

Teamwork - Issue No. 5-

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This issue of 'Teamwork' includes:

- A success story: the Orange Book on the web.
- Project Reports: some snippets.
- Division V supports the SEANAC Conference in Botswana.
- Ottawa initiative: the Division V Workshop on "New challenges for Analytical Chemists: Genomics and proteomics"
- Gleanings from the President's report to Council.

Web strikes - The Orange Book is a hit!

One feature of David Moore's time as Division President is the energy he has put into the preparation of a web version of the Orange Book (Compendium of Analytical Nomenclature).

The success of this development is indicated by the number of "hits" on the IUPAC website. In the first 3 months of 2003 the Orange Book accounted for 1/6 (99432) of the total hits (578399) on the IUPAC publication folder! This is most encouraging, especially as the "Orange Book project" has only taken the first step - a verified transcription of 'hard copy' into html.

This success does show us how much the scientific community values the information contained in the OB. But we all know that much of the content is rather dated. Therefore a process to update the Orange Book has been implemented. It has begun with the Chapters on Electrochemical techniques ([2002-002-2-500](#)) and Separation methods ([2001-063-1-500](#)), to be followed by the other chapters systematically over the next few years. Perhaps this 'success' tells us that serving the analytical chemistry community through web-based compendia such as the OB should be identified as 'core business' of the Division. [The editor notes that two other projects that will impact on the content of the OB are currently being drafted or reviewed.]

To view the on-line version of the Compendium of Analytical Nomenclature (Orange Book):
(http://www.iupac.org/publications/analytical_compendium)

Progress reports from Task Groups

The Division asks the leader of each Task Group to submit a brief project report every 6 months. These are invaluable to the Division officers as a means of monitoring the progress of projects and of identifying concerns or difficulties that may arise.

The months since the previous reporting period have been very productive! Publications completed include:

The experimental determination of solubilities, John Wiley & Sons. ISBN 0-471-49708-8, March 2003.
See [CI, 25, No. 4 \(2003\)](#).
Task Group Leader: R. Tomkins.
Project number: [2001-084-1-500](#)

Chemicals in the Atmosphere - Solubility, Sources and Reactivity. John Wiley & Sons. ISBN 0-471-98651-8. See [CI, 25, No. 4 \(2003\)](#).

Task Group Leader: Peter Fogg.
Project number: [2001-037-1-500](#)

IUPAC-NIST Solubility Data Series. 79. Alkali and Alkaline Earth Metal Pseudohalides JPCRD (2003).
Task Group Leader: J. Hala.
Project number: [2001-085-1-500](#)

Critical evaluation of stability constants for alpha-hydroxycarboxylic acid complexes with protons and metal ions and the accompanying enthalpy changes. Part II. Aliphatic 2-hydroxycarboxylic acids (IUPAC Technical Report), by R. Portanova, L. H. J. Lajunen, M. Tolazzi¹, and J. Piispanen. [Pure Appl. Chem. 75\(4\), pp. 495-540, 2003](#)

Critical review of analytical applications of Mössbauer spectroscopy illustrated by mineralogical and geological examples (IUPAC Technical Report), by E. Kuzmann, S. Nagy, and A. Vértes. [Pure Appl. Chem. 75\(6\), pp. 801-858, 2003](#)

Here are some 'snippets' from the latest round of Progress Reports:

We are finishing the project, hopefully it will be done by June 30. We have 432 pages of data sheets and evaluations. Indexes are in progress.

[Lawrence Clever: [IUPAC-NIST Solubility Data Series. Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon and Silicon and Solid Xenon Fluorides in all Solvents.](#)]

The revised final text will be send to the Division in July.

[Konstantin Popov: [Critical evaluation of Stability Constants of Metal Complexes of Complexones for Biomedical and Environmental Applications](#)]

[I am] going to attend suitable Conference in 2004 in order to disseminate results.

[Konstantin Popov: [Recommendations for NMR Measurements of high pK Values and Equilibrium Constant in Highly Basic solutions](#)]

Currently the database holds stability constant data on 8453 ligands -130 new ligands since November 2002 (all with .mol file structures) from 21254 references - nearly 800 new references (since November) - and holds 98701 records - an increase of over 4000. The interrogation software has been improved and the searching on CAS registry numbers extended.

[Leslie Pettit: [IUPAC Stability Constants database](#)]

An important new feature has been added. Experimental data (pairs of ionic strength and log K value) may now be entered interactively, or as a text file. The SIT parameters can then be calculated by on-screen curve fitting, with standard deviations. The latest version of the PC-compatible computer program is available on www.acadsoft.co.uk and will be added to the IUPAC web-site shortly. Dr Igor Sukhno is currently adding more SIT parameters and preparing a Russian version.

