

Analytical Chemistry Division (V)

General Assembly Meeting,

August 13th and 14th, 2005

Beijing Conference Centre, Beijing China

Present Committee members

Prof. K. Powell (Division President), Prof. R. Lobinski (Vice President), Dr D. S. Moore (Past President), Prof. R. M. Smith (Secretary), Prof. M. Bonardi, Dr A. Fajgelj, Prof. J. A. Jönsson, Prof. D. B. Hibbert, Prof. K. Matsumoto, Dr. Zhifang Chai, Prof. H Gamsjäger, Prof W. Kutner, Prof W. Lund, and Dr N. Torto.

Subcommittee members, Observers and Visitors

Dr D. Shaw, Prof. P. De Bièvre, Dr M. Schoenfisch (U North Carolina, US Young Observers Program); Dr Caroline Ribes (Process Analytical, Dow Chemicals Co. US Young Observers Program), Dr Al Ribes (USA), V. Gaune-Escard (France), Gadzuric Slobodan (France), S. Kocaoba (Turkey), Aicheng Chen (Canada), Prof W. Wang (Beijing. U of Chemical Technology), and Prof. Watarai (Osaka U; sponsored by Science Council, Japan).

Apologies Prof E.A.G. Zagatto

1. Welcome

The members of the Analytical Chemistry Division Committee, Subcommittees, visitors and young observers were welcomed to the meeting by the Division President (DP) and he particularly thanked those who had come on their own funding.

2. Agenda

The agenda was approved

3. Division President's Report to Council (circulated - Appendix A)

The DP thanked members of the Division for their work over the biennium and for the efforts that they had put into the work of the ACD. The report concentrated on the approach and strategy

that the ACD had adopted, in particular the setting of core priorities and the use of teams and workshops to generate ideas and new projects. Communication was a key to the success of the Division and had been supported by the ACD newsletter Teamwork, which had been the responsibility of the Division Vice-President.

The three core areas of the work of the Division were critical evaluations, quality assurance, and terminology. In addition a number of emerging issues had been identified: bioanalysis, nanotechnology, support for developing countries. These had led to potential projects areas. These emerging issues will be kept under review and may change with time.

The Division had established a reporting system, which checked on the progress of projects every 8 months and identified the progress and potential obstacles. The reports were available electronically on the IUPAC website.

The work on terminology had concentrated on the updating and development of the Orange book entries. The critical evaluations were a series of projects carried out under the umbrella of the Solubility SSED subcommittee. These studies were concentrated into three areas, human health, industrial processes, and metals in the environment.

The work on emerging countries had led to a series of articles in *Chemistry International* (CI); four had been published and 8 more were in preparation

4. Division Workshop: “Future opportunities and challenges for the ACD”

Introduction

The Chairman stated that the aims of the workshop were to generate new ideas and new project topics. Each topic was introduced by a short presentation which was followed by a chaired discussion.

a. Emerging issues in separation science applied to analytical chemistry (RMS/JAJ)

Main needs were on developing and emerging areas such as bioanalysis and “omics” and reference materials. The main future tasks were likely to be in terminology and collaboration with biochemists.

b. Challenges for analytical atomic spectroscopy (WL / RL)

The challenges facing atomic spectroscopy include the need to develop low cost equipment for emerging countries, and routine applications.

The discussion explored (i) the need for terminology for collision/ reaction cells and (ii) the requirements of emerging countries - whether they need the best technique, or the technique which is sufficient for the requirement. There was an interest in nanoanalysis using ICP-MS.

c. Critical evaluations: future challenges and opportunities (HG/ DS)

A draft proposal for a new project on the critical evaluation of heat capacity functions for exhaust gases and fuel gas components was presented. This has potential as an interdivisional project.

The discussion emphasised the need for IUPAC to consider industrial needs and the generation of usable data and to avoid an academic bias.

d. Emerging needs for developing countries (NT/ JAJ)

Dr Torto reported on the activity of SEANAC as a network bringing together analytical chemists in sub-Saharan Africa. Its work includes establishing collaboration between users of equipment and emphasising the need to involve young persons - how to develop their interest in chemistry. Possible collaboration with CCE was noted: - risk mitigation, curriculum development.

In discussion the importance of collaborating with existing structures and agencies (such as IOCD and IAEA) was emphasised. There is a need for a geopolitical involvement and understanding. So far IUPAC has only a small involvement. We need to ensure collaboration and not just be a minor partner. One initiative has been the series of articles on Developing countries in *CI*.

e. Challenges for nuclear methods in radioanalytical (and radiopharmaceutical) chemistry (MB /ZCh)

The presentations emphasised the importance of nuclear methods but also looked at “Threats and enemies” to nuclear chemistry.

The discussion questioned the role of radiochemistry in environmental analysis. Could ICP-MS replace radioactivity in monitoring? The relative reliability of these techniques would need to be tested. Could this be a possible project ?

There is disagreement within the Division as to what is meant by “nuclear methods”. For example, one view is that XRF is not a nuclear but an atomic technique. This disagreement is causing problems in formulating projects.

f. Emerging issues in bioanalytical chemistry (RL/ WL)

Looked at some emerging areas and outlined potential projects. There have been problems in the past in the identification of Se species and results were often incorrect. How should the ACD become involved in metallomics and other “omics” areas - looking at terminology and methods? There is a general question of terminology: what is bioanalytical chemistry – is it the assay of biological material, or is it the use of biological materials in sensors?

g. Molecular spectroscopy - emerging opportunities for the analytical chemist (Moore)

Molecular spectroscopy has a significant role in legal and forensic assays but is also becoming important in areas such as antiterrorism. Does IUPAC have an analytical role in this area? There is need for care in use of terms, e.g. whose terrorism?

h. Metrology and Quality Assurance: Challenges for the analytical chemistry (Fajgelj)

Quality assurance studies require the cooperation of many partners. However, if the results of a standardisation are to be marketed commercially should IUPAC be involved as a non-commercial organisation?

There are a number of potential quality assurance topics. One impediment is that BIPM has not defined “primary method of measurement”. “Recovery” has been described but this term is not widely used. How does IUPAC move beyond generating “another” report and gain authority?

5. Review of Project progress reports

Using the Progress Reports that had been recently submitted to the DVP the ACD reviewed the current projects

Number	Title	Chairman	Status	ACD Decision and actions
1999-044-2-500	Terminology for the description of peak asymmetry in chromatography	Jönsson	In Boston the Officers agree to merged with Orange book project 2001-063-1-500	To be included in 2001-063-1
1999-050-1-500	Chemical Speciation of Environmentally Significant Heavy metals and Inorganic Ligands	Sjöberg	2 papers published - 4 in preparation - to be completed by end 2007	proceeding
2000-003-1-500 (000031/500/00)	Ionic Strength Corrections for Stability Constants	Pettit	As a continuing (extended) project	Questions of distribution via the web or a CD to be followed up by DP
2000-004-2-500 (000042/500/00)	IUPAC Stability Constants Database	Pettit	Demo version available Academic software and IUPAC site	Academic Software to pass management of project to IUPAC. KP/DM/Folke negotiating
2001-038-2-500	Recommendations for NMR Measurement of high pKa values and equilibrium constant in strongly basic solutions	Popov	In final revision - being commented on by NMR experts - passed DP review	In review by 2 NMR experts.

