Metrological Traceability
&
Measurement Uncertainty

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on

Metrology in Chemistry (MiC)

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WIEN
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Comparabililty of results of chemical amount measurements is needed in:

- determination of the value of goods in border-crossing trade
- implementation of border-crossing environmental regulations (water, air, soil)
- verification of safety of border-crossing food
- border-crossing use of clinical measurements
- application of forensic science across borders
- detection of border crossing adulterated products
- verification of authenticity of border-crossing products

Measurement results can only be *compared* if they have been obtained against a common "stated reference".

PDB01130

What is traceability ?

PDB99136

Key 1 for Metrology in Chemical Measurement:

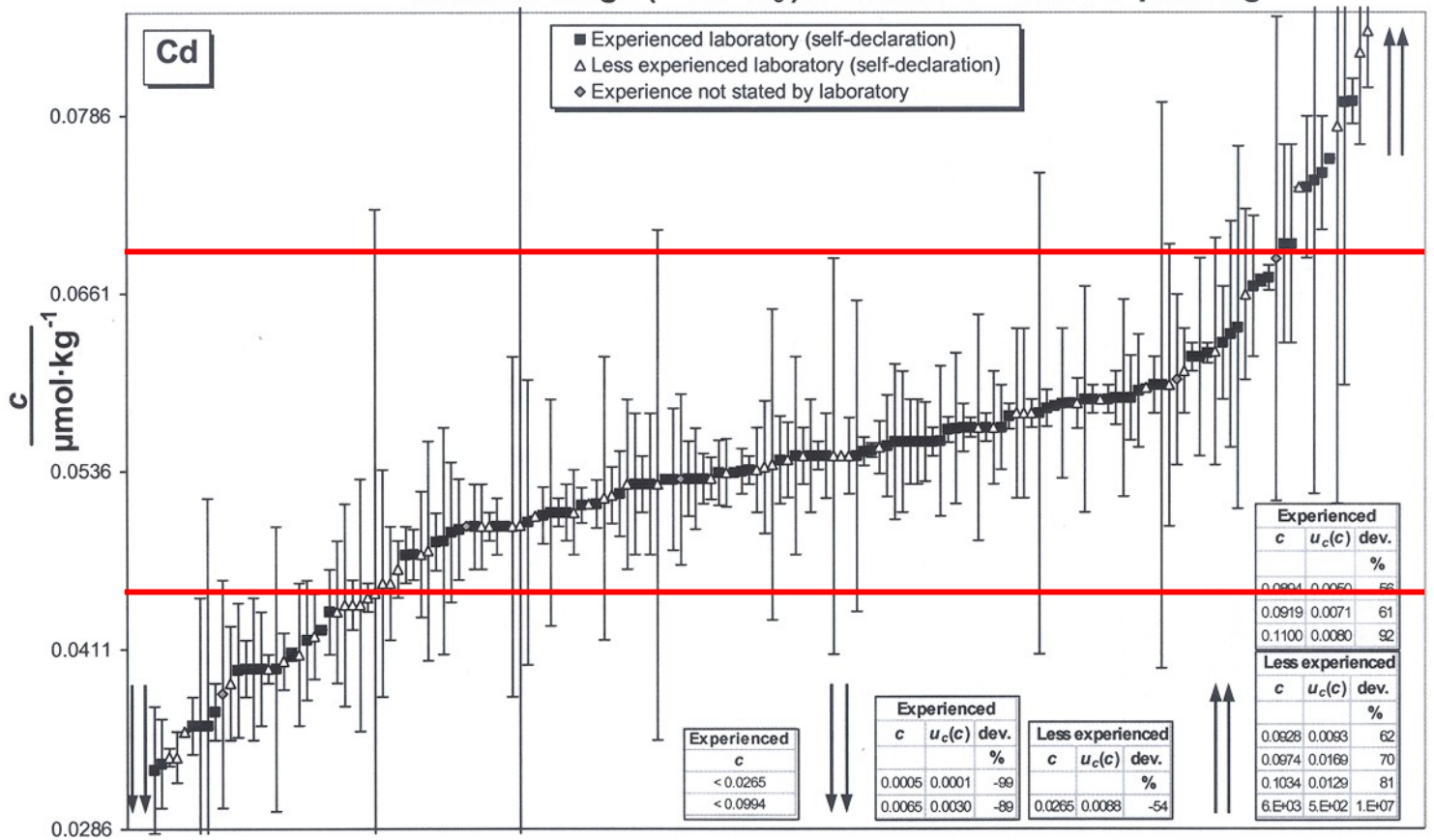
Traceability

property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties

VIM 1993

IMEP- 6 : Trace elements in water : synthetic water (sample " 1")

