Measurement of pH. Definition, Standards, and Procedures (IUPAC Recommendations 2002)

by R. P. Buck, S. Rondinini, A. K. Covington, F. G. K. Baucke, C. M. A. Brett, M. F. Camoes, M. J. T. Milton, T. Mussini, R. Naumann, K. W. Pratt, P. Spitzer, and G. S. Wilson

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The definition of a "primary method of measurement" has permitted a full consideration of the definition of primary standards for pH, determined by a primary method (cell without transference, Harned cell), of the definition of secondary standards by secondary methods, and of the question whether pH, as a conventional quantity, can be incorporated within the internationally accepted system of measurement, the International System of Units (SI, Système International d' Unités). This approach has enabled resolution of the previous compromise IUPAC 1985 Recommendations [*Pure Appl. Chem.* **57**, 531 (1985)]. Furthermore, incorporation of the uncertainties for the primary method, and for all subsequent measurements, permits the uncertainties for all procedures to be linked to the primary standards by an unbroken chain of comparisons. Thus, a rational choice can be made by the analyst of the appropriate procedure to achieve the target uncertainty of sample pH. Accordingly, this document explains IUPAC recommended definitions, procedures, and terminology relating to pH measurements in dilute aqueous solutions in the temperature range 5–50 °C. Details are given of the primary and secondary methods for measuring pH and the rationale for the assignment of pH values with appropriate uncertainties to selected primary and secondary substances.

www.iupac.org/publications/pac/2002/7411/7411x2169.html

Use of the Term "Recovery" and "Apparent Recovery" in Analytical Procedures (IUPAC Recommendations 2002)

by D. T. Burns, K. Danzer, and A. Townshend

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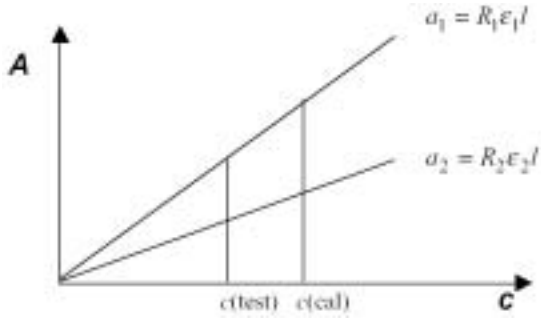
The chemical community has used the term **recovery** to deal with two quite different experimental configurations. The terms **recovery** and **apparent recovery** are recommended to avoid confusion caused by the use of the term **recovery** to cover two distinct situations. These situations deal with: (a) the **yield** of a preconcentration or extraction stage of an analytical process (where **recovery** is recommended) and (b) the quantity **observed value/reference value**, obtained using an analytical procedure that involves a calibration graph (where **apparent recovery** is recommended).



For linear calibration graphs *c*(test) is independent of the slopes a_1 or a_2. The absolute values of R_1 or R_2 do not affect the value of *c*(test) provided that $R_1\mathcal{E}_1 l$ and $R_2\mathcal{E}_2 l$ are independent of *C*.

www.iupac.org/publications/pac/2002/7411/7411x2201.html

Impact of Scientific Developments on the Chemical Weapons Convention (IUPAC Technical Report)

by G. W. Parshall, G. S. Pearson, T. D. Inch, and E. D. Becker

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This document was prepared as a report from IUPAC to the Organisation for the Prohibition of Chemical Weapons (OPCW) to provide an evaluation of scientific and technological advances in the chemical sciences relevant to the Chemical Weapons Convention (CWC). The report is intended to assist OPCW and its Member States in preparation for the First Review Conference to be held on 28 April 2003. The CWC, now ratified by 145 nations and in effect since 1997, totally prohibits the production, storage, or use of

toxic chemicals as weapons of war. This report is based on an IUPAC Workshop held in Bergen, Norway, 30 June to 3 July 2002. The report highlights developments in organic synthesis and changes in chemical plant design that will pose new challenges to the Convention, but it also describes recent and probable future developments in analytical chemistry that should assist in implementation of the Convention. The key issues identified at the Workshop are listed and the findings and observations are summarized in 18 points. Some of the lectures presented at the Workshop are published in the same issue of *PAC*.

www.iupac.org/publications/pac/2002/7412/7412x2323.html

Critical Evaluation of Stability Constants and Thermodynamic Functions of Metal Complexes of Crown Ethers (IUPAC Technical Report)

by F. Arnaud-Neu, R. Delgado, and S. Chaves

Pure and Applied Chemistry,
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Stability constants and thermodynamic functions of metal complexes of crown ethers in various solvents published between 1971 and the beginning of 2000 have been critically evaluated. The most studied crown ethers have been selected: 1,4,7,10 tetraoxacyclododecane (12C4); 1,4,7,10,13 pentaoxacyclopentadecane (15C5); and 1,4,7,10,13,16 hexaoxacyclooctadecane (18C6). The metal ions chosen are alkali and alkaline earth metal ions, Ag^{+}, Tl^{+}, $Cd2^{+}$, and $Pb2^{+}$. The solvents considered are water, methanol, ethanol, and their mixtures, as well as acetonitrile, *N,N'*-dimethylformamide, dimethylsulfoxide, and propylene carbonate. The published data have been examined and grouped into two categories, "accepted" and "rejected." The "accepted" values were considered as (i) recommended (**R**), when the standard deviations (s.d.) on the constant K or on ΔrH were inferior to 0.05 lg unit or inferior to 1 kJ mol^{-1}, respectively; (ii) provisional (**P**), when s.d. is superior to 0.05 and inferior to 0.2 for lg K or s.d. is superior to 1 and inferior to 2 kJ mol^{-1} for ΔrH; (iii) recommended 1 (**R1**), if the values were obtained by a single research group, but were considered reliable in comparison with related systems, and considering that the research team usually presents R-level values for other similar systems.

www.iupac.org/publications/pac/2003/7501/7501x0071.html

Critical Evaluation of the Chemical Properties of the Transactinide Elements

by J. V. Kratz

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In this paper, the chemical properties of the transactinide elements rutherfordium, Rf (element 104); dubnium, Db (element 105); and seaborgium, Sg (element 106) are critically reviewed. The experimental methods for performing rapid chemical separations on a time scale of seconds are reviewed, and comments are given on the special situation with the transactinides for which the chemistry has to be studied with single atoms. There follows a systematic description of theoretical predictions and experimental results on the chemistry of Rf, Db, and Sg—their mutual comparison and evaluation. The literature cited has the cutoff date of March 1999. The more recent chemical identification of bohrium, Bh (element 107), and of hassium, Hs (element 108), should be evaluated in a future part II of this report.

www.iupac.org/publications/pac/2003/7501/7501x0103.html

Current Challenges and Needs for Analytical Chemistry

This workshop, organized by the Analytical Chemistry Division, will be held during the IUPAC General Assembly on Sunday 10 August (AM).

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