2001-041-2-500	Recommendation for the Use of Countercurrent Chromatography in Analytical Chemistry	Spivakov	Main project completed - supplementary project in draft	Awaiting comments (RMS to follow up) [paper expected in Jan/Feb for ACD review]
2001-055-1-500	Critical evaluation of stability constants of Metal Complexes of Complexones for Biomedical and Environmental Applications	Popov	Completed	PAC
2001-063-1-500	Revision of terminology of separation science	Smith	slow progress	Continuing. To include 1994-044-2-
2001-072-1-500	Low activation materials for fusion technology: State and Prospects	Kolotov	limited progress - financial support offered in early 2005 for translation to generate final version - but no response	Response awaited DP to follow up
2002-002-2-500	Recent advances in electroanalytical techniques	Kutner	some delays in work	In progress
2002-003-2-500	Performance Evaluation Criteria for Preparation and Measurement of Macro and Microfabricated Ion-Selective Electrodes	Umezawa	report - working on final manuscript	Final version awaited
2002-009-2-500	Optical spectrochemical analysis using waveguide and optical fibres	Gauglitz	Status unclear	DM to contact - if no report by September should terminate.

2002-058-1-500	Definitions and fields of applications of the terms robust and rugged	Thorburn Burns	Submitted for review	Serious concern in Division review - but has also gone to external review - awaiting responses
2003-015-2-500	Terminology for radiochemistry	Bonardi	verbal report - some new publications	No expenditure yet
2003-037-1-500	Optical biosensors and bioprobes	Vo Dinh	no reports for 4 years	To be terminated
2003-056-2-500	Standard definition of terms relating to mass spectrometry	Murray	Doing very well - project consulting closely with industry - envisaged problem of acceptance with ASMS (American Society for Mass spectrometry) and editors and companies - website for discussion	Discussion led to need to collaborate with IUPAP on similar projects Should IUPAC be involved when there are problem areas or if there is a controversy / conflict? The DP to contact TGC re the responsibility of IUPAC to provide direction to the community of users.
2004-005-2-500	Comparable pH measurements by metrological traceability	Cameos	Considerable number of publications proposed - Byrnn Hibbert to join committee by invitation	Question - who will publish book? Unclear: who will send out questionnaire; has it been circulated yet?
2004-016-2-500	Guidelines for potentiometric measurements in suspensions	Oman	In MS central review - internal external review	Concern that not all TG members were involved in revision [later substantiated]
2004-041-1-500	Uncertainty estimation and figures of merit for multivariate calibration	Oliveri	Completed - ready for external review	To be reviewed [update - Part 3 accepted for PAC Oct 05]

Interdivisional Projects

Number	Title	Chairman	Status	ACD Decision and Actions
2003-011-3-600 (Division VI)	A critical compendium of pesticide physical data	Wauchope	Expanding project - limited involvement of pesticide chemists from environmental side	Cultural gap between data users and evaluation process may delay project - later completion date.
2003-060-2-400 (Division IV)	Terminology on separation of macromolecules	Chang	Progress slow - needs active participation from both Divisions	Benefits of reporting system in identifying problems. DP to alert Div (IV) President re slow progress.
2004-017-1-500 (Division V and Division VI)	Standardization of analytical approaches and analytical building capacity in Africa	Benson	Some problems in development of project. Focus now moving from Uganda to Kenya	In progress
2004-021-1-300 (Division III)	Reference methods, standards and applications of photoluminescence	San Roman	Task group increased - discussion re commercial products - data may not be open - access - non-disclosure - should recommendation refer to commercial \products of unknown properties/ composition	Committee queried if commercial materials should be approved / supported Project needs objective criteria RL to report back
2004-023-1-700 (Division VII)	Internationally agreed Terminology for observation in scientific communication	Pontet	Preparing concepts and systematic structures	Query Division VII - any progress
2005-016-1-100 (Division I)	Developments and application in solubility	Letcher	New project in conjunction with Division I. Funded by Div. I.	New project in progress

Reports from the Interdivisional WPQA

Number	Title	Chairman	Status	ACD Decision and Actions
2000-033-1-500	Soil sampling	Fajgeli	first part completed	PAC 2005, 77, 827 Ascertain possible interest of International Society of Soil Science
2001-009-1-500	Revision of the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories	Fajgelj	completed submitted to PAC	Awaiting publication
2001-010-3-500	Metrological traceability concept of chemical measurement results	De Bievre		DP to discuss on-going costs and expected life-time of project with TGC
2003-004-1-500	Interdisciplinary harmonised approach to metrological traceability of chemical measurement results	De Bievre	Completed	PAC

Reports from Subcommittee on Solubility and Equilibrium Data

Number	Title	Chairman	Status	ACD Decision and Actions
2002-025-1-500	Solubilities of Inorganic Compounds of Actinides (except carbonates)	Hala	6-9 months behind schedule, but good progress	To continue [Dec05 SDS Vol. 82, submitted]
2002-031-1-500	Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates	Vanderdeelen	Scope and Objective to be revised at next SSED meeting. Intended output: publication in JPCRD	To continue
2002-032-1-500	Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates (Mn, Fe, Co, Ni, Cu, Zn, Ag, Cd, Hg, Pb)	Gamsjäger	Slow progress - poster - at Congress - might be moved to T. Letcher book for publication - rather than JPCRD	Possibility of publication in JPCRD and Letcher's book "Solubility for Industry" discussed. Referred to SSED for decision. [SSED decided to continue project]
2002-033-1-500	Solubility data related to oceanic salt systems Part I	Balarew	Being reorganised	New working group composition awaited
2002-034-1-500	Solubility data related to oceanic salt systems Part II	Voigt	Being reorganised	New working group composition awaited
2002-035-1-500	Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis	Königsberger	Continuing. Completion: mid 2006	To continue
2002-036-1-500	Solubility data of compounds relevant to human health. Solubility	Goto and Miyamoto,	Article in preparation for JPCRD	Dissemination could be improved via vector articles

	of hydroxybenzoic acids and hydroxybenzoates			published in pharmaceutical journals and in <i>CI</i> . Refer to SSED. For all human health related papers see Div VII
2002-037-1-500	Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons	Makino, Goto and Goto	1-2 years to completion 2007	To continue
2002-038-1-500	Solubility data of compounds relevant to human health. Antibiotics: peptides antibiotics and macrocyclic lactones,	Lorimer	No progress. TG too busy.	Postponed, will not be finished in the next two years
2002-042-1-500	Solubility data related to industrial processes Lead sulphate	Lorimer	No progress. TG too busy.	Postponed, will not be finished in the next two years
2002-043-1-500	Solubility data related to industrial processes Carbon dioxide and the lower alkanes at pressure above 2 bar methane to butane	Mather	No report since July 2004	Terminate project? Referred to SSED [SSED project has been terminated]
2002-044-1-500	Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions	Scharlin	Delays in internal data evaluation process.	To continue

