INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

(CPCDS) Committee on Publications and Cheminformatics Data Standards

Meeting IUPAC – De Gruyter
Teleconference
8:30am - 9:35am EDST
September 26, 2014

Draft Minutes

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IUPAC Attendees: Hugh Burrows, Mark Cesa, Kazuhiro Hayashi, Colin Humphris, Robert Lancashire, Bonnie Lawlor, Bono Lučić, James Liu, David Martinsen, Fabienne Meyers, Miloslav Nič, Lynn Soby

De Gruyter Attendees: Katharina Butsch, Spencer McGrath, Karin Sora

Background

Bonnie Lawlor opened the meeting at 8:35am Eastern Daylight Savings Time with a review of who was in attendance. The objective of today's teleconference was to provide a forum in which De Gruyter could present a proposal for the creation of a database from IUPAC content. The motivation behind the development of such a database is to create a revenue-generating product that De Gruyter can market and sell since they cannot sell the *PAC* back files as originally planned (the back files are open access).

This concept was first discussed at the meeting of the IUPAC Committee on Publications and Cheminformatics and Data Standards (CPCDS) that was held in Berlin, Germany, July 26-27, 2014. A follow-up meeting was held in San Francisco, CA on August 11, 2014 during the meeting of the American Chemical Society. At that meeting, De Gruyter presented a database developed from the Color Books, but it became clear that there were issues that had to be resolved, especially since there is an IUPAC project already underway for the development of a Content Management System that will facilitate Color Book updating. Since the August meeting they revised the concept to maximize the use of IUPAC's *Pure and Applied Chemistry* content that they already have in-house. They remain very interested in pursuing a Color Book database, but believe that this new database will allow them to move more quickly in development and will pave the way for IUPAC and De Gruyter to collaborate on other databases in the future.

A copy of the presentation given by Katharina Busch appears at the end of these minutes for ease of reference to the relevant slides.

Introduction (slide #2)

The database being described would be created from the legacy back files of the standards and recommendations that are contained in IUPAC's *Pure and Applied Chemistry* (PAC). As noted earlier, this is data that De Gruyter already has in-house. The estimate is that there are over one thousand articles containing standards and recommendations that have been printed on some twenty-two thousand pages, first in *PAC* and then in other IUPAC products such as the Color Books, where the content is enriched. De Gruyter is fully aware that this material is already freely-available on the Internet, but they believe that the database will offer sufficient added-value to warrant a subscription fee that users will be willing to pay.

Database Added-Value (slides 3 - 10)

The main value of the database will be the ease of locating specific information of interest. Currently, the information-seeker has three channels through which he/she can access the standards and recommendations: first, by going to IUPAC.org and searching the archives of standards and recommendations, but to do this the searcher must know the year in which the material was published or the IUPAC Division that submitted the material; second, by searching *PAC* on IUPAC.org by refining the search to limit it solely to standards and recommendations; and third, through a Google search which can provide a large number of results. These Google search results may not be the most recent, but will be those most frequently accessed and opened. Also, it should be noted that only about one-quarter of the documents containing standards and recommendations are short (1-2 pages). About half are of full-article size (10-20 pages) and the remainder range from fifty-one pages to small booklets of more than one hundred pages. So searching for specific IUPAC standards and recommendations can be difficult. De Gruyter believes that the most efficient and effective tool for retrieving specific information is a dedicated database.

Database Options (Slide 11)

Three database options were put forth: 1) a core, basic database created from the standards and recommendations as they were published in *PAC*; 2) an advanced "living" database; and 3) an enriched database which would be sophisticated and contain additional information.

Core Database Option (Slides #12 - 15)

The basic database would be created from the current *PAC* content that De Gruyter already has in-house. Required actions are the conversion of PDF files into XML, the "cutting" of some of the articles into appropriate database entries, and the uploading and hosting of the database. By "cutting" the article, it is meant that there is content (e.g. definitions) that can be very easily identified during the conversion from PDF to XML for documents that are glossary or encyclopedic in format. This content would provide added-value to the database (see slide #13). However, this identification and cutting cannot be easily done for full-text articles. De Gruyter is willing to do all of the work and incur all of the expenses for this basic product (this does not include the cutting of full-text documents; additional information from full-text articles is an option – see below).

There is an *optional* action that can be considered and that is to create additional metadata for the full-text articles that cannot be "cut." These articles already have basic metadata associated with them. Creating additional metatdata would involve identifying relevant terms, figures, phrases, etc. (see slide #15) that are not among the basic keywords that have already been created for the article and that would enhance the search and retrieval process. This optional action can be done by IUPAC at its expense or by a freelancer. In the latter case the expenses would be shared by IUPAC and De Gruyter (slide #14). To estimate the cost IUPAC and De Gruyter would need to identify how many terms would be created for each full-text article.

Living Database Option (slide #16)

The more advanced version of the core database is a living database. By "living" it is meant that database entries would be worked on within the database itself and therefore would require the use of a Content Management System (CMS). The CMS system and a technical help desk can be provided by De Gruyter and they would incur the expenses for those functionalities as well.

An option to consider is if IUPAC would want to add additional information to the articles already created. This would require working in the CMS and De Gruyter is willing to provide some editorial support. This does not mean that De Gruyter will create the data – this will remain an IUPAC function. Rather, De Gruyter will provide the expertise for organizing the entries, checking for completeness, etc.

Enriched Database (slide #17)

The enriched database is the most sophisticated version as it would contain information beyond what actually appears in the standards and recommendations. This could include data such as InChI codes, links to external related content, etc. and would require the use of a freelancer. Costs of including this additional information would be shared by De Gruyter and IUPAC. No estimate can be provided until IUPAC decides what additional content would complement the core standards and recommendations.

What a Database Could Look Like (Slides #18-26)

The format shown on slide #18 is a standard database format and that would be the same for the core product as well. Search options are listed on the left hand side and the article appears on the right. The header information is taken from the metadata that is associated with the retrieved document (article title, authors, journal citation, keywords, etc.). Entries can be browsed using a "tree structure" which is a listing of major subjects along with related subheadings for each major subject (e.g. Analytical Chemistry" followed by a subheading of "actinometry" which in itself is followed by a subheading of "calibration."). De Grutyer suggested that a tree structure be developed by analyzing the articles that De Gruyter has already amassed, not by looking at all of chemistry. If the latter route is chosen, some major headings in the structure may not have sufficient related content, if any at all.

