A131 – CALA Policy on the Accreditation of Calculated Analytes
Revision 1.3 –January 9, 2019

CALA
Laboratory Accreditation

TABLE OF CONTENTS

Accreditation of Calculations

1.0 SCOPE

This policy applies to all laboratories accredited under the CALA Accreditation Program that have calculated analytes on their accredited scope.

2.0 POLICY

General

The calculation shall be supported by a valid reference method, and detection limit determinations and calculations must be valid. As well, there must be an estimate of the measurement uncertainty.

All constituent analytical analytes that are part of the calculation must be accredited by the location seeking accreditation of the calculated analyte.

Only those analytes that are a property of the item or matrix being tested can be accredited. Calculations performed for internal QC purposes or checking correctness of results (e.g., TDS-calc or Ion Balance) cannot be accredited.

The calculation shall be the result of two or more results that were obtained by measurement. This means that a measured result that is simply converted to another form using a factor cannot be accredited (e.g., SO4 by ICP cannot be accredited).

The scope will clearly indicate which analytes are calculations.

For example: Hardness (calculation)

Reporting Calculated Analytes

For analytes that are calculated, the test report must clearly indicate that the result presented is a calculation.

As per ISO/IEC 17025, all information necessary for the interpretation of the test results must be on the test report. For calculations, this is interpreted to mean that the lab must state all elements necessary for interpretation of the calculated results on their reports. For example, if "Total PAH" is reported, then reports need to state which PAHs are included.

The laboratory is required to consider the calculated analyte as suspended or withdrawn:

- If any one of the constituents is suspended or withdrawn; and/or,

- If the analyte is directly supported by Proficiency Testing (PT) and the PT is suspended or withdrawn.

While a laboratory cannot claim accreditation for SO4 by ICP, based on converting a sulphur result, the laboratory can be accredited for sulphur by ICP and report SO4, provided that the laboratory clearly states the assumptions on the test report (e.g. Sulphate result assumes that all sulphur is in the form of sulphate). As well, it must be clearly indicated that sulphate is not part of the scope of accreditation if a statement about accreditation is included in the report.

3.0 GUIDANCE ON DETECTION LIMITS AND MEASUREMENT UNCERTAINTY

Summations should either sum all component detection limits or should use the root sum of squares.

Subtractions should compute the uncertainty of the subtracted result, and the reported detection limit should never be less than this uncertainty.

Sodium Absorption Ratios (SAR) calculations should be verified to handle non-detects appropriately.

The components of a calculated value (e.g., hardness and components Ca and Mg) each have uncertainty. For simple sums, the square root of the sum of the squares is generally appropriate. However, in some cases the uncertainty of the components are correlated (e.g., something in the measurement system that causes a bias in Ca might also cause a bias in Mg). In these cases, the combined uncertainty could be reduced by the amount of the correlation. Therefore the simple (quadratic) addition of the uncertainties of the components will produce an over-estimate of the actual uncertainty.

For direction and guidance on measurement uncertainty of calculated analytes, the following document may be of use and is available free of charge on the Bureau International des Poids et Mesures (BIPM) web site.

JCGM 102:2011
Evaluation of measurement data – Supplement 2 to the “Guide to the expression of uncertainty in measurement” - Extension to any number of output quantities
http://www.bipm.org/en/publications/guides/gum.html

4.0 REVISION HISTORY

Revision 1.3 January 9, 2019

Removed reference to ISO/IEC 17025:2005

ANNEX 1:

Common Analytes that are the Result of a Calculation

There are some common tests that are typically done by calculation. Listed below are some examples of which analytes are calculated. This list is not exhaustive.

1) Using a colourimetric method:
   - Nitrate plus nitrite ($NO_3 + NO_2$)
   - Nitrite (NO_2)

   Calculated Analyte:
   - Nitrate (NO_3) = ($NO_3 + NO_2$) – NO_2

2) Using ion chromatography (IC):
   - Nitrate (NO_3)
   - Nitrite (NO_2)

   Calculated Analyte:
   $NO_3 + NO_2$ = Nitrate (NO_3) + Nitrite (NO_2)

3) Hardness

   A laboratory may be accredited to determine hardness by titration. Alternatively, hardness is calculated as follows:

   - Hardness = Calcium x meq for Ca + Magnesium x meq for Mg

Other examples:

Total Chlordane = gamma-Chlordane + alpha-Chlordane

Total Nitrogen = Total Kjeldahl Nitrogen + Nitrate + Nitrite

Organic Nitrogen = Total Kjeldahl Nitrogen – (Ammonia+Ammonium)

Aldrin + Dieldrin

Atrazine + N-dealkylated metabolites

DDT + metabolites = o,p'-DDT + p,p'-DDT +p,p'-DDD + p,p'DDE

Total Trihalomethanes = Bromodichloromethane + Bromoform + Chlorodibromomethane + Chloroform

Total Haloacetic acids

Total Xylenes = m/p-xylene + o-xylene

Heptachlor + Heptachlor Epoxide