Certified range (= ± 2 u_c) : 0.056 1 - 0.058 3 µmol·kg^{-1}



Experienced
c
< 0.0265
< 0.0994

Experienced		
c	u_c(c)	dev. %
0.0005	0.0001	-99
0.0065	0.0030	-89

Less experienced		
c	u_c(c)	dev. %
0.0265	0.0088	-54

Experienced		
c	u_c(c)	dev. %
0.0919	0.0071	61
0.1100	0.0080	92

Less experienced		
c	u_c(c)	dev. %
0.0928	0.0093	62
0.0974	0.0169	70
0.1034	0.0129	81
6.E+03	5.E+02	1.E+07

172 results from all laboratories arranged by ascending values.

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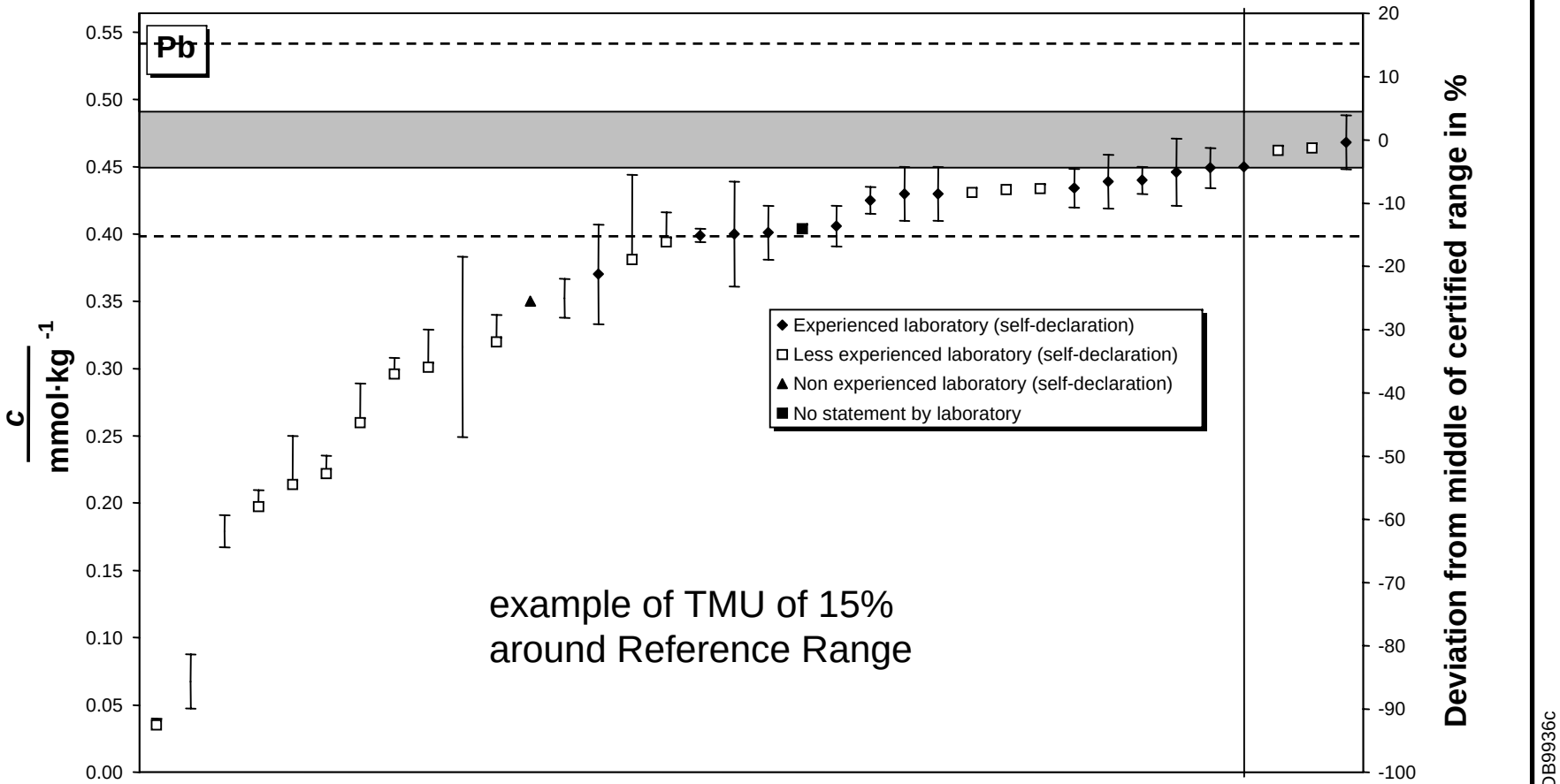
IMEP- 10 : Trace Elements in Polyethylene

Certified range [$U = k \cdot u_c$ (k =2)]: 0.449 - 0.491 mmol·kg^{-1}



Results from all participants.

