Quality assurance of analytical measurements of CO_2 parameters

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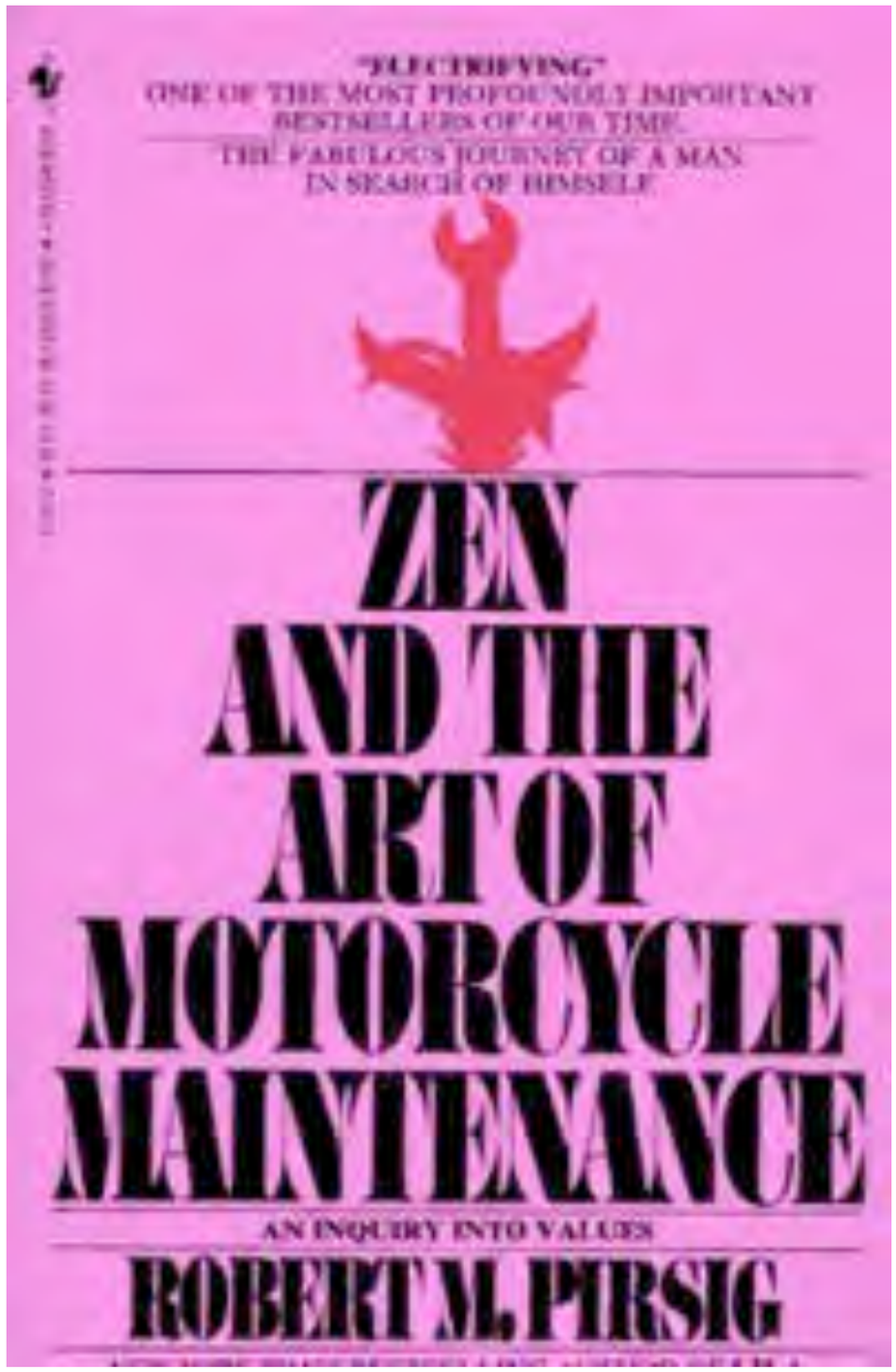
Quality assurance constitutes the system by which an analytical laboratory can assure outside users that the analytical results they produce are of proven and known quality.

