

From the past to the future: <Calibration certificates for radioactivity @PTB>

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Abstract – The XML-DCC (Digital Calibration Certificate) was developed at PTB for use in a variety of applications. This contribution refers to the field of radioactivity. It involves representing the calibration item, the measurement method, the detected nuclides and the measured activity digitally, and referring them to a specific reference time.

While this specific schema is in the tradition of 100 years of calibration certificates as defined by Hans Geiger, it also points towards the future by employing a machine-interpretable digital representation of the SI in the field of ionising radiation.

I. INTRODUCTION

A. Measuring radioactivity: A new field evolves

Accurate measurement has had an institutional home in Germany since 1887. The approval of the first budget for the Physikalisch-Technische Reichsanstalt (PTR) on 28 March 1887 marked the birth of the first large-scale state research institution and the beginning of a success story. The industrialist Werner von Siemens and the scientist Hermann von Helmholtz are regarded as the PTR's founding fathers. Thanks largely to their vision and persistent commitment, the German Reichstag finally approved the PTR's first annual budget on 28 March 1887. This laid the foundations for the first state-funded, non-university, large-scale research institution committed to basic research, free of material interests, and to supporting industry with current problems [1].

At the beginning of the 20th century, under the presidency of Emil Warburg, the PTR increasingly focused on the so-called 'New Physics'. This included X-rays, new ideas about atomic structure, Einstein's special theory of relativity, and quantum physics based on the black body and electron properties. The renewal of the PTR's research content was achieved above all by outstanding researchers such as Hans Geiger, who set up the PTR's first radioactivity laboratory and quickly turned it into a world-class scientific facility.

By the early 1900s, the effects of radioactivity were already well understood, forming the basis for the development of detectors that are still in use today. For

example, radiation can blacken a photographic plate, generate ions in gases, and trigger flashes of light, known as scintillations, when it hits certain materials.

Geiger's counting methods have a long history. Not only did they lead to the invention of various detectors, such as the counting chamber with longitudinally entering beams in the proportional range (created by Rutherford and Geiger in 1908), the sphere counter (created by Rutherford and Geiger in 1912), the tip counter (created by Geiger in 1913), the Geiger-Müller counting tube (created in 1928), and the self-extinguishing counting tube (created by Adolf Trost in 1936), but they also led to the development of recording and amplifying devices [2].

The invention of the Geiger-Müller counter tube in 1928 represented a new development in the field of ionising radiation detectors. The construction of electronic amplifiers for this tube, however, was driven forward by Geiger's students and the working groups of Walther Bothe and his colleagues in Germany, as well as various institutes in Italy, France, the USA and England.

In 1912, Hans Geiger was appointed head of the newly founded Laboratory for Radioactivity at the Physikalisch-Technische Reichsanstalt in Berlin. He had previously spent five years in Manchester as a research assistant to Ernest Rutherford, gaining experience in the new scientific field of radioactivity research. In Berlin, his role was to measure the activity of radioactive materials, maintain radioactive measurement standards, and develop new measurement methods in accordance with the PTR's mandate.

Geiger expanded the laboratory into a central testing centre for radioactive standards. By the time he left the PTR in 1925 to take up a professorship in experimental physics at Kiel University, his team had determined the activity of eighty-five radium standards, six ore samples, five radium compresses, two radioactive ointments, a radioactive bread additive and a radioactive cat fur.

Radioactivity was one of the new discoveries that attracted the interest of scientists and aroused the enthusiasm of the press and public alike. In 1896, Henri Becquerel became the first person to detect radiation emitted by uranium in Paris. By the start of the First World War, its basic properties were well understood, although they were still the subject of much controversy and debate in scientific circles. Other radioactive elements had been discovered,

and a distinction had been made between alpha, beta and gamma rays. The first radioactive decay series had been established, and the radioactive decay law had been formulated. Radioactive decay was also recognised as a random process. Important scientific discoveries were based on investigations involving radioactive rays, including the discovery of the atomic nucleus and isotopes, and then neutrons and nuclear fission in the 1930s.

