## Data Standards within IUPAC and the role of CPEP

## Robert John Lancashire

The Department of Chemistry, The University of the West Indies, Mona Campus, Jamaica, robert.lancashire@uwimona.edu.jm

The terms of reference for **CPEP** (IUPAC's Committee on Printed and Electronic Publications) include offering advice to the President, Executive Committee, other Standing Committees, Divisions, and Commissions on all aspects of the design, implementation, production and dissemination of printed and electronic publications, including computerized databases of all sorts, and to promote the compatibility of electronic transmission and storage of information.

Some of the notable successes include the following:

In 1995, IUPAC took over the responsibility for the JCAMP-DX range of data standards and initially this was handled by a working party until 2003 when it evolved into **SEDS** (the subcommittee of electronic data standards of CPEP). The protocols developed and published for instruments including IR, MS, NMR, IMS, EPR, etc. were done with open collaboration between industry and user groups. This was seen as a key to the successful development of internationally recognized data standards.

The IUPAC Compendium of Chemical Terminology (Gold Book) belongs to the IUPAC "Colour Book" series and comprises over 6000 terminology definitions that were published in *Pure and Applied Chemistry* and other "Colour Books". The last printed version of the Gold Book was in 1997. In 2002 the project "Standard XML data dictionaries for chemistry" began and 2005 saw the first public preview release of an online XML Gold Book.

The InChI project, begun in 2000 is overseen by an IUPAC Division VIII subcommittee and recently ownership of the project was assumed by the InChI Trust. Version 1.03 of the algorithm was released in June 2010 and the InChI program is believed to be the most widely used IUPAC project having gained widespread acceptance and implementation.