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Key 2 for Metrology in Chemical Measurement:

Uncertainty

Type A evaluation:

method of evaluation of a standard uncertainty by the statistical analysis of a series of observations

Type B evaluation:

method of evaluation of a standard uncertainty by means other than the statistical analysis of a series of observations

ISO BIPM GUM 1993

Current revision of the VIM:

1. improvement through decrease of
   - inconsistencies:
     - internal within VIM
     - internal within ISO Guides and Standards
     - external between ISO- and non-ISO documents

   - unclarities, since: ...
     - no clarity
     - ↓
     - no understanding
     - ↓
     - no agreement possible

       in trade
       in implementation of EC Directives
       in mutual acceptance of measurement results

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The (revision of VIM-2, yielding) VIM-3

2. takes on board chemical measurement

3. uses the “substitution principle”:
   any definition of a term for the definition of a concept must be capable of replacing that term in another definition

4. uses GUM, even if a number of GUM terms for concepts is already up for refinement in “GUM-2” (which is not yet planned)

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The (revision of VIM-2, yielding) VIM-3

5. obviously still suffers from a carry-over from 20th - and even 19th - century thinking
6. contains “counting quantities is an implicit base quantity”
7. makes uncertainty part of the measurement result
8. defines “metrological traceability”
9. defines “traceability to the SI”
10. defines “measurand” as a “quantity intended for measurement
11. includes thinking in terms of “chemical measurement” (for the first time !)
12. includes examples of chemical measurements (for the first time)
13. introduces “calibration hierarchy”
14. gives a definition of “comparability”
15. specifies any “CRM” as a “measurement standard”

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Some examples justifying a revision:

example 1: “measurand”

example 2: “measurement result”

example 3: “metrological traceability”

example 4: “measurement uncertainty”

example 5: “measurement unit” and “measurement scale”

example 6: “metrological comparability”

example 7: “target measurement uncertainty”

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Key 2: Measurement uncertainty (MU)

Measure of doubt about the measurement result.

1. an uncertainty of a measurement result is generated automatically from the very moment one starts measuring

2. measurement uncertainty is obtained through an evaluation process:

   - type A evaluation
   - type B evaluation

   (calculation comes only in at the end, after evaluation)

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3. understanding the process called measurement, is a prerequisite for evaluation of measurement uncertainty

4. measurement uncertainty should be small enough for the intended use but, need not be smaller (it *can*, but *need not* be smaller)

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Uncertainty is new to chemists !

- absent in most university curricula
- ISO/BIPM guide (GUM): only 12 years old !
- Repeatability is thought of as uncertainty
- Terra incognita !

PT0201

ISO/BIPM-guide:
the new approach

re-establishes the responsibility
of the analyst because
“evaluation of uncertainty”
is a thinking process !

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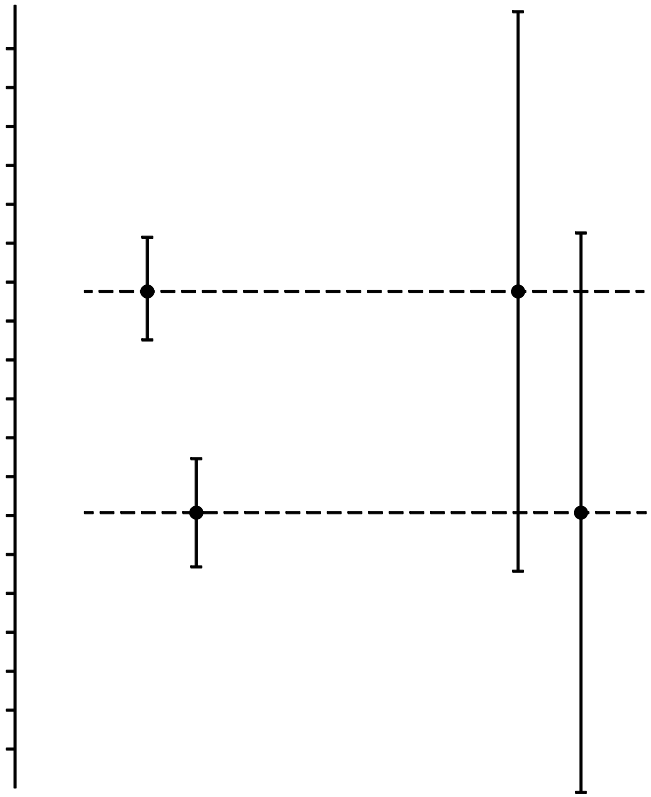