So what is quality?



The Metaphysics of Quality

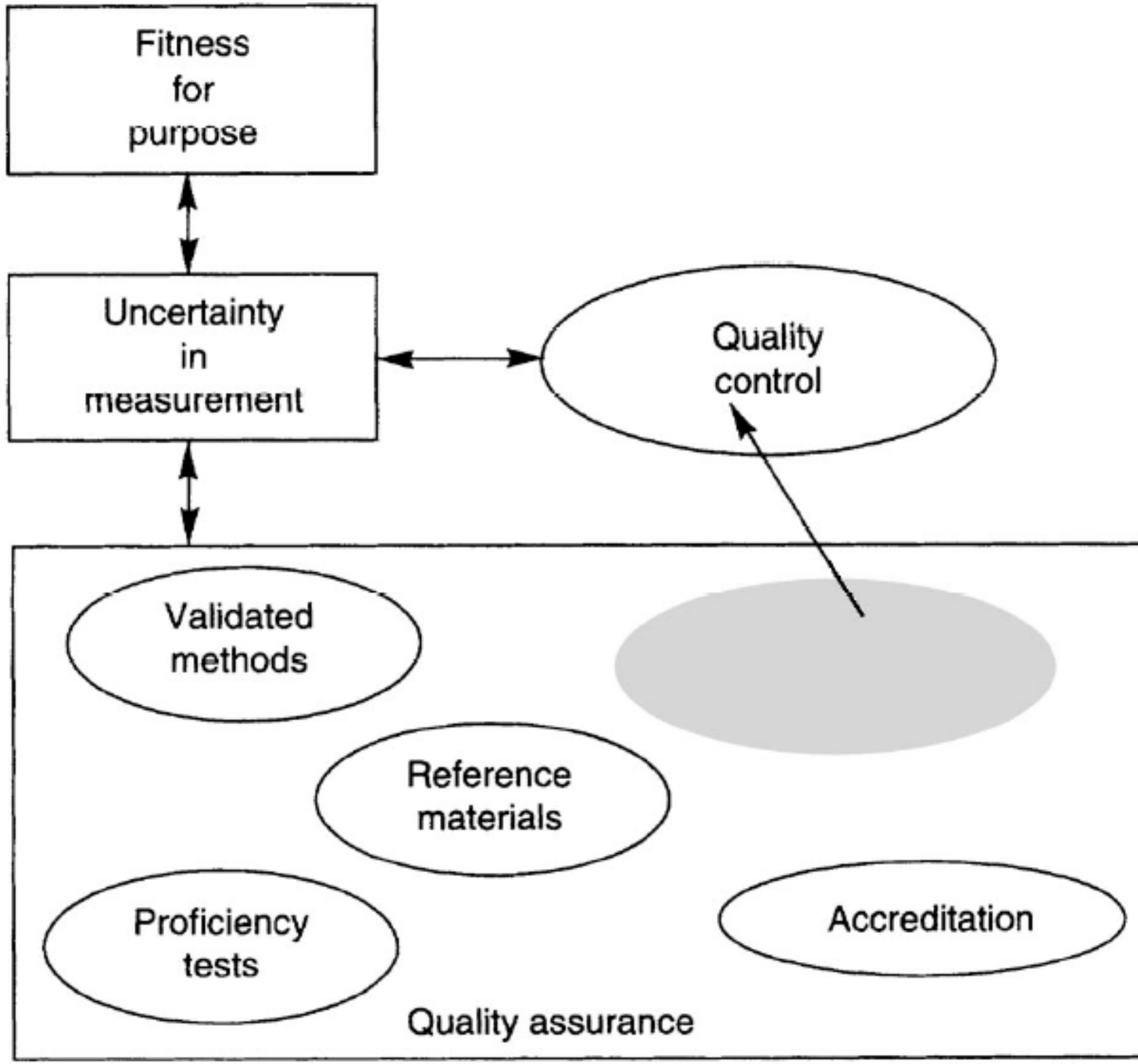
So what is quality?