2002-045-1-500	Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide	Knox	active	To continue
2002-050-1-500	Solubility data related to industrial processes; Acetonitrile: ternary and other multicomponent systems	Sazonov	95% complete but no progress since last year. Current status unclear.	SSED trying to reactivate. [SSED - has been reactivated successfully]
2003-018-1-500	Mutual solubility of hydrocarbons with water	Maczynski	Part completed	in press
2005-006-1-500	Mutual solubility of alcohols and water update of SDS Vol 15)	Maczynski	Jan 2006 completion	To continue

6. Submitted and Proposed projects

The Division then considered recently submitted project proposals

Proposal Number	Project	Chairman	Status
2003-11-17 2004-004-1	Chemical speciation study of essential and toxic elements by NAA	Z. Chai	Lacks focus – comments back to task group. TGC asked to revise. Action: RL
	Comparison of the terms: preconcentration/sample preparation as used in GMO analysis and in classical analysis:	Kazuko Matsumoto/ Elias Zagatto	Stalled. May need new focus. Action: RL.
	Terminology related to analytical chemistry of metal forms in biological systems: metallomics:	Ryszard Lobinski	In preparation
2005-014-1	IUPAC stability constants	Powell	Proposal with Project

	database		Committee [Funded September 2005.]
2005-017	Glossary of terms related to solubility	Shaw	Decision to fund approved at Assembly
2005-019	Selection and Use of Proficiency Testing Schemes for Limited Number of Participants (Chemical Analytical Laboratories)	A. Fajgelj	Under review. [Funded December 2005.]

7. Project review process

Some general conclusions arose from the review of current projects.

The request for reports needs to make it clear that the report should be about progress *since* the last report - and that the previous report has been posted on the IUPAC website. There was discussion about possible changes to the report form questions: Have the project objectives been changed? Does the work still match the original proposal? Are all the task group members still actively involved? A revised form to be circulated by RL for comment.

It would assist reviewers if the title made it clear whether the paper was a technical report or recommendation for terminology.

8. Review of Projects ‘in preparation’

A number of projects are at the formulation and assessment stages

- a. Glossary of solubility terms: David Shaw (SSED sub committee project). This had been reviewed and voted on by the ACD with a score 4.6 - agreed to fund.
- b. Solubility Constants Database - had also received a favourable score - agreed to refer to Project Committee - to be submitted to Executive for financial support from reserves
- c. In house method validation protocols – TG Chair AF. Currently being reviewed
- d. Calibration of organic and inorganic isotopic materials - Joint with Div II. Reviewed favourably by ACD - terminology involved - linked to traceability. Awaiting Division II decision.

9. Potential new projects

The Division considered a number of projects which were at the scoping or drafting stage:

- a "omics" (Chair RL): metallomics to be drafted within 6 months - potential task group members by June 2006 - proposal by end of December.
- b. Selenium speciation. Proposal in preparation: Critical evaluation and recommendations regarding the determination of selenomethionine in yeasts. Budget to be decided. Draft from task group (Mester/RL) to be submitted by December 2005.
- c Solid state speciation (ZC). The focus of the proposal is not clear. It was noted that the project must be a critical evaluation not a review. Is it to be a spectroscopic (non-nuclear) or a nuclear project? The DP indicated that a consensus was required within the Division before the project could proceed. A small group was asked discuss this (MB, BH, Chai AF and RL) and report back in February. The project must be relevant and require IUPAC involvement.
- d. ICP-MS calibration interferences. (WL) A proposal will be developed for February. (Walter Lund plus Pablo Gonzalez, Spain)
- e. Trace elements analysis: role of grain size distribution in solid reference materials. AF had a proposal from Maria Belli (APAT) ready for Division review. This project is of interest to WPQA.
- f Isotope geochronology. This is an IUGS project, in which Divisions II and V have expressed interest. IUPAC is not interested. MB and AF have been designated by the Secretary General and President to represent IUPAC in this project and to work with IUGS in formulating a joint project proposal.
- g C_p empirical functions (HG). This project was outlined in the Workshop, at which time a draft proposal was circulated. Involvement of Division I was encouraged (subsequently made a commitment). Potential industrial interest to be discussed with COCI.
- h. Orange Book, Chapter 10 (Spectrochemical analysis) - project in preparation (DM).
- i. Orange book, Chapter 8 (Electrochemical analysis) - developed from existing project (WK)
- j Orange book, Chapter 16 (Radioanalytical methods) needs revision as result of a project.
- k. MIPs role in sample preparation. JAJ doubted value of methodology and need for IUPAC critical review at this time. Noted that WK must not overcommit.

- l. Interpretation and reporting on bioanalytical results to the general public. This is a potential project raised by the CEFIC representative (Chris Humphries). Public understanding of Science needs the meaning of analytical results to be explained and the risk justified. It is of interest to WPQA and CCE and would involve aspects of publicity and risk analysis. Chris Humphries to contact Division VI.
- m. Process Analytical technology. C. Ribes will explore the need for an IUPAC input re Terminology by contacting industrial colleagues in USA.
- n. Chemometrics soft modelling. Bryn Hibbert
- o. Mark Schoenfisch expressed an interest in chemical education and curriculum. RMS to discuss possibilities at CCE. MS also in dialogue with Nelson Torto.
- p. Sample preparation terminology (JAJ). A broader topic than separation science. Will explore in February at Ex-Tech meeting in York

10. New Project Review Process

DP reported that following a request at the Vienna meeting, new projects had been circulated to the whole Division committee for comment, but few responded, so he has now reverted to a limited circulation - more successful.

11. Project completion

It is important that not just the Task Group Chair is involved. The whole task group should be involved in the revision process and response to reviewer comments, and a consensus achieved. There is evidence that this is not always the case.

There are still some problems with the review process. Working through Manuscript Central the Division review and ICTNS/ public/expert review occur in parallel, rather than sequentially as in the past. This method is flawed when a document needs major revision – which should occur after an initial Division review. W Kutner (ICTNS) offered to look at final drafts before submission to Division to minimise problems in ICTNS.

12. Project funding

In 2004 the Bureau approved an increase in the “guideline” for Division operating expenses from 25% to 30% of the biennial grant. The DP noted that the total grant was not adjusted - so the

project budget had in fact been reduced. In our Division part of the budget had been used to bring speakers to the Workshop in Vienna and to support additional attendance at the Division meeting at the GA. It is possible for a Workshop to be funded as a Project but that requires an advance commitment to Workshop outcomes (e.g. a specific project proposal) and should not be limited to attendance by Division members.

It was noted that unspent project money is lost to Division; it is returned to Reserves.

C. Ribes asked how central budget is allocated. The allocation is largely historical and reflects previous needs. The Division can also present a case to the Project Committee, or to the Executive committee for support from central Reserves. As noted by the President: “good projects will be funded”. The DP is to raise the allocation of initial budgets with the Executive. He noted that up to now the Project Committee has been very supportive.

