IUPAC Project Progress Report

Date : December 2005 **;** Period: July 2005 – February 2006

Project number: 2004-005-2-500

Project Title: Comparable pH measurements by metrological traceability

Series Titles: pH Measurements in Complex Matrices
Part I - pH Measurements in water quality monitoring and assessment Part II- pH Measurements of clinical, biochemical and environmental relevance

Task Group Leader:M. F. Camoes

Starting date: January 2005

Report:

1. Projected completion date (documents ready for external review): January 2008

2. Have the project objectives been modified during the last 6 months? No

3. Please list the task group members involved in the work during the last 6 months.
   M. Filomena Camões, Paul de Bievre, Hans Bühler, Arthur Covington, Andrew Dickson, Richard Durst, Erno Lindner, Michal Mariassy, Günther Meinrath, Martin Milton, Kenneth Pratt, Cedric Rivier, Petra Spitzer

4. Difficulties encountered (or concerns):
   Distance, funding and professional activities tend to diminish the direct productivity of task group members towards the project.

5. Please list the to-date results (outputs) of the project

MINUTES of the 2nd Meeting of the task group
TUESDAY, 18 October 2005- 09:30 h to 18:30 h (lunch from 12:30 till 13:30 h)

Address- BAM , Building 8.15, Richard- Willstätter Str. 11 room 236

Present: Hannes Buehler, M.F.Camões, Michal Mariassy, Guenther Meinrath, Keneth Pratt, Cédric Rivier, Petra Spitzer

Thanks have been addressed to:

- Petra Sptizer for having made arrangements for the meeting,
- Ralph Matschaf for having hosted the meeting and supplying coffee and lunch,
- Cédric Rivier (LNE) for having supported the costs of lunch at LNE last February.

pH: Updating of Action List for the period between 18 October 2005 and next meeting /April 2006- Paris, CCQM

Action	Dead line	REMARKS
1) update emails	Immediate	MFC to verify contacts and to write personnal letters of apology for those who may have got little information, e.g.Peter Atkins
2)Work Group Members	----------	Bjorm Kristensen and Sandra Rondinini have expressed their impossibility to integrate the group due to professional commitments in different topics
3) Letter from Broadley-James Corporation	Immediate	MFC to reply inviting an observer to next meeting and a reply to Cédric Rivier's questionnaire
4) PROJECT WEBSITE	Immediate	MFC/ul.pt
5) Documents to be circulated in PDF format or low Windows version	------	All
6) Comments to IUPAC Compendium of Chemical Terminology 2nd Edition (1997) http://www.iupac.org/goldbook/P04524.pdf entry for pH	Immediate	The whole text should be replaced by: Proposal: "pH, as defined, pH=-lg $a_{H+,}$ is immeasurable because it involves the hydrogen single ion activity coefficient. The pH(S) of international recognized primary pH buffer solutions thus approaches the defined pH as closely as present electrolyte theory permits. The primary method for pH is based on the measurement of the potential difference of an electrochemical cell without transference, containing a platinum hydrogen electrode and a silver-silver chloride reference electrode, often called a Harned cell. The primary method is used to assign pH(S) values to a restricted number of primary standards in dilute aqueous solutions between pH 3 and 10 and in a temperature range from 5 to 50 ºC. Most routine pH measurements are carried out with pH meter-glass combination electrode assemblies. The use of these electrodes is subject to various effects, like liquid junction potentials, causing uncertainties of unknown magnitude. Therefore a suitable calibration is required by certified reference buffer solutions

		whose pH is traceable to the pH(S) of primary buffer solutions. [(R.P. Buck, S. Rondinini, A.K. Covington, F.P. Baucke, C.M.A. Brett, M.F.Camões, M.J. Milton, T. Mussini, R. Naumann, K.W. Pratt, P. Spitzer and G.S. Wilson *Pure Appl. Chem.*, 74:11, pp 2169-2200 (2002)]"
7) PAPERS a) "A revolution in analytical Chemistry: Chemical Metrology and the measurement of pH" (oral presentation)	G. Meinrath, P. Spitzer and K. Pratt	GIT/American Lab Publication
b) "HOW SHOULD ONE MEASURE pH" (oral presentation)	M.F. Camões and R. Durst	AQUAL, Chemical Review, J.Chem.Ed or Analyt. Chem. To be finished by the end of December; <u>draft for comments sent out end November</u>
c) "What are the improvements in measuring pH from Sorensen" (debate)	Send contribs to G.Mein. until 20th November	THIS PAPER SHOULD CALL THE PUBLIC'S ATTENTION TO CR QUESTIONNAIRE -MFC to ask AKC a paragraph on how IUPAC became interested in pH -MFC "Education"/Motivation of people to answer CR questionnaire - PS to ask Fritz Baucke how pH meas uncert are done in Refer. Labs - PS to supply picture traceability chain -MM 2 paragraphs about Key Comparisons
d) Estimation and experimental issues concerning liquid junctions (oral presentation)	Hannes Buehler	-CR, what is wanted from the questionnaire Kenneth Pratt and Petra Spitzer to contribute
8) BOOK "pH for everyone" or "Metrological Approach to pH Measurements" Request (to Elizabeth Pritchard, Marc Priel, Philipe Charlet ???) for contributions on	PICTURES and EXAMPLES References at the end of each chapter Draft of each chapter (5-10 pages) to	20pages per chapter INTRODUCTION Historical Background- KP Basic Theory- MFC Glass Electrodes- Traceability-PS LJP- Hannes B Key Comparisons MM and CR Applications : Water, Salinity, Food, Envir, Speciation, Clinical, Pharmacy