Quality is fitness for purpose.

Fitness for purpose: the property of data produced by a measurement process that enables a user of the data to make technically correct decisions for a stated purpose.

Fitness for purpose therefore refers to the magnitude of the uncertainty associated with a measurement in relation to the needs of the application area.

Has implications for the level of resources needed!


Fitness for purpose
Uncertainty in measurement
Quality control
Validated methods
Reference materials
Proficiency tests
Accreditation
Quality assurance

Two facets of quality assurance

Quality control: The overall system of activities whose purpose is to control the quality of a measurement so it meets the need of users. The aim is to ensure that data generated are of known accuracy to some stated, quantitative, degree of probability, and thus provide quality that is satisfactory, dependable, and economic.

Quality assessment: The overall system of activities whose purpose is to provide assurance that quality control is being done effectively.

Effective quality control requires

- Well-trained people
- Suitable and properly maintained equipment and facilities
- Well documented, validated, measurement procedures
- Regular and appropriate use of reference materials to evaluate measurement performance
- Appropriate documentation of measurements and associated quality control information

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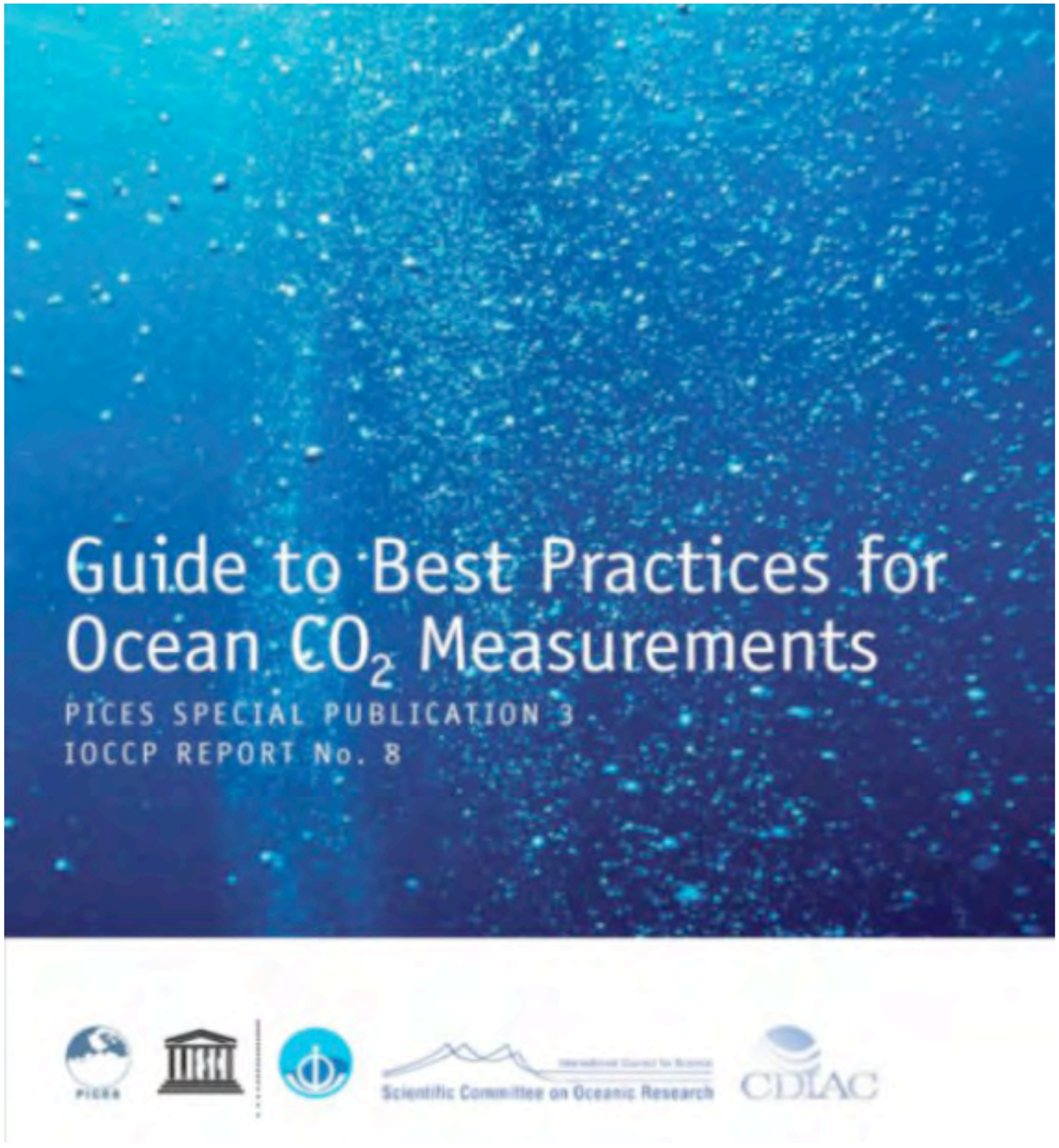