13. Strategic planning - Review of Division structures, operations, expectations. (During this item joined by IUPAC President)

The DP wants to have all TM and AM involved in project generation and activity and not just acting as liaison between project TGs and the Division. Currently the Division members give different contributions. How can we get all involved in the project system - not just administratively but as TG participants? The Division needs to generate a climate of involvement. In addition, members should use Conferences to actively seek involvement of leading scientists in IUPAC projects. AF agreed with these views and commented that within the WPQA all members are involved in projects.

C. Ribes asked what guidance is provided to new members? There is a description of TM, AM and NR responsibilities on the Division website. There is scope to provide more direct instructions on participation - not just to attend meetings and generate ideas but also to participate in the project system.

There is a particular need that the invitations to NAO should expand on the role expected from nominated representatives. The nominees must be willing to be involved in working on a project; it is not just an honorary position. Leiv Sydnes endorsed this point of view. But there is also a need for a geographic spread of Division members. It was requested that this expectation

of participation must be made clear in the letter sent to NAOs by the Secretary General (e.g. that AM and TM duties could include “participation in the project system”).

The comment was made that in the old Commissions, each member was expected to generate new ideas but that the new project system was not personal and more targeted to satisfy IUPAC objectives. President Sydnes agreed, but indicated that under the old system some projects had taken 12 years – the new system has to be more realistic. DM noted that in the ACD the present structure evolved - from commissions to projects - with no major difficulties.

14. CCE presentation

The Chairman of CCE Peter Atkins visited the ACD and discussed the work of CCE and how the Division could interact with CCE. They had appointed Eva Akesson (Lund) as a liaison contact with the Divisions.

The ACD expressed special interest in areas where the CCE might be able to help developing countries, e.g. through curriculum development and assistance and in evaluating curricula in Africa. One CCE initiative is the “flying chemist”, who could go out and help local groups or organisations to get projects off the ground. Other CCE projects were (i) to examine the role of chemistry in every day life; (ii) a comparison of degree programmes in different countries -especially attainment levels (this is linked to the Bologna agreement); (iii) a programme on organic chemistry in South America.

15. Visit by Secretariat / Chemistry International

Fabienne Meyers, the Electronic Publications Manager and Editor of *CI*, and Chris Brouwer, the Production Editor, joined the meeting. FM described the support that the Secretariat can offer the ACD: John Jost as Executive Director, Enid Weatherwax and Linda Tapp on finances, Erin Carter conferences, and Paul LeClair on membership (<http://www.iupac.org/news/contact.html>). Their job descriptions were to respond to the demands of the membership, so it is up to us to ask!

There was a discussion about the degree of “user-friendliness” of the IUPAC website. Although it served members reasonably well, there were problems with navigation for external users as it often uses terms in a specialised way. ACD members noted problems with conference information.

It was noted that the ACD under the coordination of JAJ had been active in the series of papers on “Emerging Issues in Developing Countries”. About ten articles are promised; three are in press, and two in hand; others are currently being prepared. A sequel series is possible - but not necessarily developed by Division V. This series could reflect another IUPAC goal such as “tools for international standardisation”. *CI* is now routinely distributed to all attendees at IUPAC sponsored meetings.

16. Composition of Division Committee

The Nomination Committee for the election to the next Division Committee had been asked to ensure that there were members representing the areas of: Quality Assurance, Separation methods, Spectrochemistry, Electrochemical methods, Nuclear methods and Bioanalytical methods, so that together with the expertise of the Officers all the main areas of analytical chemistry would be represented.

The meeting then considered the areas that needed to be represented by the six Associate Members. It was proposed that positions be reserved for the Chair of SSED and the Division representative on ICTNS. It was also suggested that there should be a second AM in the bioanalytical area. These three proposals were agreed.

Following a discussion it was suggested that the remaining three AM positions should be used to include a younger member on the Committee and to add an industrial analytical chemist. The geographical spread of ACD would be widened by including representation from additional NAOs. It was agreed to reserve an AM position for an industrial representative and to bear the other requirements in mind when nominating members.

17. Elections to Division Committee

a. Titular members

The Nominating Committee consisted of the past Division Chair, Dr Moore and Professor Umezawa as the Division V representative, plus three external members: Dr Stephen Wise (NIST), Dr Heiner Korte (former president of FECS) and Professor Valcarcel (President FECS). Nominations had been invited from NAOs by the Secretary General and 6 had been received. These nominations and those from the Division had been allocated to the 6 topic areas and the election had been conducted by the Secretariat. It had achieved a 73% response from the electorate (compared to 33% last time). The results were as follows - the first named being duly elected for the 2006-2007 biennium.

Quality Assurance/ Chemometrics

Prof P. De Bièvre	18 (elected)
Prof P. Minkkinen	12

Separations

Prof J.A. Jönsson	19 (elected)
Prof B. Spivakov	7
Prof H. Watarai	4

Spectrochemistry

Prof W. Lund	15 (elected)
Prof K. Murray	9
Prof T. Imasaka	6

Electrochemical methods

Prof D.B. Hibbert	18 (elected)
Prof J. M. Pingarrón	12

Nuclear methods

Prof M. Bonardi	27 (elected)
Dr D. Mohammed	2

Bioanalytical methods

Prof J. Labuda	14 (elected)
Prof U. Karst	13
Dr Jong Hoa Ok	3

b. Associate Members

The ADC then considered nominations for the six AM positions:

SSED chair Professor Heinz Gamsjäger has exceeded the formal term of office of 4 years (but the Executive Director had been notified by the DP and was willing to approve the nomination)

ICTNS Professor W. Kutner

Bioanalytical (2nd position): Prof Kermit Murray USA was nominated.

At this stage no other nominations were made and the three nominations above were accepted by a show of hands.

As no nominations were made for the Industrial position, the meeting agreed to widen the specifications for three remaining positions: The nominations were:

Professor Uwe Karst (Germany) who has expertise in bioanalytical

Professor Zhifang Chai (China) who has expertise in nuclear chemistry

Professor Pennitti Minkkinen (Finland) who has expertise in QA, solution equilibria, chemometrics, and has industrial links

These three were duly elected as AM.

c. National representatives

Although up to 10 could be nominated none could be from countries with TM or AM.

The following current NR were nominated:

Dr Zoltan Mester (Canada)

Professor Christo Balarew (Bulgaria)

Professor Klaus Danzer (Germany)

Professor Elena Dominquez (Spain)

Nominations had been received from NAOs for:

Professor Waterai (Japan)

Professor Boris Spivakov (Russia)

Professor Elias Zagatto (Brazil) subject to status of NAO (currently suspended)

The ACD nominated

Dr Sergi Kocaoba Turkey (who was attending the meeting as a Young Observer)

Professor Wenchuan Wang (China) subject to approval of the Bureau as China already has an AM.

These 9 names were accepted by the ACD for recommending to the Bureau.

One current NR, Dr Daniel Bastoni (Argentina), could not be nominated; he was not eligible as Argentina was suspended as a NAO.

d. The suggestion was made that one of the TM positions might be reserved for the SSED by the next Nominating Committee (to be discussed by the new Nominating Committee).

e. The officers for the 2006-2007 biennium had been approved at the Executive Committee meeting in Boston in January.