In the age of digitalisation and Industry 4.0, it is clear that paper-based calibration certificates are no longer sustainable. With an increasing number of sensors and devices requiring calibration, printing, mailing, storing and processing paper calibration certificates not only creates a bottleneck, but also increases the chance of errors and mistakes at each step in the chain. Electronic (digital)

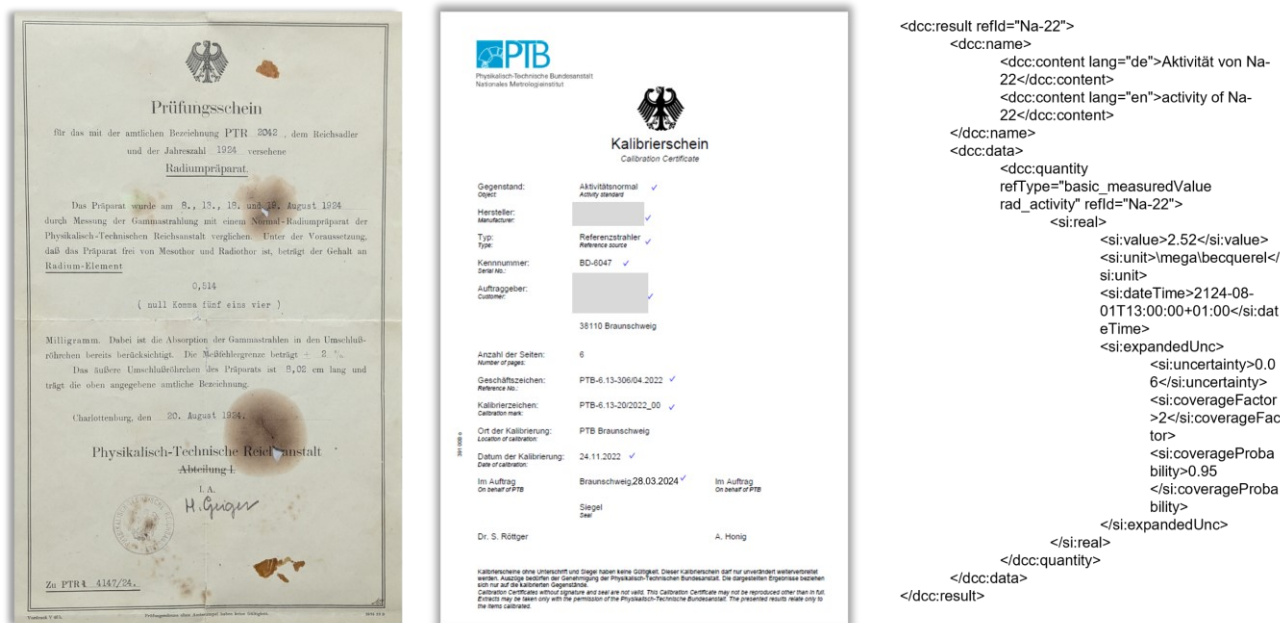


Figure 1: Calibration certificate (left) from 1924 (Hans Geiger), Typical calibration certificate (middle) from 2024 (Anja Honig) and a possible structure for a machine interpretable activity statement (right) maybe before 2124.

Radioactivity research in the early 20th century gave rise to many new fields of study, including atomic, nuclear and neutron physics, radiochemistry, radiobiology and radiology. From the time of Geiger to the present day, the history of the Laboratory for Radioactivity at the Physikalisch-Technische Bundesanstalt has been continued. For over 100 years, the results have been passed on using calibration certificates. Even if these have changed over the course of time, the field of radioactivity has its own requirements, as can be seen in the historical, current and future calibration certificates, a possible digital calibration certificate (DCC) – see Figure 1.

The information included in the radioactivity calibration certificate became more detailed and included even fundamental and nuclear data used and needed for further usage of the calibration data. Since this data might even change with new developments in physics or better experiment with smaller uncertainties, newer fundamental data might even influence the calibration results afterwards.

calibration certificates mitigate these problems. We need to distinguish between different levels of "digitalness" [3]. Here we focus on calibration certificates of level three or higher according to the extended utility model of [3] - i.e. certificates with machine-readable (level 3), machine-interpretable (level 4) and/or machine-executable (level 5) content.

Several formats for digital calibration certificates and similar documents have been proposed, including some that append machine-interpretable data to human-readable PDF documents (see e.g. [4, 5]). Other approaches focus solely on having a machine-interpretable document such as XML (Extensible Markup Language) [6]. The advantages of using pure XML over PDF-with-XML (or PDF-with-JSON [Portable Document Format; JavaScript Object Notation]) are that no additional steps are required to extract the machine-readable data from the PDF, and there is no potential for a mismatch between human-readable and machine-readable documents. On the other hand, XML certificates require additional information to enable customers to extract the information in a meaningful way, for example in the form of Extensible

II. DIGITAL CALIBRATION CERTIFICATES

Stylesheet Language Transformations (XSLT) style files. These would need to be distributed with the calibration certificate or hosted online.