http://cdiac.ornl.gov/oceans/Handbook_2007.html

Reference materials

Reference materials are stable substances for which one or more properties are established sufficiently well to calibrate a chemical analyzer or to validate a measurement process.

Ideally, such materials are based on a matrix similar to that of the sample of interest, in this case sea water.

The most useful reference materials are those for which one or more of the properties have been certified as *accurate*, preferably by the use of a definitive method in the hands of two or more analysts.

Sea water based reference material, poisoned with $HgCl_2$, stored in Schott Duran® glass sealed with a greased, ground-glass stopper.

Certified for salinity (0.005) total dissolved inorganic carbon (1 µmol kg^{-1}), and total alkalinity (1 µmol kg^{-1}).

Information values for nutrients

Stability ≥ 3 years

co2crms@ucsd.edu

Other certified materials available from my lab (in small quantities)

Equimolal tris buffer in synthetic sea water
Stored in 125 mL Schott Duran® bottle
pH certified (H_2 cell) to 0.003
Stability ~1 year

Hydrochloric acid solution (0.1 mol kg^{-1}) in a sodium chloride background (0.6 mol kg^{-1})
Stored in 1 L Schott Duran® bottle
Certified (coulometry) to 0.00002 mol kg^{-1}
stability >5 years

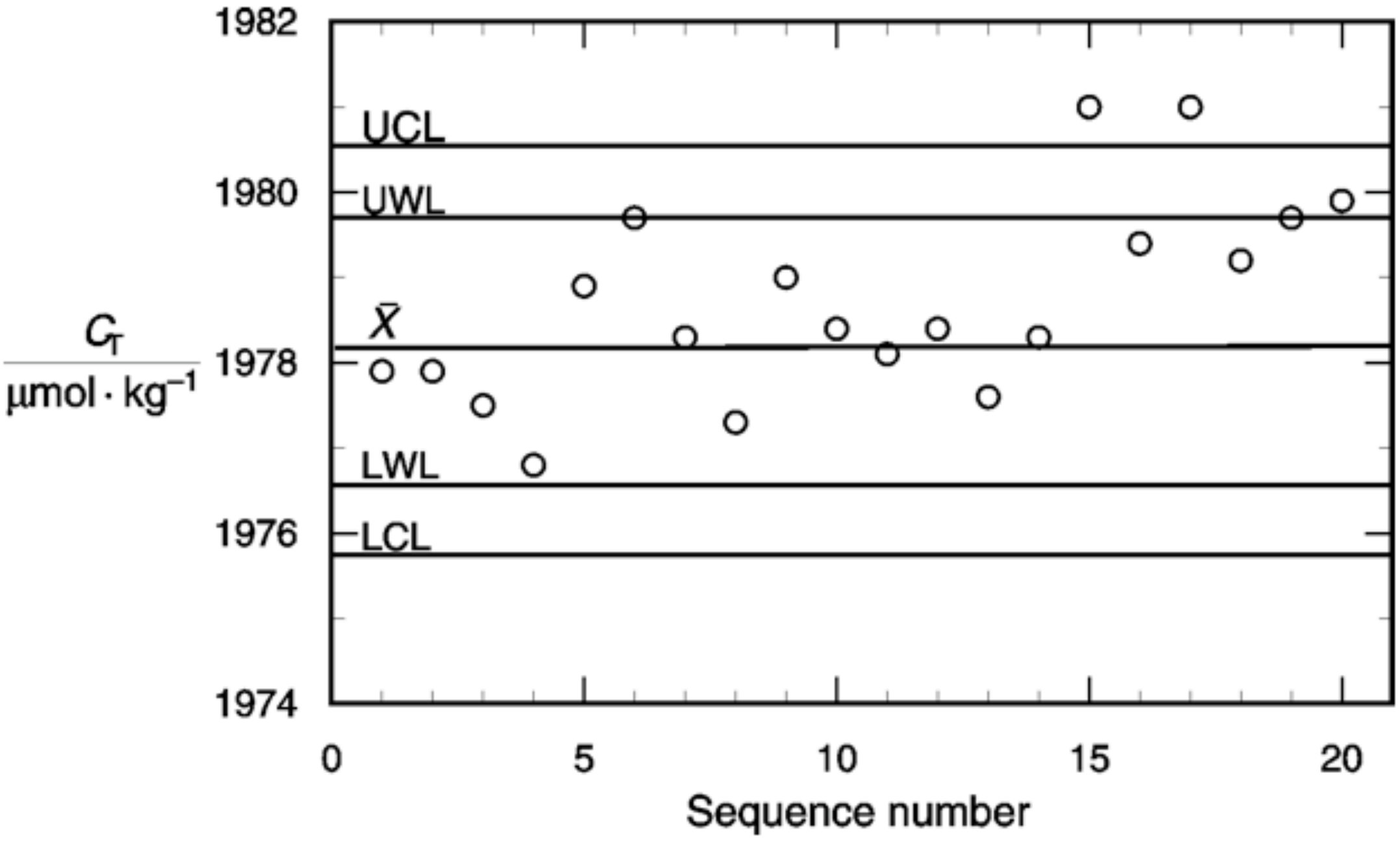
Quality control approaches

- Internal techniques
  - Repetitive measurements
- Internal test samples
  - Control charts
  - Interchange of operators
  - Interchange of equipment
  - Independent measurements
  - Measurements using a definitive method
- Audits
- External techniques
  - Collaborative tests
- Exchange of samples
  - External reference materials
  - Certified reference materials
- Audits