President: Professor R. Lobinski

Vice President: Dr Ales Fajgeli

Past President: Professor Kip Powell

Secretary: Professor Roger M. Smith

18. Membership of external committees

The follow were nominated to represent the ACD on external committees:

ICTNS Prof W Kutner

CCE Prof Roger M. Smith

COCI Dr A. Fajgelj

PAC editorial board: Prof R Lobinski (subsequently delegated to KP)

BIPM/ CCQM: Dr. A. Fajgelj

ISO/REMCO: Dr A. Fajgelj

Joint Committee on Traceability in medicine: Dr P De Bievre

Inter-Agency Meeting (IAM): Dr Roger Wood

19. Publicity

Teamwork: 97 copies are circulated. The next issue (November) will reflect on the GA.

20. WPQA Report

The WPQA has two project areas:

- Interdisciplinary harmonised approach to metrological traceability of chemical measurement results
- Metrological traceability of measurement results in chemistry

with two others recently completed.

- Terminology in soil sampling - published in PAC.
- Revision of the International Harmonised Protocol for the Proficiency Testing of Analytical Chemistry laboratories.

New projects are being proposed to fill in gaps. These will be discussed later in the GA when the WPQA meets. One draft proposal is with the DP – “Selection and Use of Proficiency Testing Schemes for Limited Number of Participants (Chemical Analytical Laboratories)”. This project is of possible interdivisional interest. Division VII (Human Health) is interested. Division VI (Environment) has not yet responded. Also of possible interest to COCI?

Many ideas for projects but not enough members - must be able to manage activity

AF will continue as Chair of WPQA - a new chair will be appointed when AF becomes DP. A lot of work was put into an ICSU project proposal that was not successful in competition for the limited funds available.

The Division meeting was followed by an open meeting promoted by WPQA to discuss “Metrological traceability of measurement results in chemistry” based on Project 2001-010-3-500.

21. Orange book update

Change in title: now “Terminology” not Nomenclature. Now in the form of a series of pdf files held as part of the Gold book project, which in due course will include all existing terminology from the different colour books. The aim is eventually to use XML which will be more readily searchable and will allow journal editors to match terms in submitted papers to check if they are correctly used. The file will serve as a data dictionary. Current ACD work is to convert descriptive chapters of the Orange book to glossary terms as well as update existing terms. Any new definition must be approved by ICTNS and published first in PAC. The eventual aim will be an annual updating of the Gold/Orange book database.

Currently, ACD has projects revising Chapter 3 Separation science, and Chapter 8 Electroanalytical; a Chapter 10 update has been proposed. It is expected that no new printed edition of the Orange book will be produced but it might be marketed on a CD. Currently there are problems with mathematical terms in XML but new methods are being developed.

22. Report from SSED

Heinz Gamsjäger reported that *CI* has been used to report on the activities of SSED in a number of short papers since March 2003. It is now using Manuscript Central for reviewing project reports. The committee would be reviewing their work during the GA and considering the removal of non-active old projects; final decisions to be made at SSED annual meeting 26/8/06. Three new projects need approval: formal submission and DP approval is needed in order to enter the projects into the tracking system - even if projects are under an SSED umbrella proposal.

Re: the proposed Trevor Letcher book “Solubility for Industry”: (i) critical evaluation team to review chapter on solubility data banks, (ii) concern at over-commitment by specific authors.

23. Report from ICTNS

Dr Kutner indicated that the ICTNS report from Dr Lorimer to Council had raised the problems of conflicts between proposed new terms and existing terms.

The Chair and Secretary of ICTNS are now on the editorial board of PAC and will be able to monitor progress of papers. New procedures and guidelines on document preparation had been prepared.

Technical reports and recommendations: It is harder to get agreement on recommendations so these should be separated from technical reports and submitted separately other wise they could cause delays. Guidelines will appear in the Blue book and web-pages.

See attached Appendix B of a report from Dr Kutner on the meeting of ICTNS at the GA.

24. Journal editors

Because of concern that many journals were not following IUPAC recommended terminology, an exercise had been carried out by Brynn Hibbert to ascertain journal practice as listed in Instructions to Authors. He reported that usage in following IUPAC terminology varied - the RSC good, ACS patchy/poor, but Elsevier variable. It was suggested that Division members who are on editorial boards should try to influence more editors. He encouraged them to act to encourage good practice. Possible larger IUPAC project.

25. Review of Division Responsibilities

The DP proposed that all Division members should be involved in projects. This is an expectation, but also necessary to give practice in the formulation and evaluation of projects. Changes to the TM and AM Responsibilities on the ACD web page were approved.

26. Next Meeting of ACD

RL proposed that the meeting in early 2006 should be in Europe and a number of venues were considered. It was subsequently arranged to hold it in Rome on 4- 5th March at the offices of APAT (Italian Environmental Protection Agency). It will be followed by a workshop on “Combining and reporting analytical results” - The role of (metrological) traceability and (measurement) uncertainty for comparing analytical results.

27. Closing remarks

The DP expressed his thanks to observers, current, past and future members.

Special thanks were expressed to Dr David Moore for his work in IUPAC over many years and for his guidance, enthusiasm and energy from 1987 as he had risen from a young observer to almost every possible level in the Union. He was especially thanked for being a Friend of the ACD Division.

Appendix A Division President's report to IUPAC Council

IUPAC Analytical Chemistry Division (V)

Report to Council, 2003 – 2005

I. Executive Summary

- The Division has made significant moves to build partnerships with organizations that have experience in developing countries (IAEA, UNIDO, IOCD, SEANAC), other unions and expert bodies (IUPAP, BIPM, IUGS).
- The Division is coordinating a series of articles for *Chemistry International* on the topic of “*Emerging needs of developing countries*”. This series should run for 8-10 issues and will carry contributions from several Divisions.
- The Division has started a significant number of inter-Divisional projects. These link us with Divisions I, III, IV, VI and VII, and with COCI.
- To ensure attention to critical areas it has identified a limited number of “priorities” for the biennium. It has focused its energy on these.
- To cultivate a spirit of “collective responsibility” it has formed seven Teams, each with responsibility for one priority area. All NR, AM and TM are assigned to one or two teams. The Team structure should facilitate continuity of effort into the next biennium.
- Communication within the Division and with other officers of the union is maintained through the electronic newsletter “*Teamwork*”.
- The Division is working on the maintenance and updating of two key IUPAC publications, *The Compendium of Analytical Nomenclature* (Orange Book) and the *IUPAC Stability Constant Database* (SCDB).
- To facilitate the development of new projects the Division involved external experts in a mini-symposium on “*Metrological traceability*” held at the IAEA in conjunction with its even-year meeting.

II. Report on Division activities in relation to IUPAC goals

2.1. *IUPAC will provide leadership as a worldwide scientific organisation that objectively addresses global issues involving the chemical sciences.*

The Division has ‘Core activities’ as on-going responsibilities. But it also identified a set of priorities that are based on perceived emerging needs of the scientific community.