[Leslie Pettit: [Ionic Strength Corrections for Stability Constants](#)]

Southern and Eastern Africa Network of Analytical Chemists (SEANAC)

The objectives of this [inaugural conference in Botswana \(7-10 July\)](#) are to develop networks between analytical chemists on the African continent, to facilitate the sharing of information and the limited resources available.

All Divisions in IUPAC have a responsibility to further the worldwide dissemination of information and understanding in the chemical sciences. A very tangible commitment that Division V has made to

Chemistry Education in this biennium is to sponsor one of its TM (Roger Smith) to attend the SEANAC meeting in Botswana.

Division V wished to identify with this group of analytical chemists who are seeking solutions to real challenges in teaching and research in analytical chemistry, in countries that are less well resourced than most. As well as providing encouragement we wanted to listen to their initiatives and concerns, identify any areas in which we can be of help, and identify ways in which African analytical chemists can contribute to the work of the Division. The next issue of '**Teamwork**' will have a report from Roger.

A new initiative in Ottawa

The Division has been seeking ways to improve its links with stakeholders/end-users. It has also noted the capacity for the Division Committee itself to be much more pro-active in identifying projects. The Committee meetings could, in part, assume the role of a 'think tank' and so generate Project proposals 'from the top down' (the inverse of the present process).

To help achieve both of these objectives we are holding a half-day workshop, a forum with input from external experts, as part of the General Assembly meeting in Ottawa (Sunday 10 August at 9.00 a.m.). The topic will be "***New challenges for Analytical Chemists: Genomics and proteomics***"

The rapidly changing face of analytical chemistry has indeed posed new challenges to the role of IUPAC. Among the emerging needs are analysis of genetically modified organisms (GMOs), functional proteomics and combinatorial analysis, to mention but a few.

In order to generate ideas for new generic projects at the cutting edges of analytical chemistry this workshop will include presentations by invited participants as well as contributions from members of the Division Committee. External experts will include:

- A. Edwards, Director of Structure Genomics Consortium, Department of Medical Research, University of Toronto.
- T. Kodadek, Center for Biomedical Inventions at the UT-Southwestern Medical Center, Dallas, TX.
- J. McLaren, Director of Chemical and Mechanical Standards Department, National Research Council, Canada.

An anticipated outcome of this workshop will be identification of possible new projects for the Division to initiate through its TM and AM, and identification of key contributors from the scientific and industrial community.

Spreading the word

CI (Chemistry International) has a readership of 9,000. It is a great vehicle in which to 'advertise' what we have been doing.

Issues this year report on five of our projects that are in progress:

- Recent advances in electroanalytical techniques: characterisation, classification and terminology.
- Metrological traceability of measurement results in chemistry.
- Solubility of substances related to urolithiasis
- Solubility of hydroxybenzoic acids
- Solubility of halogenated aromatic hydrocarbons.

The May-June issue reports on 4 projects that have been completed and published in the latter part of 2002 or early 2003:

- Measurement of pH: definition, Standards and Procedures.
- Use of the terms "Recovery" and "Apparent Recovery" in Analytical Procedures.
- Critical evaluation of stability constants of metal complexes of crown ethers.
- Critical evaluation of the chemical properties of the transactinide elements.

Well done! The Division is keen to see 'an article for **CI**' as one component of every dissemination plan for Division V projects.

The Editor also saw a note in **CI** about David Shaw (previously chair of Commission V.8) who has been appointed to the editorial board of the Journal of Physical and Chemical reference Data. Congratulations David!

David Moore reports to Council

The biennial meeting of Council is a time for Division Presidents to report on what their Divisions have achieved. As well as successful outcomes, David's report covers 'new initiatives' and 'concerns'.

Amongst the new initiatives David notes:

- Revision of the Division web pages.
- Use of the web to solicit projects and to present guidelines for preparation of project proposals.
- The newsletter "Teamwork".
- The formation of 'advisor' groups to support each TM.
- The Directory of Expertise.
- The introduction of a six-monthly report for each project.

Amongst his concerns expressed to Council:

- Few advisor groups have been appointed; only one of these has generated a new project.
- Most projects are originating with analytical chemists previously involved with the Commissions or task groups.
- Too few project proposals are being submitted.
- There are major hold-ups of completed projects at the ITCNS.

These concerns should stimulate some lively debate in Ottawa!

On reflection, after reading David's report and thinking about the Workshop that we have planned for Ottawa:

Should the DC be more willing to invest project funds in order to generate projects (e.g. via workshops)?

Is it time for the DC to take a greater role in the initiation and development of project ideas and proposals; i.e. invert the process of project generation, with the DC acting as a "think tank"?

Ottawa homework

If you are attending the GA in Ottawa, please try to come prepared with at least one idea for a new project initiative by the Division. Now, that is a challenge!

[Kip Powell](#)
July, 2003.

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