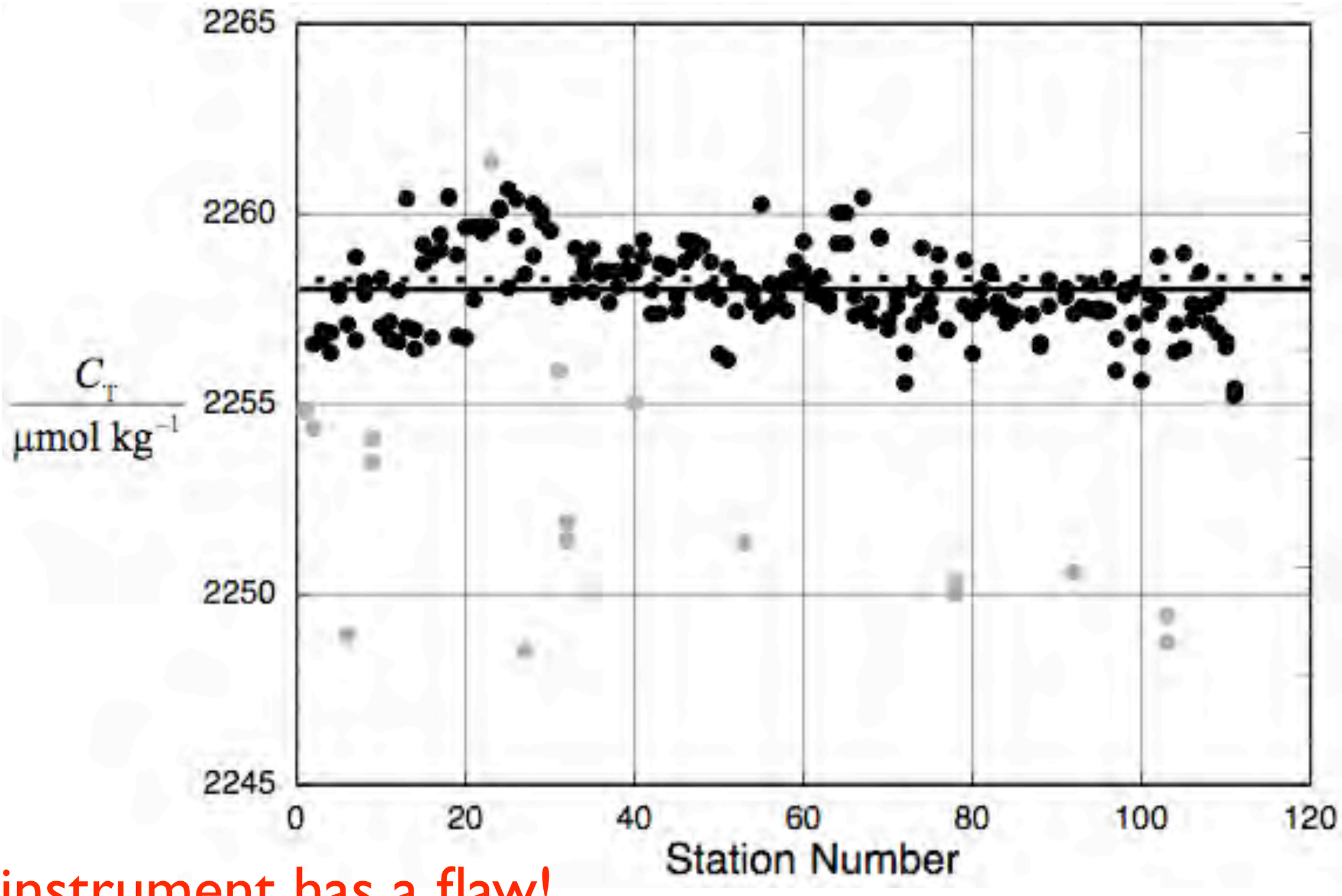
Remember, need quality control for both the sampling and the measurement process.

Using a control chart

not "in control"



Cruise data control chart (using CRMs)



instrument has a flaw!