These ‘Emerging issues’ are more time-dependent and are likely to change to some degree from one biennium to the next:

Core Activities:

Communication

Project initiation and management in the areas of:

- Quality Assurance
- Terminology – Orange Book: maintaining and updating
- Critical evaluation of data

Emerging issues in analytical chemistry:

- in bioanalytical chemistry
- in process chemistry and nano-chemistry
- in developing countries and scientific communities.

Teams of 4-6 members (TM + AM + NR) are formed for each priority area. Each Team has a collective responsibility and is encouraged to:

- Determine the scope of its responsibility and activities;
- Develop a strategy for effective communication between and by its members.
- Identify activities that advance the goals of IUPAC in its designated area.
- Achieve at least one significant output each year (*e.g.* letters to Editors; an IUPAC or ACD presentation at a Conference; an article for *CI*; a Project Proposal; etc.)
- Accept responsibility for leading Division activities in its designated area
- Facilitate a ‘roll-over’ of its activities at the end of the current biennium.

Communication.

The Division maintains communication with all its members, and officers of other Divisions and Operational committees, through its newsletter *Teamwork*.

The Division interacts with all Task Groups on a half-yearly basis (to be changed to eight-monthly) via a Project reporting system. The reports are read by all Division members and are reviewed at Division meetings. They provide an ‘early warning system’ for any projects that are struggling, alert the Division to the need for reviewers and allow re-assessment of Dissemination plans as the projects near completion. As from November 2004 these reports are appended to the respective Project pages on the IUPAC website, so that Project progress is in the public domain.

Global issues.

One global issue being addressed is the measurement of pH, through the project: *Comparable pH measurements by metrological traceability. Part I: Water quality monitoring and assessment; Part II: Clinical and biochemical matrices*. This project sees a continuation of work by the “pH task group” [Measurement of pH. Definition, Standards and Procedures. 2002] and it has the financial and professional backing of three Divisions and COCI.

Another global issue addressed is the concept of 'fair trade'. Fair Trade can only arise between nations when all have adequate and *quality-assured laboratories* and their methodology meets the current requirements for *metrological traceability*. These issues are particularly relevant to the less developed nations. These concepts were the basis of:

- (a) A successful joint project proposal with IOCD which includes two Division V members, titled: "*Standardisation of analytical approaches and analytical capacity building in Africa*". This project involves a melding of IUPAC technical expertise with IOCD appreciation of geopolitical issues in developing countries.
- (b) Division V support for the WPQA in the preparation of an ICSU proposal on "*Measurement traceability – a fair basis for trade*". This application for funds was not successful but the process of preparing the proposal generated very positive interactions with project partners UNIDO and IUPAP (including their participation in a WPQA/Division V workshop).

Symposia and Workshops.

The Division attempts to capture external expertise to introduce and scope emerging issues or opportunities in analytical chemistry. This is assisted through mini-symposia held in conjunction with the Division even-year meeting and the GA.

>From the mini-symposium on "*New Challenges for Analytical Chemists in Genomics, Proteomics, and Genetically Modified Organisms*" held during the Ottawa GA, two new projects were identified. One has been funded in this biennium ("*Standard definition of terms related to mass spectrometry*") while the other on "*Terminology related to analytical chemistry of metal forms in biological systems: metallomics*" has been thoroughly scoped and a Task Group identified.

At the even-year meeting in Vienna 2004 a mini-symposium on "*Metrological traceability*" was held jointly with IAEA staff and the WPQA. It attracted speakers from IUPAP, UNIDO, BIPM, IAEA and WPQA. The meeting identified several areas in which IUPAC expertise might be applied. We now try to identify possible 'concrete' outcomes from that meeting - IUPAC projects that could be crafted around the ideas and concerns that were shared. IUPAC will benefit through any projects that link it with agencies that are working much closer to the geopolitical coal-face.

2.2. IUPAC will facilitate advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion

Division V actively pursues these goals through its program of critical evaluations of data, the establishment of guidelines for Quality Assurance in chemical methods and associated sampling, and by the updating of analytical nomenclature and making it readily available via the web:

- (a) **The Orange Book.** This is now on-line at (http://www.iupac.org/publications/analytical_compendium/)

The route for updating terminology in the OB is via formal publication in *PAC*. Examples of issues being currently addressed through projects are: *Glossary of Terms related to Solubility*; *Revision of terminology in separation science*; *Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry*; *Internationally agreed terminology for observations in scientific communications*; *Standard definitions of terms relating to mass spectrometry*.

The text will be progressively converted to ICTNS-accepted format; it will also be aligned with the Gold book version, so that there is only one version of terminology within the IUPAC database.

- (b) ***The IUPAC Stability Constants Database*** (SCDB) is the most comprehensive compilation of stability constants available, covering the years 1877 to 2002. It is the primary source of data for the Critical evaluations of Stability Constants that are published on a regular basis by Division V. It is a major research tool for those involved in equilibrium modelling of environmental, biological and industrial systems.

Division V has in place a Project to continue the evaluation, collection and entry of data through to 2008. To minimise risk the data collection team has been expanded from one site to now involve experts in four countries.

The future of SCDB was the subject of a Division V presentation to the Bureau meeting in 2004. All aspects of the management of the database – program development, data conflation, advertising, marketing – have for the last 16 years been undertaken on behalf of IUPAC by the developers of the current database, Academic Software. This company has now signaled that it wishes to transfer the responsibility for management and maintenance of SCDB to IUPAC within about 3 years.

Division V has formed a consultative team (Folke Ingman, David Moore and Kip Powell) to work with Academic Software and the Executive to effect a successful transition to management by IUPAC or an alternative external systems manager. The Bureau meeting identified the future management of commercial databases as a generic issue that now needs to be addressed by IUPAC. It is possible that appropriate secretariat resources may need to be assigned in future.

- (c) ***The Working Party on Quality Assurance*** continues to produce publications that are of value to chemists in analytical laboratories; e.g. *Revision of the IUPAC/ISO/AOAC protocol for proficiency testing*; *Harmonised guidelines for single-laboratory validation of methods of analysis*; and *Terminology for soil sampling*. The WPQA will make a major presentation at the GA on “*Metrological Traceability of Results in Chemical Measurement*.”
- (d) ***The Solubility and Solution Equilibrium Data sub-committee (SSED)*** has a very active program of projects that embrace the critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) industrial processes, (c) human health. The outputs appear as papers in the *Journal of Physical and Chemical Reference Data* or as book volumes and are thence transferred to the NIST-IUPAC Solubility Database: <http://srdata.nist.gov/solubility/>. A significant new project is a 25-Chapter book volume on “*Solubility for Industry*”. Another project is concerned with *Chemical speciation of environmentally significant heavy metals with inorganic ligands*.

2.3. IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement of the quality of life.

Chemistry-related industry is served by the active program of critical evaluations of solubility data and of solution equilibrium data, and by the continuance of data evaluation and compilation for the IUPAC

Stability Constant Database. The current projects on pH (*Comparable pH measurements by metrological traceability.*) and metrological traceability (*Metrological Traceability of Results in Chemical Measurement*) are highly relevant to industry. The SSED were joint organisers of the 11th International Symposium on solubility phenomena (Aviero, 2004) at which there was significant emphasis on industrial issues and involvement of industrial chemists (*PAC*, 77(3), 2005).