We decided to implement calibration certificates in the XML format developed and hosted by PTB (Physikalisch-Technische Bundesanstalt), which is described in the next section.

III. PTB DCC

In this document, the XML-based format for digital calibration certificates developed at PTB is referred to by the abbreviation "DCC" [6, 3]. This DCC is based on an XML schema in XSD format. It is maintained and hosted by PTB¹. The current release is version 3.3.0². The schema is complemented by a vocabulary database³, good practice examples⁴, and usage guides (e.g., [7, 8]). The vocabulary database and usage guides are developed and maintained by technical committees (TCs) within DKD⁵, the German Calibration Service at PTB.

XSLT style sheets may be used to render XML DCCs for human readability [9]. External files, including a human-readable representation of the document, may also be included in the DCC (where permitted by the schema) as base 64 binary strings.

The DCC schema depends on the D-SI schema [10] for the representation of physical quantities such as measurement results, and on a modified version of the W3C xmldsig schema for digital signatures, and otherwise stands alone. Further harmonisation and modularisation of the digital quality infrastructure has been proposed, which would involve the introduction of a generic schema "DX" on which the schemas for the DCC and other documents, such as Digital Reference Materials or Digital Test Certificates, could be based. [11].

Each DCC document contains different sections (and an optional signature(s)) which are: administrative data, measurement results, comments and included documents.

Many elements of the DCC can have the optional "refType" attribute. RefTypes allow information to be stored and extracted in a harmonised way, making DCCs truly machine-interpretable. To that end, each calibration community maintains a list of community-specific refTypes with definitions and usage notes. Currently, PTB hosts a database of refTypes⁶. RefTypes consist of a prefix and base, separated by an underscore. The prefix indicates

the domain or metrological area, while the prefix "basic" is reserved for refTypes used by several communities. Only the combination of prefix and base uniquely identifies a refType.

Future versions of the DCC schema⁷ will support definitions of measurands in external vocabulary databases, reducing the need for measurand-specific refTypes.

IV. DCC FOR RADIOACTIVITY

The steps to implement a DCCs for a new calibration community are: identifying community-specific information that needs to be represented in a DCC. This must then be prepared as: A list of refTypes (with definitions and usage notes) to encode the information in a machine interpretable way. Ideally, all this would be documented in a DKD expert report or similar publication.

We are currently in the process of implementing DCCs for radioactivity, that is, the calibration of radionuclide standards with calibrated activity (or activity concentration), and the calibration of detectors that measure activities in Becquerel and related quantities. Since this is very much work in progress - input and feedback from the community is very welcome and necessary at this stage.

B. Prefixes and refTypes

Ionising radiation metrology, which includes the BIPM service categories of dosimetry, radioactivity, and neutron measurements, is part of DKD TC 2, "high frequency and optics". The structure of refTypes and refType prefixes for the fields of metrology included in TC 2 are currently under discussion. In this text, we use the symbol "Y_" as a placeholder for the future refType prefix that will cover the new refTypes for radioactivity.

C. Calibration Item

Calibration items in the field of radioactivity comprise devices and artefacts. Artefacts are available in different shapes including point-like sources, area sources, liquid solutions, volume samples in complex matrices, and gaseous samples. The simplest case: A single-nuclide radioactivity standard provided in the form of a liquid solution, characterised in terms of its activity. Other cases, as well as DCCs for devices measuring radioactivity, will have to be considered in future works.

¹ See <https://www.ptb.de/dcc/>

² <https://www.ptb.de/dcc/dcc.xsd>

³ <https://digilab.ptb.de/dkd/refType/vocab/>

⁴ https://wiki.dcc.ptb.de/en/gp_home

⁵ <https://www.ptb.de/cms/en/metrological-services/dkd.html>

⁶ <https://digilab.ptb.de/dkd/refType/vocab/>

⁷ <https://www.ptb.de/dcc/v3.4.0-rc.1/>

The definition of the calibration item(s) is part of the administrative data section of the DCC. In general, a DCC may have multiple calibration items (e.g., a set of weights). In the field of radioactivity, each calibration certificate commonly only covers a single calibration item. Still, we propose to assign an `id` attribute to the calibration item, to keep this structure as general as possible.