"Legal Issues of Metrology" for publication in Journal (?) and Book	Rome Conference/ March	Recommendations
9) French PTS on pH measurements in water (Oral presentation)	Cédric Rivier…	Look for PTs in SeaWater
10) PTS organized by BAM and others until 2003 (Oral presentation)	Petra Spitzer	
11) Questionnaire (Oral Presentation and discussion)	Cédric Rivier	
12) Conferences	- APAT/IUPAC Rome , March 2006 -Pittcon (2006); - Euroanalysis (2007); FECS (2006); National meetings	The Group will produce some contribution; dead line 15th Dec 2005
13) Collect "funny" stories/jokes about pH	On going	All
14) Next WG Meeting	On the occasion of CCQM-Paris/April 2006	The Group Members who are not coming to CCQM will be able to use part of the budget from the Project.

6. Please list the dissemination events (viz. articles, CD, conference presentations; etc.)
   (i) already accomplished

Articles

- Reassessment of pH Reference Values with Improved Methodology for the Evaluation of Ionic Strength
  M. J. Guiomar H.M.Lito and M. Filomena G.F.C. Camões,

Anal. Chim. Acta, 531, 2005,141-146

Conference Presentations

- COMO É QUE SE MEDE pH?
M. Filomena G. F. C. Camõesa, c, M. J. Guiomar H. M. Litob, c, Catarina M. Viçosoc
4deq, SPQ, Lx 27-28 Oct 2005

-COMPARABILIDADE DE VALORES DE ACIDEZ/Invited Lecture
Maria Filomena G. F. C. Camões, Catarina Viçoso, Maria J.Guiomar H.M.Lito-
1 Confer Nac. SPMet, 28 e 29 de Novembro de 2005 – Lisboa

Results from Profficiecy Tests conducted for fresh waters, by Petra Spitzer/BAM and Cedric Rivier/LNE have been analysed and will be incorporated in publications; they have also contributed to the revision of the questionnaire which will soon be sent to pertaining laboratories.

Project webpage
http://quimica.fc.ul.pt/pH IUPAC

Comments to IUPAC Compendium of Chemical Terminology 2nd Edition (1997)
Sent in/ ongoing discussion
(ii) planned

- Publications under completion:
- "A revolution in analytical chemistry"- Metrology and the measurement of pH: New concepts and new responsibilities in chemical measurement
G. Meinrath, P. Spitzer & K. Pratt

- “How Should One Measure pH”
M.F. Camões and R. Durst

- “What are the improvements in measuring pH from Sorensen”
Guenther Meinrath

- “Estimation and experimental issues concerning liquid junctions”
Hannes Buehler

BOOK - ”pH for everyone” or “Metrological Approach to pH Measurements”

Conferences

“Traceability of pH in a metrological context”
Workshop-APAT-IUPAC, Rome, March 2006

7. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project?
Not applicable

8. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them.

The aims and scope of the project have been well stated in the application form and so agreed the **Analytical Chemistry Division (V)** and **Physical and Biophysical Chemistry Division (I) Chemistry and the Environment Division (VI),** which is a clear recognition of the current problems and challenges ahead in multiple disciplinary areas.

May be the novelty and the direction in which the working group is investing is well put in the following phrase which is part of a paper under preparation:

"In the light of the importance of pH, especially in the context of medical treatment, food quality and cosmetic products, it seems surprising that the values produced at different locations and different times by different equipment and different procedures were all accepted as valid determinations of the quantity pH - despite the fact that the quantity pH by its own definition is an immeasurable quantity."