100 volumes of IUPAC’s Solubility Data Series

by David Shaw

The year 2014 marked the publication of Volume 100 of IUPAC’s Solubility Data Series. Since publication began in 1979, each volume has presented an exhaustive compilation from the published chemical literature of experimentally determined solubility data for a group of related and chemically well defined systems, such as methane in liquids (vol. 27/28, 1987), liquid and solid hydrocarbons with water and seawater (vol. 81, 2005), or potassium sulfate in water (vol. 93, 2012). Whenever two or more sets of independent experimental data have been reported in the primary chemical literature and are judged to be free of obvious errors, the data are critically evaluated in an effort to guide the user to the most reliable data.

A Symposium during the August 2014 Annual Meeting of the American Chemical Society marked the publication of 100 volumes and looked forward to continuation of IUPAC’s Solubility Data Project, both in its current print form as articles in the Journal of Physical and Chemical Reference Data and in electronic formats. Presentations at the symposium covered a range of topics including the history and evolution of the project, contemporary issues related to the compilation and evaluation of solubility data, and new approaches to the dissemination of solubility and other equilibrium data.

The work of data compilation and evaluation necessary for the preparation of each volume is carried out by an international group of experts operating under a set of guidelines that ensure uniformity in the approach to the work and format of the volumes. Participants in the Solubility Data Project have met annually since the mid-1970s. In the early years of the project international communication was slow, difficult and expensive. Although global web-based communication is now convenient, participants still find it valuable to meet face to face each year.

The requirements for compilation are straightforward: an exhaustive search of the published primary chemical literature for published experimental data, together with a summary of experimental methods and estimates of experimental error where those are provided in the published work or can be estimated by the compiler. Solubility values from review articles and handbooks are not used unless they can be traced to original experimental work.

The guidelines for critical evaluation of the data allow flexibility based on expert scientific judgment. Flexibility is required to accommodate both the range of data precision that exists over chemical systems studied and the considerable variation in theoretical frameworks for data interpretation between, say, gases in nonpolar liquids and salts in water. But in every evaluation the goal is to indicate the reliability and precision of solubility data and to clearly explain the evaluation method used to reach the assessment presented.

CI readers are invited to view the related article published recently in Chemical Information Bulletin Vol. 66, No. 4: Winter 2014, online at http://bulletin.acscinf.org/node/668. Detailed information about the Solubility Data Series, including lists of volumes (published and in preparation) as well as guidelines for the preparation and use of these volumes is available at www.iupac.org/body/502. Suggestions and proposals for collaboration on future volumes are always welcome.

www.iupac.org/project/2014-012-2-500

FloHet-2014

by Eric Scriven

The 15th Annual Florida Heterocyclic and Synthetic Conference took place at the University of Florida in Gainesville, 2-5 March 2014. The theme of the conference was catalysis in organic chemistry. This was reflected in the course, Pd-catalyzed Cross-coupling Reactions: From Fundamental Steps to Catalytic Cycles, given by Bert Maes, University of Antwerp, Belgium.
Conference Call

Eleven plenary lectures, four short courses, and 50 invited lectures were delivered. Towards the end of the conference a Hot Topics in Catalysis Session was led by Professors Beller and Maes. There was a poster session that attracted 60 posters and a small exhibition at which publishers, chemical manufacturers, and scientific instrument companies exhibited. Two hundred delegates from over thirty countries attended the conference.

The plenary lectures were given by: Mathias Beller, University of Rostock, Germany, Catalysis: A Key Technology for Sustainable Synthesis; Carolyn R. Bertozzi, UC Berkeley, USA, In vivo Chemistry; Jonathan Clayden, University of Manchester, UK, Asymmetric Arylation and Vinylation of Carbanions; Peter J. Dunn, Pfizer, UK, Green Heterocyclic Chemistry; Paul Feldman, Glaxo-SmithKline, USA, Organic Chemistry Aiding Medicinal Chemistry Advances; Stephen Hanessian, University of Montreal, PQ, Canada, Exploring the Unique Reactivities of Heterobicyclic Tetrazoles – Access to Functionally Diverse and Versatile Heterocyclic Scaffolds; Sebastien Lemaire, Janssen Pharmaceutica, Belgium, Stereoselective C-Glycosylation Reactions with Aryl-zinc Reagents; Erik J. Sorensen, Princeton University, USA, Taking Risks in Complex Synthesis Design; Jim Thomas, University of Manchester, UK, Approaches to the Synthesis of Some Biologically Active Compounds; M. Christina White, University of Illinois, USA, Site Selective C-H Oxidation; Tony Wood, Worldwide Medicinal Chemistry, Pfizer, USA, Heterocycles and Medicinal Chemistry: The importance of Innovative Synthesis.