Katharina Butsch showed the current structure used to search for standards and recommendations (slide #20) which is basically a list of the IUPAC Divisions. She then showed the major headings for the type of tree structure that De Gruyter is proposing (slide#21). This was then followed by an example of how the structure for each major heading might be constructed (slides #22-24). The headings use terms that serve the needs of the information seeker so that the searcher can intuitively find the information that they want. An arrow represents a unique level. The structure shown is simply an example and De Gruyter recommends that the final structure have more sublevels for the fine-tuning of searches.
Katharina also discussed other database features such as linking to relevant external sites (see slide #26).

Advantages of Creating a Database with De Gruyter (Slide #27)

Katharina closed her presentation with a summary of the benefits of creating an IUPAC-dedicated database and why it would work well with De Gruyter. These are as follows:

- The visibility of IUPAC's standards and recommendations would be increased
- IUPAC branding would be strengthened (can be marketed and sold with other IUPAC products)
- De Gruyter provides the required infrastructure to create a complex database
- De Gruyter as a company has experience in launching databases and the individual staff members that IUPAC works with also have experience and expertise in this area; (The concept is similar to a database that Karin Sora had developed while at Springer (see http://www.springermaterials.com).

- The already-established contacts between IUPAC and De Gruyter will be used to build the database
- IUPAC customers now have established contacts with De Gruyter who can promote and sell the database

Question and Answers

The formal presentation was followed by a period of questions and answers.

1. Can IUPAC move from the core database to the most sophisticated version over time as finances and labor availability permits? (Bonnie Lawlor)

Yes, but De Gruyter needs to know upfront if the Content Management System is needed because they would need to apply for this right away. They also need to get internal approvals to move forward. Depending on the type of database that IUPAC chooses (core, living, enriched), they also may need to hire additional staff. They would like to know from the beginning the IUPAC vision for the database.

2. Is metadata created during the process of converting PDF to XML? (James Liu)

The tentative answer was "No," but Katharina is going to check. She said that they use freelancers to do the conversion and as she understands, they are not permitted to touch the metadata. James questioned whether the basic metadata (title, authors/publication date, etc.) has already been captured for the articles and the answer is "yes."

3. What Content Management System does De Gruyter use? (James Liu)

It is a customized solution and Katharina will get more information on this. *Note:* Since the meeting Katharina has provided the following information:

The De Gruyter CMS is a customized solution and has the following key features:

Technical
Customized Content Management System based on MarkLogic XML Database and Search

Technology
Web-based application (optimized for Google Chrome)
High-Availability setup including monitoring and backup mechanisms

Functional
Comprehensive search (XQuery-Search) with export option for results

Easy text-editing with embedded CKEditor (including MathML)

Optional: Full-fledged XML Editor "Oxygen" is also available
Multimedia asset management

PDF and HTML previews on the fly

Role-specific access to data
Customized metadata management (key words, size limits, ...)

Dashboard with user-specific "My tasks" list
- Automatic e-mail notifications, e.g. for initial invitations and overdue tasks
- Elaborate reports
- Version history
- Support for Thesauri and Taxonomies
- Supports hierarchically structured content

4. What data will be used to create the database – legacy data, new data or both? (Dave Martinsen)

De Gruyter will create the database from legacy data and at the end of each year, data from that year will be added, e.g., 2014 data will be added to the database at the beginning of 2015.

5. The PAC/Color Book workflow is very much geared towards the print publications. Should the workflow be modified so that if we choose to include additional tagging for the database going forward it can be added during the normal workflow and not afterwards? The added tags would be "invisible" to the journal, but would be extractable for the database. (David Martinsen)

Spencer McGrath said that this would be a question for Kevin in De Gruyter's production area. Spencer was thinking that if IUPAC chooses to do additional tagging for the database Ge Gruyter might change the vendor currently that is currently used for *PAC* production so that there would not need to be two production passes – the first for normal production and a second for the enhanced XML. De Gruyter needs to check with their production team to make sure that they could change the work flow to a single process. Karin Sora said that production will be involved if the database is given the go-ahead as they will need to provide input to the business plan.

6. Currently the standards and recommendations appear in *PAC* and then are later extracted for the Color Books. There have been a lot of challenges in taking the data created for a print model and transforming that data into a database. Are there efficiencies to be gained in having those who are responsible for the Color Books make use of the CMS system? Are there examples of De Gruyter using the CMS as a "master database" from which print products are extracted? (David Martinsen)

Karin Sora said that De Gruyter currently uses the CMS from which to extract print products, with a prime example being in the field of medicine – the *Pschyrembel Clinical Dictionary.* It is a database, and a series of products are generated from it. Both Karin and Katharina re-iterated that De Gruyter is very much interested in pursuing a Color Book database and hope that such a database would be possible in the future.

7. If a database of IUPAC Standards and Recommendations becomes a reality, what will be the access *to Pure and Applied Chemistry* journals? (Colin Humphris)

Karin Sora stated that access to *PAC* will be open access – that is the point of creating a database since De Gruyter cannot sell the back files. The database will provide search capabilities that are not presently available and will require a subscription fee. Colin said that this was his understanding as well.

8. Since De Gruyter will be marketing and selling the product, what are the key features that the De Gruyter team believes are important to making the database marketable? (Colin Humphris)

Katharina Butsch replied that she believes that the ease of access provided by the database and the tree structure that will facilitate searching and browsing will attract users. She added that additional information would be beneficial and Karin Sora agreed.

9. Is the core database sufficient for De Gruyter to regain the revenue perceived to have been lost as a result of not being able to sell the back files or do we need to move on to the more sophisticated databases for that to happen? (Colin Humphris)

Karin Sora noted that while a contract exists no one currently involved at either De Gruyter or IUPAC had any say in that contract. De Gruyter does not see the contract as a problem. They just need to adjust and identify a common way in which they and IUPAC can move forward together. They are very much interested in creating a database and believe that it is a stepwise process. We start with the core product (although from the beginning we must consider the living database because that involves the CMS. In a sense they are one and the same – the only difference is the inclusion of the CMS system). The eventual inclusion of InChI codes would be helpful because of the added-value.

10. How does De Gruyter see the revenue sharing taking place? Will it flow back based upon how things are detailed in the current *PAC* contract? (Colin Humphris)

Karin Sora said that the revenue sharing will be based upon how much effort/resources each organization puts into the project. If IUPAC gives the go-ahead for the database, De Gruyter will need to develop a plan with input from all areas of their company that will be involved. The sales group will be asked how many units they will be able to sell in order to develop a realistic revenue stream, production will need to look at how the workflow may need to be revised, etc.
Katharina noted that this will be a separate project and will require its own business plan and its own contract. It will not be governed by the current *PAC* contract. Karin concurred. Colin noted that just as De Grutyer needs to look at what it needs to invest, IUPAC will need to have a similar discussion.