DISCREPANCY → PROBLEM

NO DISCREPANCY → NO PROBLEM

DISCREPANCY PROBLEMS CAN BE CAUSED UNNECESSARILY BY LACK OF "ORTHODOX" UNCERTAINTY ASSESSMENT

PDB9952

Fresenius J Anal Chem (2000) 368:567–573 (Continued from 2002 as Anal Bioanal Chem)

SPECIAL ISSUE PAPER

Paul De Bièvre · Philip D. P. Taylor

"Demonstration" vs. "designation" of measurement competence: the need to link accreditation to metrology

PDB04001

Metrology

creates

respect for the law

Lack of Metrology

creates

contempt of the law

PDB9833

The task is
to demonstrate
the authority of the result
of the measurement.

This needs
underpinning (“Untermauerung”)
of the measurement result
in order to lead to
the necessary credibility.

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Key 3: Target Measurement Uncertainty (TMU)

Range of uncertainties from which the analyst claims it contains a specified "traceable" value for the measurand

1. The analyst needs a "target" for the measurement uncertainty he must attempt to achieve
2. A TMU usually originates from a requirement put down by regulatory authorities

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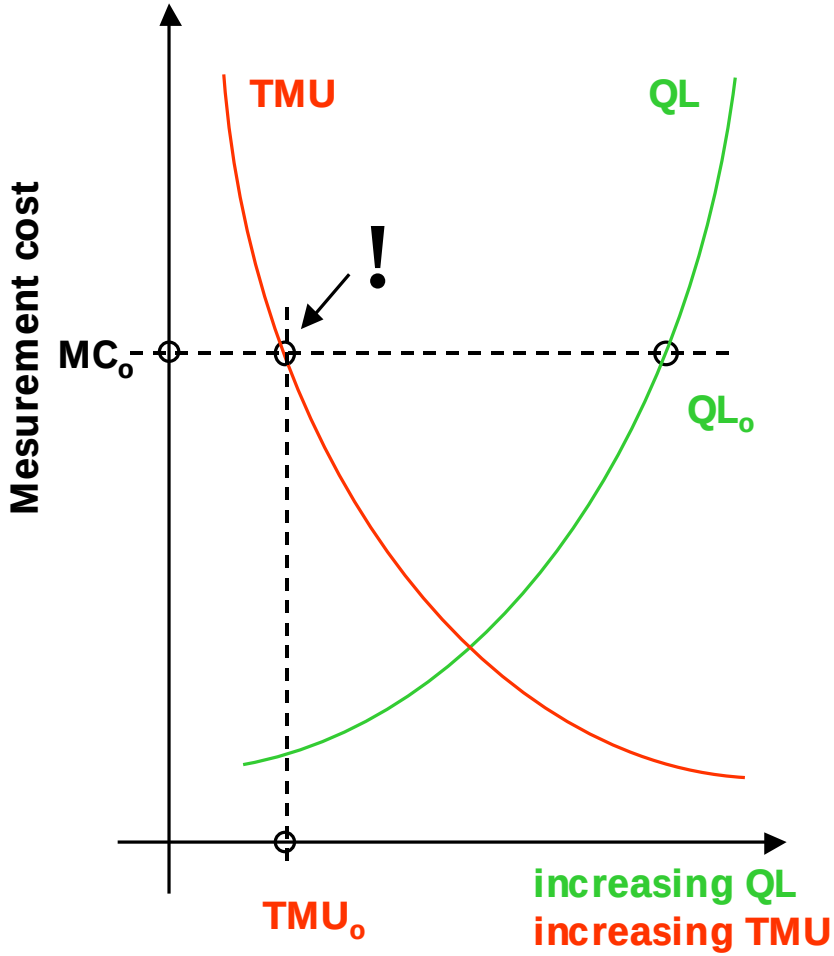

PDB2003077

Metrology in chemistry : The Hubble telescope ...

BEFORE

AFTER

= the ‘spectacles’ of the analytical chemist

PDB01144