2.4. IUPAC will foster communication among individual chemists and scientific organisations, with special emphasis on the needs of chemists in developing nations.

Analytical Chemistry in Developing countries

The Division seeks to expand activities in this area. “Emerging needs in developing countries” is one of its priority areas and is the responsibility of one Team. The Division is fortunate in having several members with established professional links with the African continent (Jan-Åke Jönsson, Walter Lund and Roger Smith). Nelson Torto (Botswana) has joined the ACD as a Provisional Member representing the IUPAC Associate Organisation, SEANAC. The Division is significantly involved in the project with IOCD: “*Standardisation of analytical approaches and analytical capacity building in Africa*”.

To increase awareness of the needs of developing countries the Division has arranged a series of 8-10 articles for *Chemistry International*. These articles on *Emerging issues in developing countries* commenced in the March 2005 issue. Division V is well-supported by other Divisions in this venture.

Building bridges with other organisations.

The SSED works actively with NIST in the preparation of critical evaluations for publication in the NIST-IUPAC Solubility Data Series. The joint Division V - WPQA meeting in Vienna showed that many new dynamics can be brought to our activities by discussion and collaboration with other organizations, in this case IUPAP, IAEA, UNIDO.

Through the WPQA the Division is represented on the Coordinating Committee on Chemistry and Materials, ISO-Committee on Reference Materials, the International Committee on Weights and Measures, the Consultative Committee for Amount of Substance (BIPM), EURACHEM and CITAC.

Better Communication.

Dissemination of project outcomes is a crucial issue for improving the impact of our work in the chemistry community. This is overseen by the “Communications” team. The ACD website has been made more intuitive. Working with Dr. Meyers we are attempting to make it better attuned to the needs of those who are not familiar with the IUPAC system and processes. Improved lines of communication between TG chairs and the Division have been facilitated by the establishment of a 6-monthly Project reporting system in which the TGC responds to questions re progress, milestones, difficulties, and opportunities for further work, etc. These progress reports are now filed on the web on the respective project pages.

The Division has been pro-active in recommendations for improved IUPAC representation at conferences. It considers that there is scope for enhanced involvement of IUPAC representatives at IUPAC-sponsored conferences. This could be aided if conference organisers were required to discuss the nomination of an IUPAC representative with the relevant Division ahead of submitting the AIS. It is all too easy for Conference programs to be ‘finalised’ ahead of representative appointment, or without reference to IUPAC requirements.

2.5. IUPAC will utilise its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

The Division was represented in the Task Group for the project: *Chemistry's contributions to humanity*. It actively participates in the General Assembly Young Observers scheme. The question of career development for young chemists from developing countries was raised in one of the *CI* articles.

2.6. IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender and age.

Division V has in place a strategy, which is communicated to the Nominations' Committee, to ensure the widest possible geographic representation. The Division actively sought participation of Nelson Torto as a Provisional Member representing the ANO, SEANAC. Within its own structures, the Division works to ensure **active** involvement of all AM, TM and NR.

III. Challenges and Solutions

The principal challenges to the ACD are typical of many IUPAC Divisions:

- The breadth of its portfolio.
- The generation of members' collective responsibility for
 - the goals of the Division
 - the needs of countries not represented
 - the long-range goals of IUPAC
- Maintaining momentum through the biennium and with the change of biennia.

Strategy adopted by the ACD to address these challenges:

- Identification of a manageable number of priorities for the biennium.
- Formation of Teams, each with collective responsibility for one priority area.
- Effort focused on the needs of developing countries and on links with other agencies.
- Use of mini-symposia to bring in external expertise.
- Maintaining active communication between members, e.g. through the newsletter, *Teamwork*.

IV. CURRENT PROJECTS

*Interdivisional projects

1999-044-2-500 - Terminology for the description of peak asymmetry in chromatography
1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands
2000-003-1-500 - Ionic strength corrections for stability constants
2000-004-2-500 - IUPAC stability constants database - completion of data collection up to 2000+
2001-041-2-500 - Recommendation on the use of countercurrent chromatography in analytical chemistry
2001-063-1-500 - Revision of terminology of separation science
2001-072-1-500 - Low activation materials for fusion technology: State and prospects
2002-002-2-500 - Recent advances in electroanalytical techniques: characterization, classification and terminology
2002-003-2-500 - Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes
2002-009-2-500 - Optical spectrochemical analysis using waveguides and optical fibers; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis
2002-058-1-500 - Definitions and fields of application of the terms robust and rugged and the characteristics or qualities of robustness and ruggedness in analytical chemistry

- 2003-015-2-500 - Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry
 2003-037-1-500 - Optical biosensors and bioprobes; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis
 2003-056-2-500 - Standard definitions of terms relating to mass spectrometry*
 2004-005-2-500 - Comparable pH measurements by metrological traceability*
 2004-016-2-500 - Guidelines for potentiometric measurements in suspensions
 2004-017-1-500 - Standardization of analytical approaches and analytical capacity-building in Africa*
 2004-041-1-500 - Uncertainty estimation and figures of merit for multivariate calibration

INTERDIVISIONAL WORKING PARTY ON HARMONIZATION OF QUALITY ASSURANCE

- 2001-010-3-500 - Metrological traceability of measurement results in chemistry
 2003-004-1-500 - Interdisciplinary harmonised approach to metrological traceability of chemical measurement results

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

- 2001-052-1-500 - Solubility of volatile and gaseous fluorides in all solvents
 2002-025-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds
 2002-031-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates
 2002-032-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates
 2002-033-1-500 - Solubility data related to oceanic salt systems. Part I - Binary systems containing sodium, potassium, and ammonium sulfate
 2002-034-1-500 - Solubility data related to oceanic salt systems. Part II - magnesium chloride-water and calcium chloride-water and their mixtures
 2002-035-1-500 - Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis
 2002-036-1-500 - Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates
 2002-037-1-500 - Solubility data of compounds relevant to human health. Solubility of halogenated aromatic hydrocarbons
 2002-038-1-500 - Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics
 2002-042-1-500 - Solubility data related to industrial processes. Lead sulfate
 2002-043-1-500 - Solubility data related to industrial processes. Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane
 2002-044-1-500 - Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions
 2002-045-1-500 - Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide
 2002-050-1-500 - Solubility data related to industrial processes. Acetonitrile: ternary and other multicomponent systems
 2003-018-1-500 - Mutual solubility of hydrocarbons and water (update of SDS Vol 37 & 38)
 2005-006-1-500: Mutual solubility of alcohols and water (update of SDS Vol 15)

OTHER INTERDIVISIONAL PROJECT

- 2003-011-3-600 - A critical compendium of pesticide physical chemistry data
 2003-060-2-400 - Terminology on separation of macromolecules
 2004-021-1-300 - Reference methods, standards and applications of photoluminescence
 2004-023-1-700 - Internationally agreed terminology for observations in scientific communication