11. If InChI codes are eventually added, could they be used to search *PAC*? (Robert Lancashire)

Katharina said that this would not be possible because the database structure would differ from that of *PAC*. Karin noted that what happens within the database stays within the database. Also, the InChI codes would be part of the added-value of the database and therefore should not be part of *PAC*.

12. Are there other projects that De Gruyter can use as a point of reference for estimating the time and cost of developing the core database (Lynn Soby)

Karin said that for the core database and the living database IUPAC will not incur any costs unless additional data is included, e.g. the metadata option. Costs will enter into the project when content is added and will depend on the type and amount of content. De Gruyter provides a CMS system to all of its users.

Katharina noted that for the core project with no added metadata, one year is a reasonable time estimate assuming that no significant problems arise with the data. She does not expect there to be problems because they already have everything in PDF format. If additional metadata is desired, they would need to identify a freelancer who not only has the technical savvy to do the conversion, but who also has the scientific knowledge and finding such a person can take some time. Karin added

that converting content into a database is something that De Grutyer does every day. She said that when she was at Springer and created the database of Springer Materials (see: http://www.springermaterials.com), it cost forty thousand Euros to convert nine hundred thousand pages for the creation of a database with all of the bells and whistles.

13. How will the CMS that De Gruyter is discussing "fit" with the IUPAC CMS project for the Gold book that is currently underway? Are there synergies to be considered for the future? (Fabienne Meyers)

Bonnie Lawlor said that this is still an issue that needs to be resolved and is very much related to the comments made by Dave Martinsen earlier when discussing the challenges of taking the *PAC* data to feed into the Color Books. She will discuss this with Brynn Hibbert who could not participate in today's meeting. She did not make contact with Mark Kinna during the ACS meeting in San Francisco but has been in contact with him.
Katharina stated there need not be a connection between the two CMS systems.

14. If we start with the basic database what decisions need to be made up front to ensure that nothing inhibits the creation of an enhanced version at some future time? Do we need to know what additional data will be included so that appropriate fields are built in? (Bonnie Lawlor)

Katharina said that the only significant up-front decision is the inclusion of a CMS for reasons internal to de Gruyter. For marketing purposes it would be ideal to have an IUPAC vision for the database (this will also have an impact on the name of the database). Karin added that the tree structure needs to be determined at the beginning as well and that she believes that this should be done as a joint IUPAC- De Gruyter effort.

Other Comments:

Hugh Burrows noted that the added-value of the database will be the advantages of the search feature if it is more efficient and quicker than the process used now to access and retrieve IUPAC standards and recommendations. This added-value could create new markets; e.g. clinical laboratories and instrument manufacturers that need access to definitions, standards and recommendations.

Milo commented that based upon his experience, the content management system will be needed and should be used from the beginning.

There being no further questions or comments, the meeting was adjourned at 9:35am. Bonnie Lawlor thanked Katharina, Karin, and Spencer for taking the time to re-do the San Francisco presentation in order to make the overall concept much clearer. She also noted that IUPAC will now need to discuss the revised presentation and determine if and how it wants to proceed. She promised to get back to them as soon as possible. She asked that De Grutyer to the questions that were raised earlier and said that she will contact them if additional questions need to be answered.

Next Step

The IUPAC attendees stayed on the line and after some discussion agreed to hold a teleconference within the next two weeks with a broader audience if possible. The objective is to be able to get back to De Gruyter as soon as possible.

after today's meeting Bonnie Lawlor polled the group as well as additional persons recommended by Fabienne Meyers to determine the date/time for the abovementioned teleconference It is scheduled as follows:

DATE: October 10, 2014 (Friday)

TIME: 11:00am Easter Daylight Savings Time

The call-in information will be sent at a later date.

Respectfully submitted,

Bonnie Lawlor
Chair CPCDS
October 6, 2014

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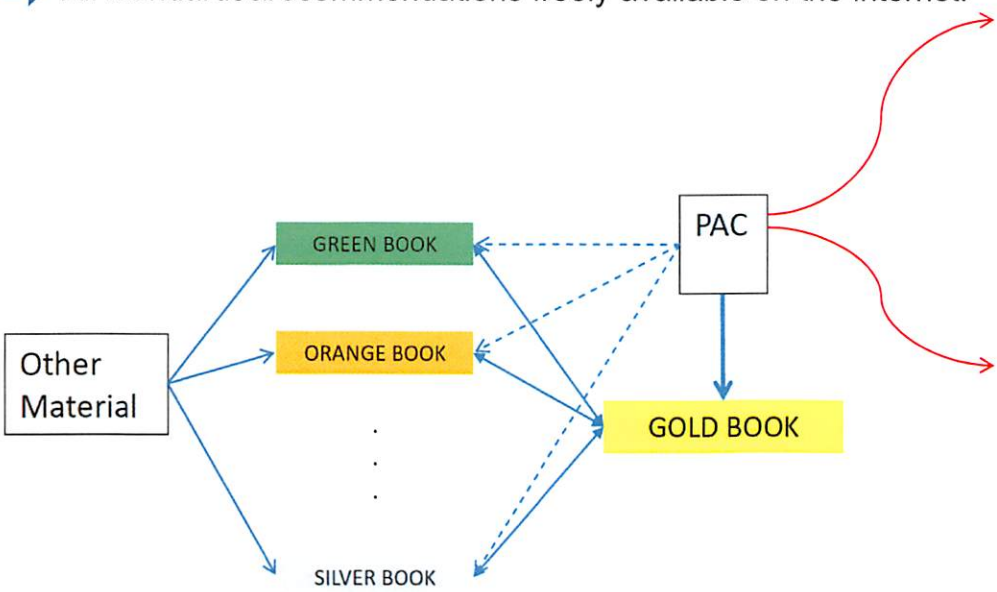
IUPAC Database

September 2014

PAC / Current Workflow

- Total of over **1000** standards&recommendations ~**22000** pages.
- All standards&recommendations freely available on the internet.



Recommendations:

- glossary terms
- definitions
- nomenclature
- terminology, symbols, units
- classifications
- conventions and standards for practices

Technical Reports:

- compilations and evaluations of data, parameters & equations
- critical assessment of methods and techniques
- determinations of elements and compounds in selected samples
- studies of biodegradability and properties of specific materials
- chemical process control aspects

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IUPAC Technical Reports and Recommendations

By year

2013 2012 2011
2010 2009 2008 2007 2006 2005 2004 2003 2002 2001
2000 1999 1998 1997 1996 1995 1994 1993 1992 1991
1990 1989 1988 1987 1986 1985 1984 1983 1982 1981
1980 1979 1978 1977 1976 1975 1974 1973 1972 1971
1970 1969 1968 1967 1966 1965 1964 1963 1962 1961
1960

By division

- ANALYTICAL CHEMISTRY DIVISION
- CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION
- CHEMISTRY AND HUMAN HEALTH DIVISION
- CHEMISTRY AND THE ENVIRONMENT DIVISION
- COMMITTEE ON CHEMISTRY EDUCATION
- COMMITTEE ON PRINTED AND ELECTRONIC PUBLICATIONS
- EXECUTIVE COMMITTEE
- INORGANIC CHEMISTRY DIVISION
- INTERNATIONAL UNION OF PURE AND APPLIED PHYSICS
- ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION
- PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION
- POLYMER DIVISION
- Other (bodies that are not part of the current IUPAC structure - historical, obsolete or renamed)

Selected recommendations translated into German are available from Angewandte Chemie website.