Invited lectures were given by: H. Amri (Tunisia), M. Azam (Saudi Arabia), R. Bavantula (India), P. Belmonte (France), E. Biehl (USA), U. Braendli (Switzerland), K. Campos (USA), A. Campbell (USA), J. Christensen (Denmark), C. Chung (USA), F. Cossio (Spain), N. Downer-Riley (Jamaica), G. Dudley (USA), P. Erdhardt (USA), S. Florio (Italy), M. Francisco (USA), R. Hanes (USA), F. Hansen (Germany), H. Ihmels (Germany), Y. Iwabuchi (Japan), Y. Jackson (Jamaica), R. Kargbo (USA), D. Ketcha (USA), J. Kocevar (Poland), S. Kotha (India), S. Kumar (India), M. Laksman (USA), J. Madelengoita (USA), V. Mamedov (Russia), A. Mattson (USA), C. Meyer (France), V. Milata (Slovakia), T. Moss (UK), A. Nefzi (USA), D. Onicui (France), R. Orru (Netherlands), D. Otte (Germany), S. Parumal (India), V. Patil (India), N. Peet (USA), Z. Pei (USA), H. Sintim (USA), J. Soloduchko (Poland), J. Svete (Czech Republic), K. Tanaka (Japan), W. van Otterlo (South Africa), A. Verma (India), D. Virieux (France), C. Williams (Australia), B. Zajc (USA).

The next Florida Heterocyclic and Synthetic Conference, FloHet-2015, will take place at the University of Florida, Gainesville, March 1-4, 2015. The Katritzky Memorial Lecture will be given by Albert Padwa, Emory University, USA. Plenary lecturers will include, Huw Davies, Emory University, USA; Veronique Gouverneur, Oxford University, UK; Timothy Jamison, MIT, USA; Peter Maienfisch, Syngenta, Switzerland; Christel Menet, Galapagos, Belgium; Tobias Ritter, Harvard University, USA; Paul Scola, BMS, USA; Jay Siegel, Tianjin University, PRC; Oliver Thiel, Amgen, USA; Yoshinori Yamamoto, Tohoku University, Japan. The short course entitled: Selective Direct Fluorination Strategies: Batch and Flow will be given by Graham Sandford, University of Durham, UK.

Nanomaterials and Human Health: The Trends and Future

by Vladimir Gubala

A workshop was held 15-16 September 2014, as a joint venture of the IUPAC Chemistry and Human Health Division (Div VII) and the University of Kent. The workshop received support from the Peptide Research Network of Excellence (PeReNE). 37 participants from 9 countries (Ukraine, Slovakia, Italy, France, Germany, Spain, Ireland, England, and Egypt) attended the symposium. There were 17 oral presentations, with poster sessions in the breaks.

After a welcome and the introduction of IUPAC and the University of Kent by Dr. Vladimir Gubala, 17 talks and 15 posters were presented. This included a poster dedicated to IUPAC, highlighting the main goals of IUPAC and specific contributions of the Division VII, and in particular two ongoing IUPAC projects: 2013-007-1-700 and 2010-051-1-700. Both deal with various aspects of nanomaterial preparation and advances in immunochemistry and their applications to human health.

The speakers presented original research work on a wide range of potential theranostic applications of nanoparticles. These included gas-filled nanobubbles that improve ultrasound signals of blood vessel walls, specific nanoparticles targeted to diseased tissues or across natural barriers (such as the blood-brain barrier), and specific signal transduction into lymphocytes. There is a clear need for more specific therapy and diagnosis (theranostics) for many diseases, notably for very aggressive tumours where known pathogenesis