chief, and Jack Lorimer became chair in 1987. Unfortunately, Kertes died suddenly in July 1988, a great blow to the project. Fortunately, Lorimer quickly and firmly took control and worked to see the project move ahead. As both editor in chief and chair of Commission V.8, he developed needed systems and brought order to the production of the Solubility Data Project volumes.

In 1996 Mark Salomon, U.S. Army Electronics Command, (USA) became editor in chief. Early on he negotiated an agreement with NIST and the *Journal of Physical and Chemical Reference Data* to publish the series. In 1992 the chairperson and editor in chief positions were divided, with Jack Lorimer continuing as editor in chief and Mark Salomon as the chair. In 1996 David Shaw, University of Alaska, (USA), became chair and Mark Salomon editor in chief.

Stevan Kertes acted as secretary of the Solubility Data Project from the beginning until 1979 when L. H. Gevantman, Office of Standard Reference Data, NBS (now NIST), was elected to the position. Gevantman served the project well with good advice and attention to detail, and set a good example for the commission secretaries who were to follow: R.P.T. Tomkins, New Jersey Institute of Technology (USA), and H. Gamsjäger, Montanuniversität Leoben (Austria), both of whom have done outstanding work.


### Subcommittees

From the first meeting, the Solubility Data Project was organized into three subcommittees with responsibility for ensuring that the volumes were prepared, properly edited, and reviewed before publication. Upon attaining commission status these subcommittees were designated as follows:

- V.8.1 Gases in Liquids. Chair H. L. Clever (USA), 1976–1992; P. G. T. Fogg (UK) 1992–2000; Pirketta Scharlin (Finland), 2000–2001
- V.8.2 Liquids with Liquids. Chair A. F. M. Barton (Australia), 1976–1984; F. W. Getzen (USA), 1984–1998; A. Skrzecz (Poland), 1998–2001
- V.8.3 Solids in Liquids. Chair Mark Salomon (USA), 1976–1992; M.-Th. Saugier-Cohen Adad (France); 1992–2000; W. Voigt (Germany), 2000–2001

In addition to the subcommittees, Colin Young acted as a committee of one to prepare and edit the three cumulative indexes of the volumes (Volumes 19, 39 and 53) for the 53 volumes published by Pergamon

## The IUPAC Solubility Data Project: A Brief History

Press. No index volumes have yet been prepared for the 12 volumes published by Oxford University Press and the volumes published by NIST. 

The author thanks Rubin Battino, Heinz Gamsjäger, David Shaw, and Mark Salomon and others who have read and commented on the manuscript. He has special thanks for Jack Lorimer who has carefully read the manuscript several times and made many valuable suggestions.

**Editor's Note:** Due to space constraints, this abbreviated article omits a number of sections. However, the following sections are included in the online version: Organization of the Printed Volumes, Guidelines, Databases and Electronic Publishing, International

Symposium on Solubility Phenomena, Solubility Data Center, A Book on the Experimental Determination of Solubilities, the Franzosini Award, References, and Appendixes.

Professor H. Lawrence Clever <hclever@att.net> retired in 1992 from the Department of Chemistry at Emory University, Atlanta, Georgia, USA, but he is still active and is preparing volume 80.

 [www.iupac.org/divisions/V/502](http://www.iupac.org/divisions/V/502)

A description of the latest volume of the *Solubility Data Series*, volume 79, appears on page 30.

## The CCE Seeks Expressions of Interest in Hosting the International Conference on Chemical Education

The International Conference on Chemical Education is a biennial event planned by the IUPAC Committee on Chemistry Education (CCE). The 18th conference in the series will be held 3-8 August, 2004, in Istanbul, Turkey. In 2006, the event will be held in Korea. CCE plans to identify possible hosts for the 2008 venue by the time of the conference in Istanbul. The CCE will make a final decision on the location at IUPAC's General Assembly in Beijing in 2005.

A letter expressing interest should be sent to Peter Atkins, CCE chairman, by 15 July 2004; e-mail <peter.atkins@lincoln.ox.ac.uk>.

**Korea, Seoul, 2006**  
**Turkey, Istanbul, 2004**  
**China, Beijing, 2002**  
**Hungary, Budapest, 2000**  
**Egypt, Cairo, 1998**  
**Australia, Brisbane, 1996**  
**Puerto Rico, San Juan, 1994**  
**Thailand, Bangkok, 1992**  
**England, York, 1991**  
**Canada, Waterloo, 1989**  
**Brazil, São Paulo, 1987**  
**Japan, Tokyo, 1985**