PROJECTS NEAR COMPLETION / IN PRESS

510/31/95 - Nomenclature for X-ray emission spectroscopy
550/64/97 - Non-selective sensors arrays ("Electronic Nose", "Electronic Tongue") chemical analysis: classification and characterization
2001-055-1-500 - Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications
2001-038-2-500 - Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions
2001-009-1-500 - Revision in the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories

PUBLISHED REPORTS (2004-2005)

523/2/89 - Determination of trace elements bound to soil and sediment fractions. *Pure Appl. Chem.* 76(2), 415-442, 2004
550/47/89 - Electrochemical detection in flowing media: Classification and recommendation. *Pure Appl. Chem.* 76(6), 1119-1138, 2004
510/35/97 - Guidelines for calibration in analytical chemistry. Part 2: multicomponent calibration. *Pure Appl. Chem.* 76(6), 1215-1225, 2004
550/62/97 - Electroanalysis with piezo-electric devices. *Pure Appl. Chem.* 76(6), 1139-1160, 2004
1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands. Part I Mercury. *Pure Appl. Chem.*, 77(4), 739-800, 2005. Chemical speciation of Hg(II) with environmental inorganic ligands. *Australian J.Chem.*, 57, 1-8 (2004)
2000-033-1-500 - Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban and contaminated environments (SOILSAMP). *Pure Appl. Chem.* 77(5), 827-841, 2005
2001-021-1-500 - Analytical electromigration techniques. *Pure Appl. Chem.* 76(2), 443-451, 2004.
2001-025-1-500 - Critical evaluation of the state of the art of the analysis of light elements in thin films. *Pure Appl. Chem.* 76(6), 1161-1213, 2004
2001-075-1-500 - Compilation of k₀ and related data for NAA in the form of electronic database. *Pure Appl. Chem.* 76(10), 1921-1925, 2004
2001-085-1-500 - IA and IIA azoles, cyanates, cyanides and thiocyanates. *J. Phys. Chem. Ref. Data* 2004, 33, No. 1, 1-176.

IUPAC REPRESENTATION AT CONFERENCES

Inaugural Conference for the Southern and Eastern Africa Network of Analytical Chemists (SEANAC), 7-10 July 2003, Gaborone, Botswana.

Colloquium Spectroscopicum Internationale 33rd Colloquium Spectroscopicum Internationale, 2003, 7-12 September 2003, Granada, Spain.

Solubility Phenomena 11th International Symposium on Solubility Phenomena, Including Related Equilibrium Processes (11th ISSP), 25-29 July 2004, Aveiro, Portugal.

Trace Elements in Food, 2nd International Symposium on Trace Elements in Food (TEF 2), 7-8 October 2004, Brussels, Belgium.

Analytical Forum 2004, July 2004, Warsaw, Poland.

8th International Conference on Nuclear Analytical Methods in the Life Sciences - NAMLS8. Rio de Janeiro, Brazil; April 2005

Analytical Chemistry and Chemical Analysis, (AC&CA-05). Kiev, Ukraine; September 2005.

Appendix B Report from Dr Kutner on the meeting of ICTNS, held on August 16-17, 2005, during GA of IUPAC.

1. Based on your Report on a two-year (2003-2005) activity of ACD, I emphasized in my report to ICTNS only those aspects of activity of ACD that were important from the point of view of this Commission. That is, I mostly discussed publications of ACD. It was pointed out that project 2000-033-1-500 'Terminology in soil sampling', which was indicated in your Report as 'Under review by ICTNS or authors', had already been published (Pure Appl. Chem. 77, 827-841 (2005)). For the purpose of updating the 'Green Book', the definition of pH recommended in the document prepared by the Working Party on pH (Measurement of pH. Definition, standards, and procedures, Pure Appl. Chem. 74, 2169-2200 (2002)) was edited and modified in such a way that non-recommended adjective 'molal' was avoided. ACD was prompted to update its 'IUPAC Compendium of Analytical Chemistry Nomenclature' ('Orange Book') with respect to the pH issue in the same way, i.e., by incorporating the same document and definition of pH.
2. Based on the Report of Dr. D. S. Moore, I presented a status of updating the 'Orange Book'. That is, the third edition of this Book published in 1997, was uploaded on the IUPAC website on one hand and five (not three, as indicated in his report) projects aiming at its updating were initiated within ACD on the other.
3. Often, authors of the IUPAC projects do not conform to instructions for authors on preparation of the IUPAC documents to be published in PAC. Being prompted by ACD, I passed to ICTNS a suggestion that the IUPAC Secretariat, upon notifying the authors on approval of their project proposals, should inform them about the exact location of these instructions on the web. ICTNS supported this suggestion.
4. A recently submitted to ACD project proposal, entitled 'Specific heat capacity functions of combustion gases and fuel gas components' with Prof. H. Gamsjaeger as the Task Group Chairman, was considered by ICTNS as being well suited as a technical report rather than a recommendation type document of IUPAC. This was because data would be compiled and critically evaluated, despite that the formulas rather than terminology, symbols or nomenclature would be recommended. Several IUPAC documents of similar type of recommendations of formulas have been published in Pure Appl. Chem. in the past. ICTNS suggested that authors of this project proposal should get in touch with NIST with respect to their project.
5. ICTNS was concerned with regard to commercial aspects of the IUPAC Stability Constants Database. That is, the Database is now available at the IUPAC website on commercial bases. Such a status of this Database is in contradiction with the IUPAC mission to serve a global society as an international non-profit organization. A hope has been expressed that this Database will be made available free to the chemical community after three years from now, i.e., after its copyright will be transferred to IUPAC. It was suggested that Division V officers should prompt Dr. G. Pettit and Dr. L.D. Pettit of Academic Software to supplement obsolete terminology, symbols, and nomenclature, used all throughout the Database, with newly approved ones. *[The Division President has made a comprehensive response to ICTNS which has been incorporated in the Minutes of the ICTNS meeting.]*

Among other points, it clarifies the difference between “freely available” and “non-profit”, pointing out the considerable cost of maintaining the database.]

6. I informed ICTNS about an initiative, undertaken within ACD by Prof. D. B. Hibbert. That is, he proposed to urge editors of international analytical chemistry journals to implement in instructions for authors of their journals exact information where IUPAC recommendations on terminology, symbols and nomenclature relevant to analytical chemistry could be found. Representatives of other divisions were suggested to do the same within their fields. Moreover, an issue was discussed of approaching editors of major publishing houses and prompt them to update their students' chemistry textbooks with respect to recently approved changes in terminology, symbols, and nomenclature. ICTNS has already assisted the European Union Customs in preparation of directory of chemical substances with the IUPAC-approved nomenclature being implemented in it.
7. The submitted to ICTNS for reviewing ACD project PAC-REC-05-07-05 'Guidelines for Potentiometric Measurements in Suspensions' with S. F. Oman as a Task Group Chairman, will be sent for reviewing also to Dr. A. Fajgelj, in response to his request. In the past, Dr. Fajgelj extensively commented on this project as an ACD referee and had so far no chances to check how the authors responded to his comments.