

IUPAC Committee on Printed and Electronic Publications

Report to Council for 2005-2006

I. Highlights

Three major developments of significance to IUPAC as a whole have occurred over the recent biennium. The first is the movement of the IUPAC Website (<http://www.iupac.org>) to FIZ-Chemie in Berlin at most favourable terms. This change permits greater control of the operations of the Website, enhancing both content and interactivity. The second is the publication online and on CD-ROM of the “Gold Book” (IUPAC Compendium of Chemical Terminology) in an enhanced, interactive XML version (<http://goldbook.iupac.org>). The third is the availability online of *Pure and Applied Chemistry*, now from vol. 45 (1976); the format of the most recent online volumes (from 2007) represents major enhancements of their usability, now including ‘out-bound linking’ of the references to their sources, through IUPAC’s membership of CrossRef.

II. Overall Report

b) IUPAC provides research tools

The new version of the “Gold Book” is an important resource for the chemical community in providing ready access to definitive information on chemical terminology.

d) IUPAC fosters communication

The enhanced Website and the provision of ready access to *PAC* and *CI* enhance the IUPAC image.

III. Other Information

CPEP met in Beijing in 2005 and in Berlin on 14-16 July, 2006. On each occasion, the publication parameters (content, schedules, self-publication, prices and currency) of the IUPAC publications, *Chemistry International* and *Pure and Applied Chemistry*, and of books, were considered. Publication of the periodicals has been eased by the process of electronic submission and control through Manuscript Central. Control by the Scientific Editor, Prof. James Bull, of the contents of *PAC* has seen an enhancement of the appropriateness of material submitted, and of the speed of publication. In acknowledgement of the movement towards open access, it has subsequently been agreed that pdf copies of articles in *PAC* could be made available on author’s own sites without any delay following publication.

A proposal was made in Beijing that the Divisions be requested to review their published numerical data collections and identify which should be considered for digitization

to make them available electronically. This review should then be reported back to CPEP so that a common procedure can be instituted. However, no response has been received as yet.

JCAMP (Joint Committee on Atomic and Molecular Physical Data) is the acronym under which IUPAC is developing and refining standard spectrometric data formats. CPEP's Subcommittee for Electronic Data Standards (SEDS) has oversight within IUPAC for all activities in either the JCAMP-DX sphere or the XML in Chemistry area. The website under which it formerly operated (jcamp.org) has recently been "high-jacked", and the relevant SEDS files have been transferred to the IUPAC website at <http://www.iupac.org/jcamp/>. The information contained therein is, however, not yet fully updated.

IV. Tabular Material

CPEP is responsible for four recent projects (one still in progress), two new projects, and for the publications of IUPAC.

Project #1999-046-2-024: Data exchange standard for electron paramagnetic resonance data types (incl. ESR EMR etc.). Chair: R. J. Lancashire – completed 2006.

Project #2002-022-1-024: Standard XML data dictionaries for chemistry (Gold Book). Chair: Steve Stein – completed 2007.

Project #2002-055-3-024 - XML-based IUPAC standard for experimental and critically evaluated thermodynamic property data storage and capture (ThermoML) Chair: M. Frenkel – completed 2006.

Project #2002-020-2-024: Data exchange standard for near infrared spectra and general spectroscopic calibration data types Chair: G. Downey – in progress.

Two new projects dealing with the conversion of Colour Books to interactive XML versions have been submitted by members of the team which produced the XML version of the "Gold Book" and subsequently approved:

2007-016-1	Enhancement of the electronic version of the IUPAC Compendium of Chemical Terminology
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024	Bedrich Kosata	Date submitted: 18-Apr-07
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This project aims to maintain the currency of the Gold Book, to ease electronic access to individual entries, and to publicise its availability.

2007-014-1	Software framework for transformation of IUPAC Color Books to XML
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024	Bohumir Valter	Date submitted: 06-Apr-07
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This project is intended to provide a common basis for conversion of the Colour Books to XML, thus easing the conversion processes.

CPEP's Subcommittee on Electronic Data Standards is working with ASTM International Committee E13.15 on an XML standard for analytical data—the Analytical Information Markup Language (AnIML). It is expected that this group will meet in Torino, ahead of the CPEP meeting.

Publications 2005-6

Subcommittee on Electronic Data Standards (R. Lancashire)

"JCAMP-DX for electron magnetic resonance (EMR)" (IUPAC Recommendations 2006)

Pure Appl. Chem. 78(3), 613-631, 2006

<http://dx.doi.org/10.1351/pac200678030613>

"Spectroscopic Data: The Quest for a Universal Format", by Robert Lancashire and Tony Davies Chem. Int. Jan-Feb 2006, p. 10 - see the many links therein.

http://www.iupac.org/publications/ci/2006/2801/3_lancashire.html

ThermoML Project (M. Frenkel)

"ThermoML - an XML-based IUPAC Standard for storage and exchange of experimental thermophysical and thermochemical property data",

Pure Appl. Chem., 2006, 78, 541-612.

<http://dx.doi.org/10.1351/pac200678030541>

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