(V2, 27 May 2024)

Guide to updating **Calibration and Measurement Capabilities** (CMCs) for **ozone** amount fraction with the adoption of the **CCQM.O3.2019 ozone absorption cross-section value**

Rational

The CCQM Task Group for Ozone Cross-Section is working with stakeholders worldwide to implement a change in the value of the ozone absorption cross section that is used for surface ozone amount fraction measurements. The new value of the cross section, referred to as the CCQM.O3.2019 value, will start to be used from 1 January 2025 and is expected to be fully in use worldwide by 1 January 2026. The comparison exercise for ozone standards (photometers), BIPM.QM-K1, will also adopt the new cross section value from 1 January 2025. It is expected that NMIs' clients will wish to have access to ozone calibration services using the new cross section value from 1 January 2025, and as a result CMCs reported by National Metrology Institutes (NMIs) and Designated Institutes (DIs) to the BIPM KCDB need to be updated to incorporate a changed absorption cross section value and uncertainty. Current ozone amount fraction CMCs are based on the Hearn.1961 ozone absorption cross section value, although this is not specifically stated in current CMCs, which is not consistent with the recommendation made by the CCQM Task Group to clearly identify which cross section value is being used. Further background and explanatory information on the different cross section values is available.

The CCQM-GAWG has recommended that NMIs with CMCs for ozone amount fractions should update these as soon as possible, so that they can be published in 2025.

NMIs may decide to implement one or more of the following changes:

1) Update the uncertainty equation to be consistent with the CCQM.O3.2019 ozone cross section value uncertainty and identify that the CCQM.O3.2019 ozone cross section value is being used

2) Retain the uncertainty equation that is consistent with the Hearn.1961 ozone cross section value uncertainty and identify that the Hearn.1961 ozone cross section value is being used

3) Retain a CMC that is consistent with the Hearn.1961 ozone cross section value uncertainty and add a new CMC that is consistent with the CCQM.O3.2019 ozone cross section value uncertainty, identifying which ozone cross section value is being used in each case (this is for the case when a NMI provides calibrations with either identified cross section, which maybe for a transitional period only)

This document aims at describing how to update ozone CMCs.

Two specific items of the CMCs need to be modified: the uncertainty equation and the reference to the absorption cross section. Both are further described below.

Modifying uncertainty equations

Ozone CMCs currently include an uncertainty equation such as:

$$Q[1.04, 0.022\ x(O_3)]$$

with the added information:

The uncertainty is expressed in nmol/mol.

The notation Q[a, b] stands for the root-sum-square of the terms between brackets: $Q[a, b] = [a^2 + b^2]^{1/2}$

This formulation uses the expanded uncertainty at a 95% confidence level (for the values of (a) and (b))[1]. This includes a contribution for a device under test in the first term (a), which is the absolute part of the measurement uncertainty. The second term (b) represents the relative part and has been required to be larger than $0.022x(O_3)$ (2.2% of the ozone amount fraction) to include the uncertainty contribution from the Hearn.1961 ozone cross section value.

Using the CCQM.O3.2019 ozone cross section value uncertainty, the formulation will keep the same format:

$$Q[a, b]$$

Where:

- a is the absolute part of the expanded measurement uncertainty, expected to be larger than 1.04 nmol mol^{-1}
- b is the relative part of the expanded measurement uncertainty, expected to be larger than $0.0091x(O_3)$ (0.91% of the ozone amount fraction)

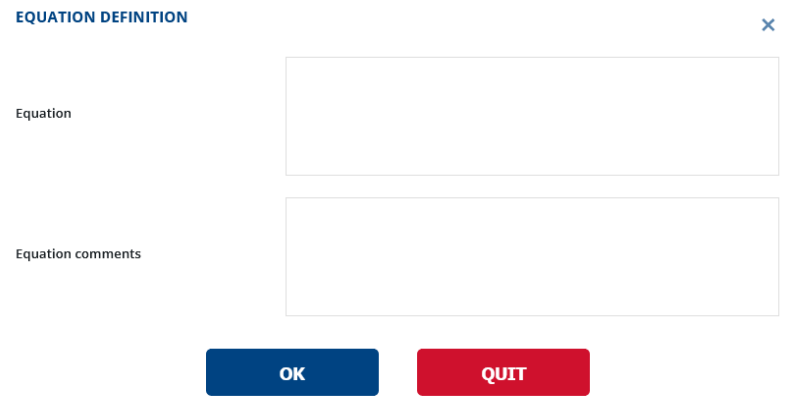
The minimum value of the absolute part of the expanded measurement uncertainty is equal to 1.04 nmol mol^{-1} or 2×0.52 nmol mol^{-1} and includes a contribution for the device under test equal to 0.36 nmol mol^{-1}.

The minimum value of the relative part of the expanded measurement uncertainty is equal to :

$$b_{min} = 2\sqrt{(0.003)^2 + (0.0034)^2}$$

which combines the ozone cross-section relative standard uncertainty (0.003) and other terms that are linear with the ozone amount fraction, using the case of the ozone standards maintained by the BIPM Headquarters Laboratory (0.0034).

The formulation will be entered in the KCDB using the box “equation” displayed in web-based tools for CMC writers, as displayed on the screenshot below:



[1] This formulation is numerically equivalent to using 2Q as described in the document GAWG/2010-03, where only standard uncertainties are used for these terms.

Identification of ozone absorption cross-section value in use

Ozone CMCs also need to display clearly what value of the ozone absorption cross-section is being used, by referring either to the **CCQM.O3.2019**, or **Hearn.1961** identifier as recommended by the CCQM. This information should be added using the box "Equation comments" of the web-based tool for CMC writers displayed above.

Comments are expected to contain either:

The expanded uncertainty is expressed in nmol/mol.

The notation Q[a, b] stands for the root-sum-square of the terms between brackets: $Q[a, b] = [a^2 + b^2]^{1/2}$

The CCQM.O3.2019 ozone absorption cross-section value and uncertainty is used.

or:

The expanded uncertainty is expressed in nmol/mol.

The notation Q[a, b] stands for the root-sum-square of the terms between brackets: $Q[a, b] = [a^2 + b^2]^{1/2}$

The Hearn.1961 ozone absorption cross-section value and uncertainty is used.