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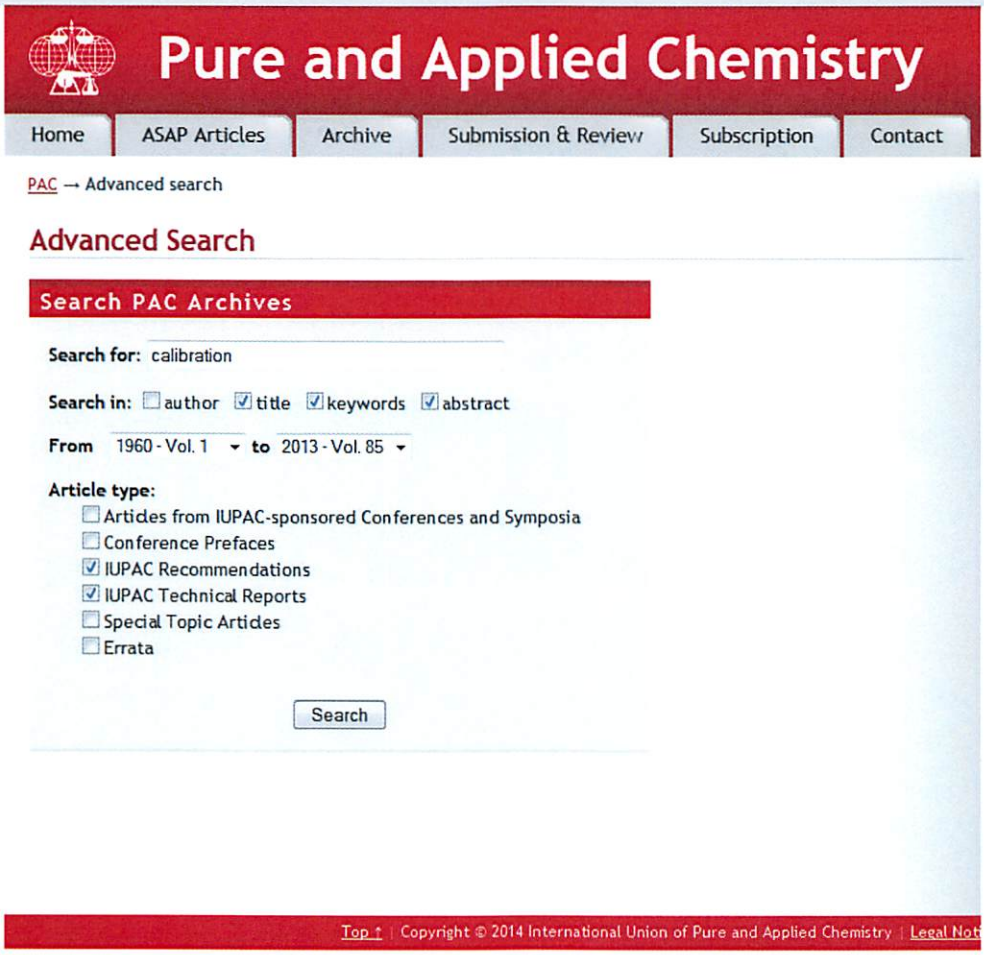
Searching Standards and Recommendations on IUPAc.org



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PAC → Advanced search → Search results

Search results

Search for "calibration", articles 1-19 of 19

Alejandro C. Olivieri, Nicolaas M. Faber, Joan Ferré, Ricard Boqué, John H. Kalivas and Howard Mark
Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report)
2006, Vol. 78, Issue 3, pp. 633-661 [Details + Abstract] [Full text - pdf 645 kB]

Giuseppe Della Gatta, Michael J. Richardson, Stefan M. Sarge and Svein Stølen
Standards, calibration, and guidelines in microcalorimetry. Part 2. Calibration standards for differential scanning calorimetry* (IUPAC Technical Report)
2006, Vol. 78, Issue 7, pp. 1455-1476 [Details + Abstract] [Full text - pdf 402 kB]

K. Danzer, M. Otto and L. A. Currie
Guidelines for calibration in analytical chemistry. Part 2: Multicomponent calibration (IUPAC Technical Report)
2004, Vol. 76, Issue 6, pp. 1215-1225 [Details + Abstract] [Full text - pdf 249 kB]

K. Danzer and L. A. Currie
Guidelines for calibration in analytical chemistry. Part I. Fundamentals and single component calibration (IUPAC Recommendations 1998)
1998, Vol. 70, Issue 4, pp. 993-1014 [Details] [Full text - pdf 1090 kB]

R. P. Buck and V. V. Cosofret
Recommended procedures for calibration of ion-selective electrodes (Technical Report)
1993, Vol. 65, Issue 8, pp. 1849-1858 [Details] [Full text - pdf 684 kB]

M. Grasserbauer
Critical evaluation of calibration procedures for distribution analysis of dopant elements in silicon and gallium arsenides

How to find Standards and Recommendations on Internet?

