

## IUPAC Committee on Printed and Electronic Publications

Report to Council, 2003-2004

CPEP met in Ottawa, Canada, in 2003 and in London, UK, on 26-27 June, 2004. The two-day annual meeting is currently structured so that project business and strategic electronic publishing issues are discussed on one day and operational issues, such as reviewing reports on IUPAC publications, are dealt with on the alternate day. On its first (reporting) day, the London meeting was attended by both the Secretary General and by Dr Wendy Warr, the latter in her capacity as ICSTI representative. Other invited attendees were Dr Steve Heller (Div. VIII representative) and Prof. Robert Lancashire (leader of a Data Standards group). Between annual meetings, the committee members have communicated regularly with each other, and the Secretariat, mainly by Email.

CPEP is currently responsible for four projects and for the publications of IUPAC.

1999-046-2-024 - [Data exchange standard for electron paramagnetic resonance data types \(incl. ESR EMR etc.\)](#)

2002-020-2-024 - [Data exchange standard for near infrared spectra and general spectroscopic calibration data types](#)

2002-022-1-024 - [Standard XML data dictionaries for chemistry](#)

2002-055-3-024 - [XML-based IUPAC standard for experimental and critically evaluated thermodynamic property data storage and capture](#)

**Data Exchange Standards:** The projects under this heading are organized by a Subcommittee of CPEP (coordinated by Tony Davies, Secretary of CPEP, and reported by him) and constitute a series of projects with the purpose of providing a common framework for electronic data exchange. Collaborative work with ASTM International is proceeding on the new Analytical Information Mark-up Language, AnIML, which will be a series of XML standards.

### **Standard XML Data Dictionaries:**

These projects (under the guidance of Steve Stein and Michael Frenkel, both associated with NIST) are intended to provide interoperability solutions for interpretation and use of chemical data, a critical objective for data use across the board.

**INChI (International Chemical Identifier):** This is a project of Div. VIII, about which CPEP has an intimate concern and which maintains an interest in its very successful progress.

**Colour Books:** The standard XML data dictionaries for chemistry are important projects intended to facilitate electronic intercommunication. As such, they will complement (and update) the IUPAC Gold and Green Books (respectively, "Compendium of Chemical Terminology", 1997, and "Quantities, Units and Symbols in Physical Chemistry", 1993). Work on the Gold Book has proceeded apace, but the contents of the Green Book (which is out of print) had not been provided by the author so that progress was halted.

The Purple Book (“Compendium of Macromolecular Nomenclature”, 1991) is also out of print while updates to the Red Book (“Nomenclature of Inorganic Chemistry”, 2000) and Blue Book (“A Guide to IUPAC Nomenclature of Organic Compounds”, 1994) were reported in 2004 to be in review status. The Orange Book (“Compendium of Analytical Nomenclature”, 1997) was made available online in August, 2002. The Silver Book (“Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences”, 1995) and White Book (“IUBMB Biochemical Nomenclature”, 1992) were reported to be available. A Website for the latter is maintained by Dr Gerry Moss at <http://www.chem.qmul.ac.uk/iupac/bibliog/white.html>; there has been some discussion with Dr Moss (as yet fruitless) regarding the transfer of this site to the IUPAC Webserver.

### **Pure and Applied Chemistry (PAC)**

The publication process for PAC has been much facilitated by the successful review and implementation of recommendations on electronic submission and control systems. Problems still remain with regard to ensuring that plenary speakers at IUPAC Congresses meet their obligation to publish their contributions in PAC.

The Editorial Advisory Board (EAB), in its earlier form, had been abolished and James Bull, in his capacity as Scientific Editor, has drafted proposals for the re-establishment of the EAB, in a revised format.

Pricing for PAC was proposed as follows: Standard USD1500; Electronic USD900; Individual USD99; Single Copies USD150; and Single Articles USD25. The last price was set so as to make it more expensive to generate (in effect) a Single Copy by purchase of the set of Single Articles!

The important task of generating Web access to back numbers was being efficiently organized by Bohumir Valter, a Committee member (back to 1965 at the time of the London meeting.)

### **Chemistry International (CI)**

The much improved format and content of CI has been noted, and Fabienne Meyers (as Editor) congratulated on the progress. The Institutional Subscription price was set as USD99.

### **Web Access (<http://www.iupac.org>)**

Web access to IUPAC information is of increasing importance for members, subscribers and interested persons. Considerable effort is being expended in improving access, in terms of organization, linking, and provision of material. The hosting and services have recently undergone formal review and a series of recommendations for improvement will be implemented by the secretariat. The important assistance of Bohumir Valter is gratefully acknowledged.

### **Membership of outside bodies:**

ICSTI and IUPAP: Wendy Warr; CODATA: Tony Davies; ICSU: John Jost.

Two projects were submitted in the name of IUPAC to CODATA for funding at the 2004 CODATA GA and rejected. The submissions were not known to the Secretariat or the Secretary General and were not presented by the IUPAC representative to the meeting who was forced to admit that he had no knowledge of the submissions. We have good arguments for receiving additional CODATA funding for our projects but a substantial improvement in the way we approach such applications would be helpful.

**CPEP Membership**

Chairmanship of CPEP transferred to Leslie Glasser (Australia) in 2004.

Leslie Glasser  
Chair, CPEP  
8<sup>th</sup> July, 2005