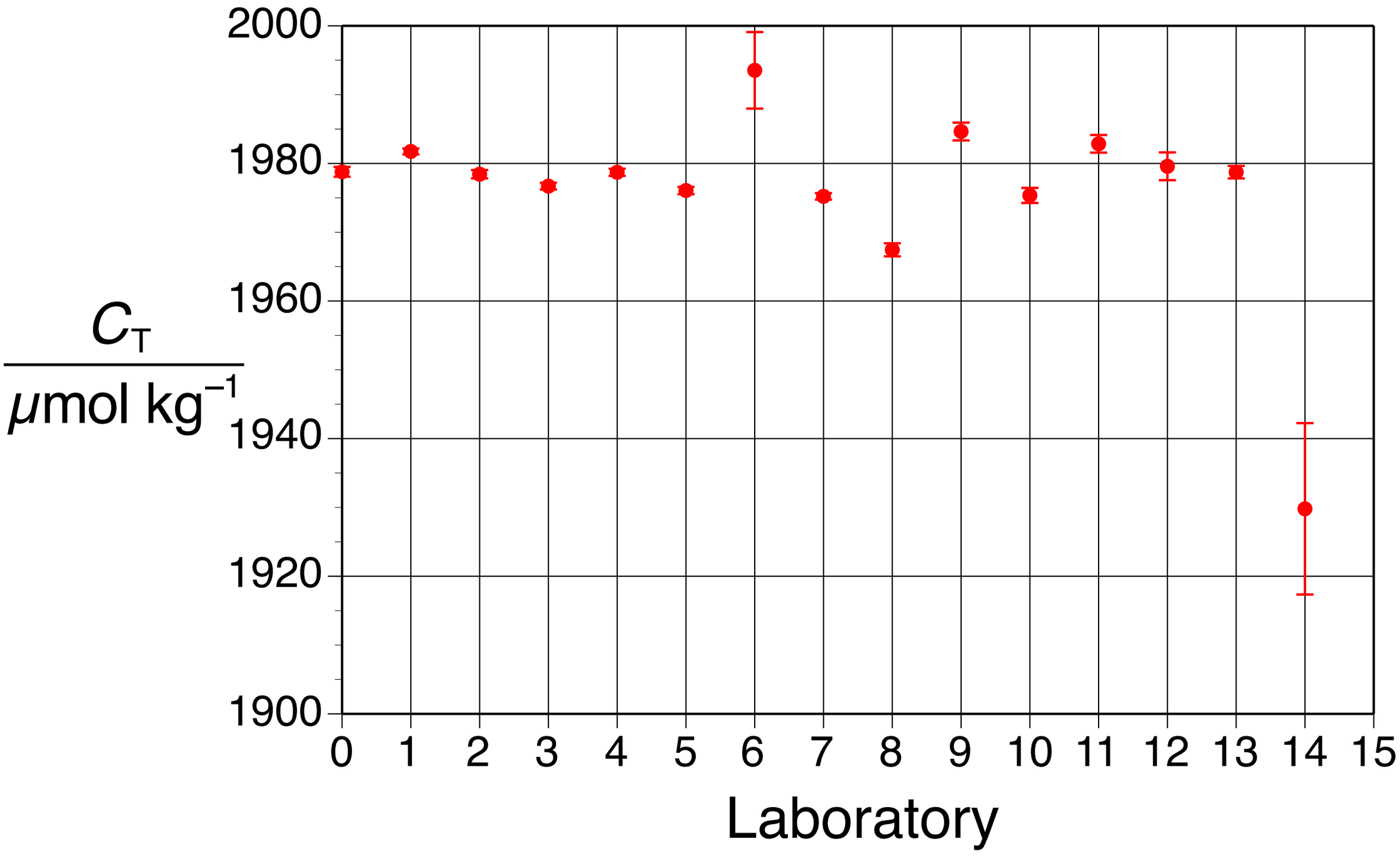
Interlaboratory comparisons

Collaborative testing of methods

Comparisons of alternate methods

Proficiency tests

Interlaboratory comparison (1991) of extraction / coulometry methods



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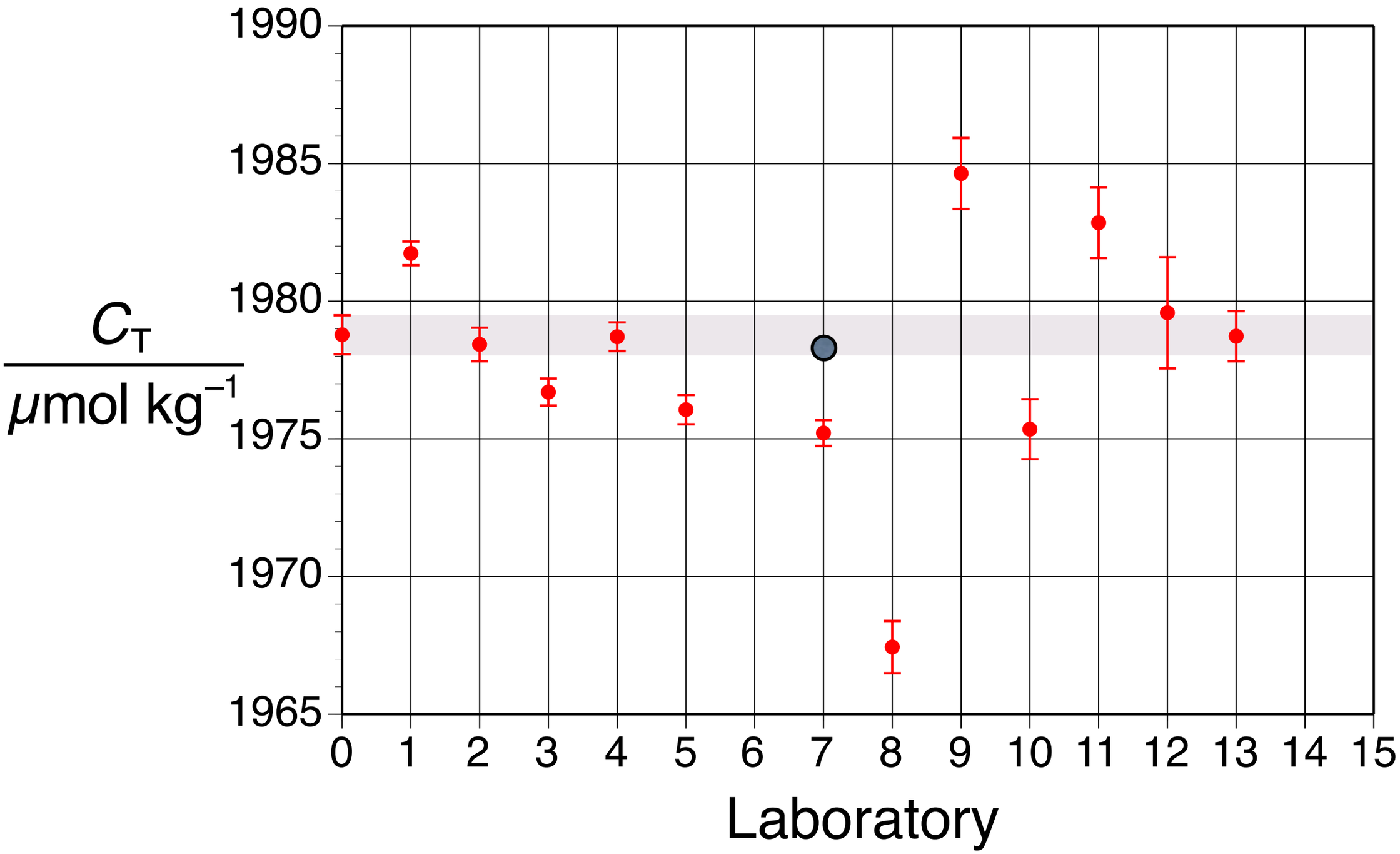

pooled std. dev. 1.6 µmol kg^{-1}

What's needed for OA research?

Robust, reliable, analytical techniques that can be used conveniently (ideally on small samples)

Each will need a suitable QA/QC plan including

1. Development of standard methods
   a. Written SOPs
   b. Collaborative testing of methods
   c. Establishment of *figures of merit*
2. Regular use of reference materials in quality control
3. Proficiency tests using blind samples

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