> Searching on IUPAC.org

> Searching on google

Searching Standards and Recommendations on google

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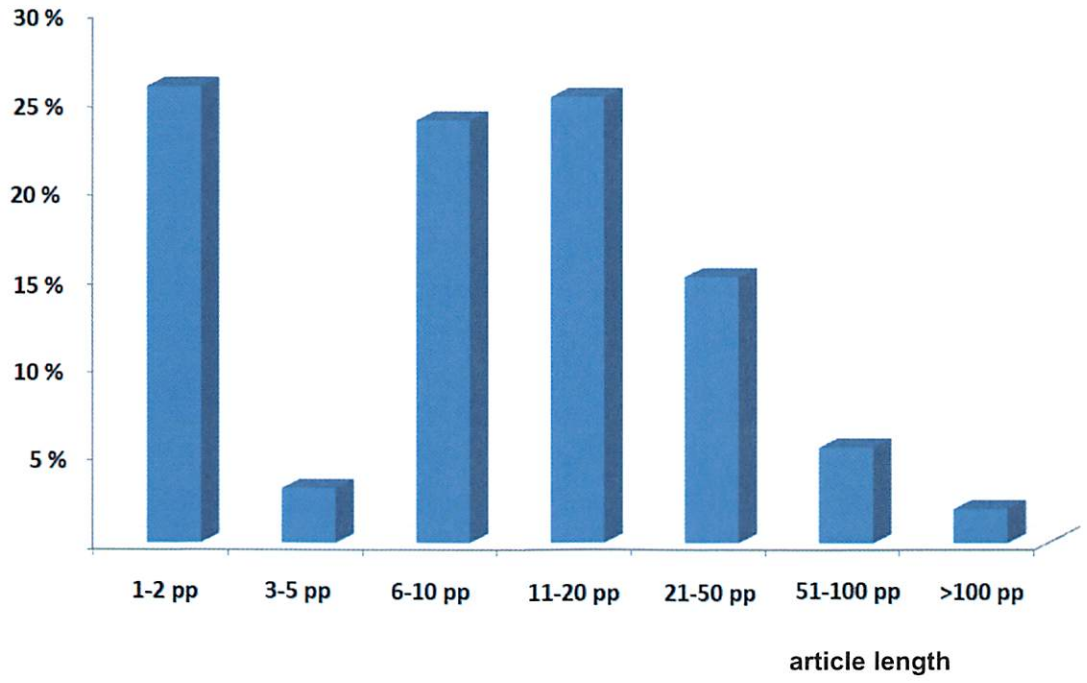
Finding the needle in the haystack



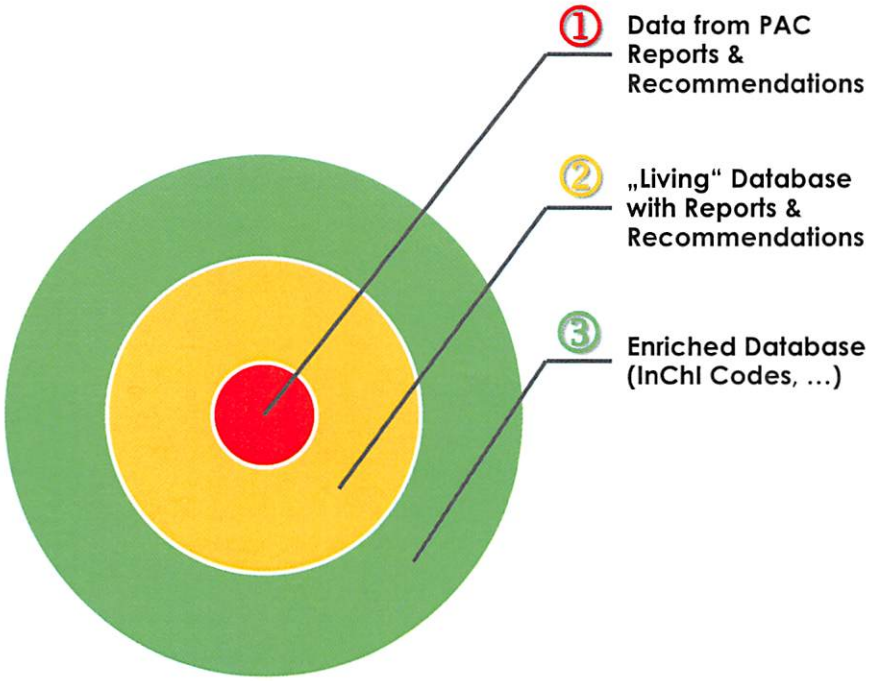
How to find Standards and Recommendations on Internet?

> Searching on IUPAC.org

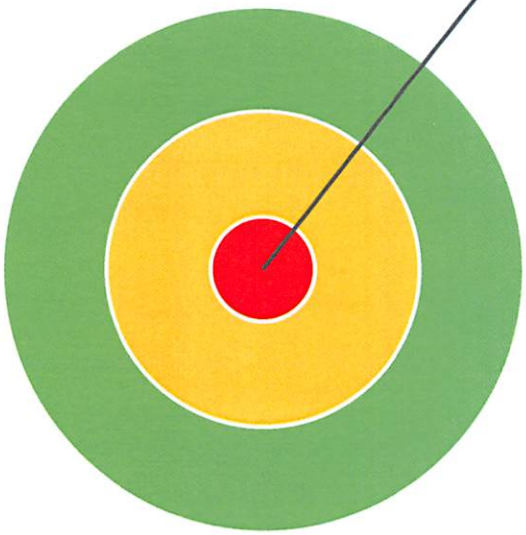
> Searching on google

> Searching in a dedicated database

Options for a Dedicated IUPAC Database



Dedicated IUPAC Database



① **Data from PAC Reports & Recommendations**

Required Actions:

- Conversion of content (pdf to xml)
- Cutting articles into appropriate database entries
- Uploading and hosting data

➡ All tasks performed by DG
All expenses born by DG

Backfile Content – Definitions, Tables, Encyclopedias

	Term	*Definition*
1	ablation	Removal of surface layers of polymers through heat generated by external forces, such as by the action of high-speed hot-gas flow or a laser beam.
2	ablator	A substance that forms a protective surface on a space craft or a missile, and is consumed in an ablation process.
3	abrasion	Removal of surface material from a solid, particularly through the frictional action of solids, liquids, or gases.
4	aging	Processes that occur in a polymeric material during a specified period of time, and that usually result in changes in physical and/or chemical structure and the values of the properties of the material. *Notes* 1. Thermodynamic processes that produce reversible changes in the physical structure of a polymeric material are termed physical aging. 2. If desired, the term aging may be qualified. For example, aging by the action of water or aqueous solutions is termed aqueous aging; aging by the direct or indirect effect of living organisms is termed biologically-induced aging; aging in extraterrestrial space or under conditions that simulate outer-space is termed cosmic aging; aging through contact with ground or soil is termed underground aging; aging caused by the action of an oxidizing agent, especially oxygen, is termed oxidative aging; aging induced by the combined action of light and oxygen is termed photo-oxidative aging, by the action of heat and oxygen thermo-oxidative aging, by the action of heat alone thermal aging, and by the action of visible or ultraviolet light photochemical aging.
5	antagonism	The opposing action of two or more agents that results in an effect smaller than would be expected from the individual action of each. *Note* Used especially for antioxidants and stabilizers.

6	anti-fatigue agent	An agent used to inhibit the fatigue of a polymer.
7	antioxidant	A substance that inhibits or retards oxidation.

Notes
1. Antioxidants acting under specified conditions may be referred to as thermal antioxidants, photo-antioxidants, mechano-antioxidants, etc.
2. See also chain-terminating antioxidant.