We propose at least the following information to be included:

- An `id` attribute to uniquely identify the calibration item within the DCC.
- A `refType` attribute specifying the type of sample.
- Child elements `name`, `description`, and `manufacturer` filled according to the DCC schema.
- The `identifications` element should contain at least one identification with `refType` `basic_serialNumber`, with a value corresponding to the serial number that the physical source is labelled with. Further identifiers may be listed.
- Physical properties of the calibration item of interest to the customer are listed under the `itemQuantities` element. These depend on the source type. Simple physical quantities, such as the mass of the sample solution, can be listed immediately, using the embedded D-SI schema. We propose to specify complex properties, such as the composition of the solution, within the `statements` element, and use the `refId` formalism to refer to them from the calibration item description.

D. Further definitions

The `statements` element within the administrative data section may contain general statements about the calibration laboratory or calibration certificate. This is also the element where further detailed information shall be placed that can then be referenced from elsewhere in the DCC. We propose to place definitions of complex properties of the calibration item here.

All radionuclides referenced in the results section should be listed, even if they were not detected in the sample. We propose to identify nuclides unambiguously by their InChI string `InChI` and isomeric state as given by the J (nuclear spin), π (parity), and n (energy level) quantum numbers. Additional information of interest to the customer may be listed here, such as the half-life to be used when converting the activity to a different reference time. Another option currently under consideration is to reference an external database of radionuclides.

E. Measurement results

For a single-nuclide radioactivity standard, the quantity of interest is typically the activity at a given reference time. This quantity will be listed in the measurement results section in the form of a `si:real` quantity, whose child elements contain `value`, `unit`, and `measurement uncertainty`. It is important that the activity value be unambiguously associated to the reference time for which it is valid. We propose to list the reference time in the `si:dateTime` child element of `si:real`. The element `si:dateTime` contains a time stamp in ISO 8061 format [12], with the timezone defined by its offset to UTC.

An example for a single-nuclide measurement result contains the `refTypes` `basic_measuredValue` and `Y_activity`, in combination with the reference back to the previously defined `nuclide_Am241`, identify this result as the measured activity of Am-241, with value e.g. 2.52 MBq at 13:00 Central European Time (UTC+1) on August 1, 2022. For mixture samples comprising multiple radionuclides, we propose to add one `result` element per nuclide within the same `measurementResult` element.

The DCC schema specifies a general structure for each of the metadata elements. However, the details of how to implement information in a manner that is machine readable in the field of radionuclide metrology is still under development.

We propose to define `refTypes` for all measurement quantities needed for radionuclide metrology calibration certificates, such as activity, activity per mass, activity per volume, and activity ratios. A full list of proposed `refTypes` is in preparation.

We also propose to define `refTypes` for the decision threshold and limit of detection, to quantify the absence of impurities. These would be used in conjunction with a `refType` defining a quantity, such as `Y_activity`.

V. SUMMARY AND CONCLUSION

Digital calibration certificates (DCCs) are becoming increasingly relevant in metrology, quality assurance, and compliance-driven industries due to their efficiency, traceability, and interoperability.

Main advantages are:

1. **Enhanced Traceability and Authenticity:**
Digital certificates can be cryptographically signed, ensuring they are tamper-proof and traceable to the issuing authority. This boosts trust and simplifies audits.
2. **Automation and Integration:**
DCCs can be directly integrated into laboratory information management systems (LIMS), and

- quality control platforms. This enables automated updates, flagging of overdue calibrations, and better lifecycle management of instruments.
3. **Reduced Errors and Administrative Load:**
Manual transcription from paper certificates is error-prone. DCCs eliminate this by using standardized formats (e.g., XML, JSON, or formats aligned with the Digital Calibration Certificate standard by PTB), reducing human error and time spent on data entry.
 4. **Interoperability and Standardization:**
Efforts like the SI Digital Framework, D-SI (Digital System of Units), and PTB's Digital Calibration Certificate initiative aim to harmonize DCCs globally. This facilitates cross-border calibration recognition and cooperation between labs and regulatory bodies.
 5. **Support for Industry 4.0:**
DCCs are foundational for smart manufacturing and the Industrial Internet of Things (IIoT), where equipment needs to autonomously verify calibration status to ensure process accuracy in real time.
 6. **Regulatory and Compliance Pressure:**
Regulatory agencies and quality standards (e.g., ISO/IEC 17025) increasingly expect digital traceability. DCCs support easier compliance with such requirements.
 7. **Sustainability and Cost-Effectiveness:**
Eliminating paper and reducing manual processes align with sustainability goals and reduce long-term operational costs.

In summary, digital calibration certificates are becoming essential for modern, automated, and data-driven operations for calibration laboratories, research institutes and industry. They're not just a convenience but a strategic enabler for digital transformation in metrology and beyond. It is therefore essential to adopt them in every field of metrology.

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