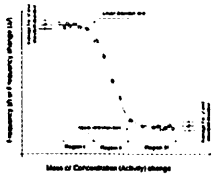


Fig. 1 Calibration plot of a quartz crystal microbalance (QCM) or electrochemical quartz crystal microbalance (EQCM).

tory and preconditioning should be reported. Moreover, parameters like flow rate, stirring rate, temperature, pressure, etc. should be given.

2.2.3 *Drift, standard deviation, hysteresis, and reproducibility: Terms related to short- and long-term stability*

2.2.3.1 Drift

Drift is a slow, nonrandom change of the measured signal of a piezoelectric sensing device under unchanged experimental conditions. The drift is determined by fitting a linear function to the data set collected in a given period of time. The slope of the line of the measured variable *vs.* time is called drift. The random deviation of the measured variable around the fitted line defines the *standard deviation* of the measured variable.

2.2.3.2 Hysteresis

Hysteresis is defined by the failure of the measured signal that has been altered through changes in the ambient conditions (e.g., concentration) to return to its original value when the alteration is removed. Usually, hysteresis has kinetic origins. Therefore, reversible values of the measured signals are expected if sufficient time is allowed for the system to return to its initial condition.

2.2.3.3 Repeatability

Repeatability of the measured signal with the piezoelectric chemical sensor is determined similarly to other sensing devices [23] as repeated experiments under the same ambient conditions (e.g., concentration), but following diverse preceding ambient conditions. The standard deviation of the measured signal (e.g., frequency) in these repeated experiments is called *repeatability*. If hysteresis of the piezoelectric device is distinct, then the repeatability will be poor.

Repeatability is defined by the International Organization for Standardization (ISO) as the precision under repeatability conditions, i.e., conditions where independent test results are obtained with the same method on identical items in the same laboratory by the same operator using the same equipment within short intervals of time (ISO 3534-1) [24]. Repeatability of results of measurements is defined by IUPAC as the closeness of the agreement between the results of successive measurement of the same measurand and carried out under the same conditions of measurement [23].

2.2.3.4 Reproducibility

Reproducibility of the signal measured with the piezoelectric c
experiments under the same conditions in different laborat
International Organization for Standardization (ISO) as the pr
i.e., conditions where test results are obtained with the same m
operators by different operators using different equipment (ISO

2.2.4 *Interfering substance and selectivity*

2.2.4.1 Interfering substance

Interfering substance is any substance, other than analyte, w
measured signal of a *piezoelectric sensing device*. Interfering
"device" interfering substances and *"method" interfering sub*

"Device" interfering substances induce a device respon
change) similar to that generated by the analyte. The presence
category generally results in an apparent increase in the con
These interfering substances interact with the selective surface
as the analytes. At high solution concentrations, even highly di
vice" interference as they are absorbed into the selective surfa
ion exchange, extraction, etc.

"Method" interfering substances interact with the analyt
presence of interfering substances falling into this category de
tations) of the analytes.

2.2.4.2 Selectivity

The *selectivity* of a piezoelectric device refers to the degree to w
species contained in the sample matrix. Selectivity is a measur
sound to the changes to the measured variables (e.g., to the a
compared to the contributions of similar substances. Piezoelec
Typically, selectivity is induced by both a selective surface film
Selectivity can be improved by the discrimination of the total
tributions of individual substances via concentration and time
and kinetically controlled conditions. In fact, an apparent sig
other than the mass increase of the surface film due to uptake

2.2.5 *Response time*

2.2.5.1 Short- and long-time constants

The *short-time constant* is the shortest time required to establi
time is typically about 2.5 cycles of the mass indicating frequ
In practice, the time needed to achieve readings of the frequen
sound by the counter.

The *long-time constant* is determined by the time elapse
(or activity) of the analyte and the establishment of a new stab
long-time constant is controlled by the rate of mass transport
film deposited onto it. If the transport rate is controlled by diff
stant is in the order of d^2/D where d is a diffusion boundary la
ent diffusion coefficient. In polymeric selective surface films,
organization, may occur over an extremely large time span. I
cases, the long-time constant can be viewed as the time requir
quartz crystal and the adjacent film. Its magnitude is of the or

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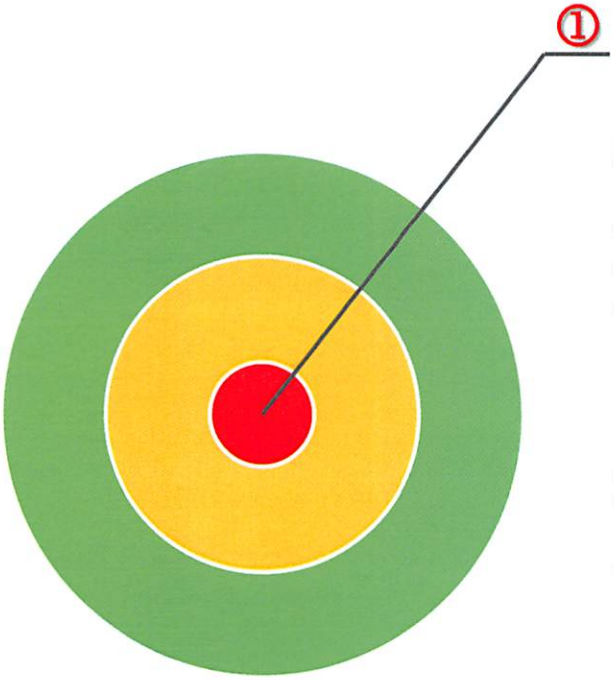

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$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2m} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3m} \end{pmatrix} \tag{8}$$

instead of eq. 5. The number of wavelengths (sensors, detecting channels), m, is usually much higher than the number of species n (here, $n = 3$). Estimation of the coefficients is then carried out by multivariate calibration.

Depending on whether the spectra Y are calibrated as dependent on concentrations X or conversely, on different methods of multispecies calibration, see Fig. 3, can be used.

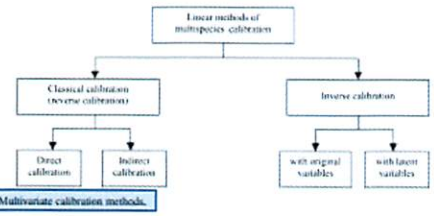

Fig. 3 Multivariate calibration methods.

2. CLASSICAL MULTIVARIATE CALIBRATION

Classical multivariate calibration represents the transition of common single species analysis from one dependent variable (measured value, or measurand) to m dependent variables, e.g., wavelengths or sensors which can be simultaneously included in the calibration model. It is possible to determine $n \geq 1$ species in the analytical system. The classical linear calibration [2] is therefore represented by the generalized matrix relation

$$Y = X A \tag{9}$$

where Y is the $(p \times m)$-matrix of dependent variables (e.g., absorbances at m wavelengths or responses at m sensors), X is the $(p \times n)$-matrix of independent variables (e.g., concentrations of n species), and A is the $(n \times m)$-matrix of the calibration coefficients, often called "sensitivity matrix" [3–5]; p is the number of calibration standards (mixtures), which is identical with the number of spectra or similar measurements. The rows of the matrix correspond to the spectra of the pure species, which can be directly measured or indirectly estimated.

Direct calibration can be applied when the calibration coefficients are known, otherwise—in the case of *indirect calibration*—the calibration coefficients are computed by means of experimentally estimated spectra-concentrations relations.

Classical calibration procedure can only be applied when all the species that contribute to the shape of the spectra are known and can be included into the calibration. Additionally, there is the constraint that no interactions between the analytes and other species (e.g., solvent) or effects (e.g., of temperature) should occur.

The analytical values (concentrations) are estimated by

$$\hat{X} = Y A^{+} \tag{10}$$

where A^{+} is the so-called Moore–Penrose generalized pseudo inverse

$$A^{+} = (A^{T}A)^{-1}A^{T} \tag{11}$$

with the same dimensions $(m \times p)$ as the transposed matrix.

In case of baseline shift, the sensitivity matrix in eqs. 9 and 10 must be complemented by a vector I:

$$A = (I\ A) = \begin{pmatrix} 1\ a_{11} & \cdots & a_{1m} \\ \vdots\ \ \vdots & \ddots & \vdots \\ 1\ a_{p1} & \cdots & a_{pm} \end{pmatrix} \tag{12}$$

Instead of the addition of the I-vector the calibration data may be centered ($y_i = \bar{y}$ and $x_i = \bar{x}$, respectively). Even if the spectra of the pure species cannot be measured directly then the A-matrix can be estimated indirectly from the spectra *provided that all species of the analytical system are known*

$$\hat{A} = (X^{T}X)^{-1}X^{T}Y \tag{13}$$

Note: Instead of the symbol A and the term sensitivity matrix also the symbol K (matrix of calibration coefficients, matrix of linear response constants, and so on) is used. Because of the direct metrological and analytical meaning of the sensitivities a_{ij} in the A-matrix, the term *sensitivity matrix* is preferred.

For inversion of the matrix $X^{T}X$, it is necessary that a sufficient number of spectra for different concentration steps have been measured. The concentration vectors must vary independently from each other. For this reason, experimental design [8] should be used. In the case that the preparation of samples of defined composition is impossible, then the samples should be selected as representative and as uncorrelated as possible (natural design [3]).

The prediction of analytical values X according to the classical indirect calibration model follows eq. 10

$$\hat{X} = Y \hat{A} \tag{14}$$

The desired independence between the variables of the different analytical signals corresponds directly with the *selectivity* of the analytical system [6,7]. In the case of multivariate calibration, the selectivity is characterized by means of the condition number

$$\mathrm{cond}(A) = \|A\| \cdot \|A^{-1}\| \tag{15}$$

where $\|A\|$ is the matrix norm of A and $\|A^{-1}\|$ the norm of the inverse matrix. The matrix norm of A is calculated from $\sqrt{\lambda_{max}}$, the square root of the largest eigenvalue λ_{max}, and the norm of A^{-1} from the reciprocal square root of the lowest eigenvalue λ_{min}:

$$\mathrm{cond}(A) = \sqrt{\lambda_{max}} \cdot \frac{1}{\sqrt{\lambda_{min}}} \tag{16}$$

Equation 14 is valid for exactly determined systems ($m = n$). In the case of overdetermined systems, $m > n$, the condition number is given by

$$\mathrm{cond}(A) = \sqrt{\mathrm{cond}(A^{T}A)} \tag{17}$$

If systems are well conditioned, the selectivity is expressed by condition numbers close to 1.

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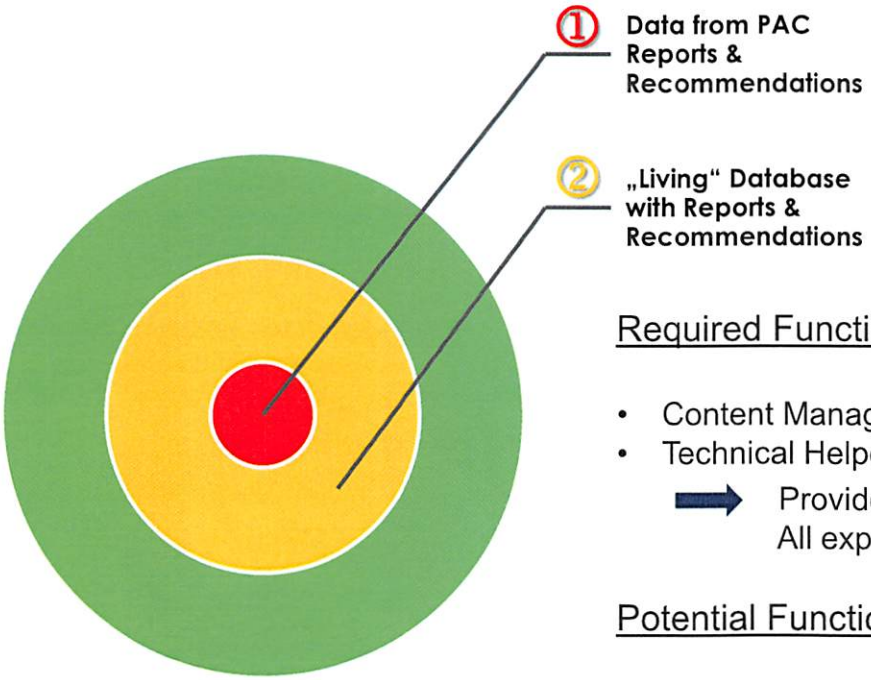

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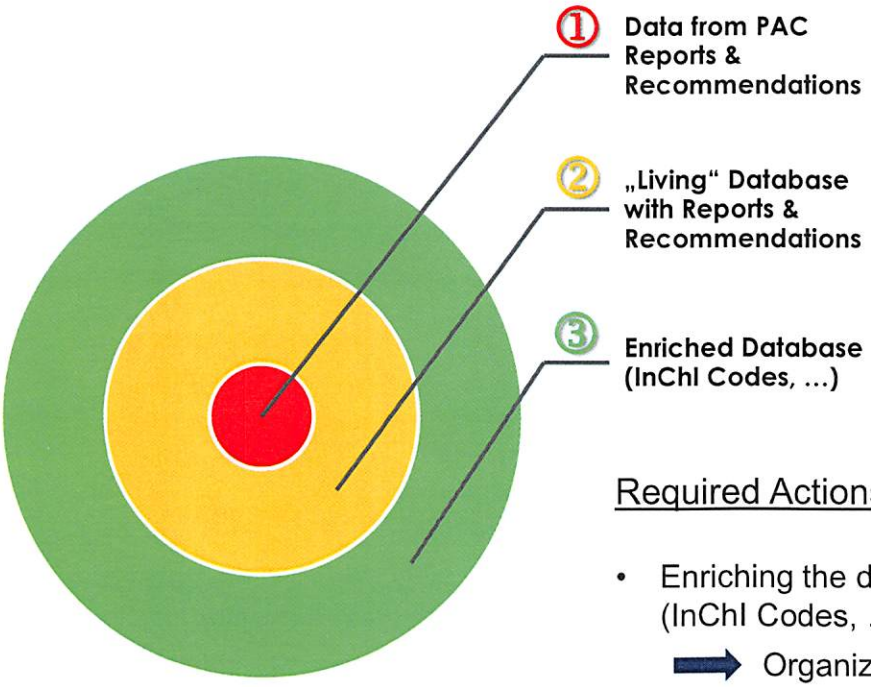

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Author(s): Klaus Danzer, Matthias Otto, and Lloyd A. Currie

Pure Appl. Chem., Vol. 76, No. 6, pp. 1215-1225, 2004

Article type: IUPAC Technical Report

Keywords: Chromatography; Error diagnosis; Sample preparation

Guidelines for Calibration in Analytical Chemistry, Part 2: Multispecies Calibration

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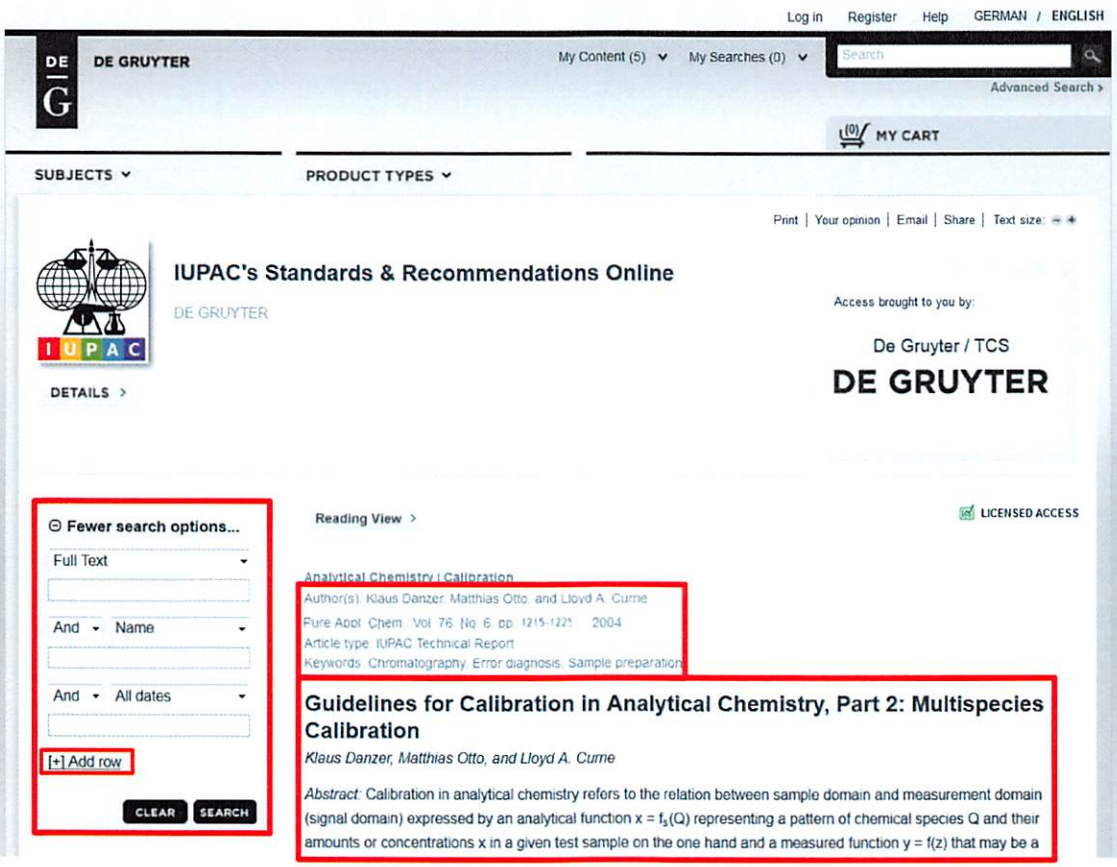

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Source: Piezoelectric Chemical Sensors. Pure Appl. Chem. Vol. 76, No. 6, pp. 1139–1160, 2004

Article type: Definition

Keywords: Hysteresis, Piezoelectric measurement

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⊖ Further Reading

[1] Physical Chemistry > Piezoelectricity > Repeatability

[2] Physical Chemistry > Piezoelectricity > Response Time

[3] Figure "Calibration plot of a quartz crystal microbalance (QCM) or electrochemical quartz crystal microbalance (EQCM)."

[4] Physical Chemistry > Piezoelectricity > Short- and long-term stability

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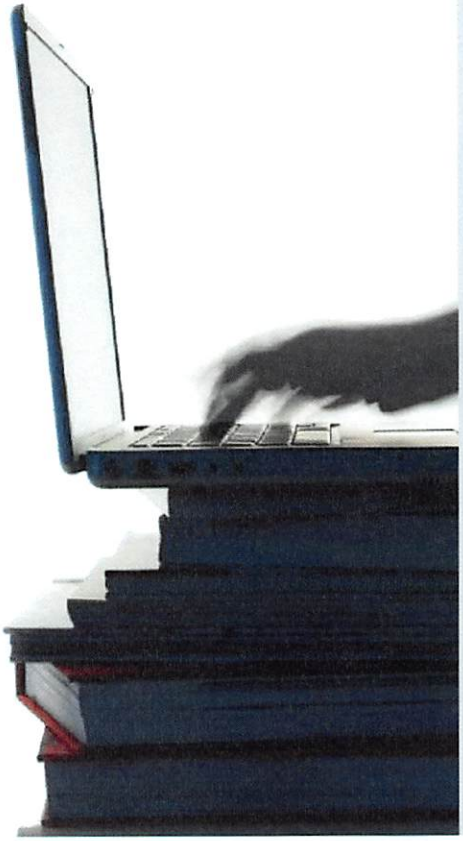

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