Report from the CCQM Gas Analysis Working Group (April 2024 – April 2025)

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1. CCQM-GAWG meetings

The 49th and 50th CCQM-GAWG meetings were held as hybrid meetings on 23rd and 24th April 2024 at the BIPM and on 21st and 22nd October 2024 at the Korean Research Institute of Standards and Science (KRISS), respectively. The 49th meeting was attended by 80 delegates (39 in person) from 42 institutes and the 50th meeting was attended by 71 delegates (38 in person) from 41 institutes. A two-day workshop was organised alongside the 50th meeting on global and national greenhouse gas monitoring initiatives. It focussed on the evolving needs for underpinning the expansion of global and national greenhouse gas monitoring initiatives (e.g. the global greenhouse gas watch (G3W), led by the World Meteorological Organisation). The role of metrology and the measurement infrastructure to support these developments was a key consideration. There was particular focus on research activities to meet the increased demand for calibration reference materials linked to global greenhouse gas scales and advances in measurement techniques. The workshop also focussed on the requirements and challenges for extending national and global greenhouse gas monitoring capabilities and the associated research and development activities. Two additional virtual meetings were organised in September 2024 and March 2025 by the CCQM-GAWG to discuss the draft A reports for CCQM-K164 and CCQM-K174, respectively.

2. Demonstrating and documenting the global comparability of measurements

At the 29th meeting of the CCQM, CCQM-76.2026 (track A comparison on sulfur dioxide in nitrogen) and CCQM-K71.2024 (track C comparison on stack gases) were approved.

Reports from the following key comparisons were published: BIPM.QM-K1 (Ozone) with several laboratories and CCQM-P229 (pilot study on the line intensities of selected $^{12}C^{16}O$). Figure 1 shows the list of active key comparisons and pilot studies.

		Track	Coordinator	Guidance	Participants	Registered	Model
K175	HCl in N_2	C	KRISS	NPL	VSL PTB VNIIM NPL NIST	2020	1
K164	H_2 purity	C	NPL	VSL	KRISS VSL NIM NMIA BAM NMISA	2019	1
K10.2018.1	BTEX	C	LNE	-	METAS, UBA	2023	1
K174	Oxygenated VOCs	C	VSL	METAS	NPL NIM METAS LNE NMISA CMI	2020	1
K26b.2019	SO_2 in air	C	NPL	*KRISS*	UBA NMISA FMI LNE KRISS VSL NIM VNIIM EAA JRC CERI CHMI UME	2019	1
K82.2023	Ambient CH_4	C	BIPM	*NIST*	NPL, UME, LNE, NOAA, NIST, NPLI, VSL, NMISA, VNIIM, KRISS, NMIJ, NIMT, NIM	2023	2
P236	Ambient CH_4	C	BIPM	*NIST*	ICOS	2023	2
K185	Particle charge and number	C	NPL	tbc	KRISS, LNE, METAS, NIM, A*STAR, NMIJ, NPLI, PTB, NRC	2023	-
P237	Particle charge and number	C	NPL	-	TROPOS, UBA	2023	-
K3.2019.1	Automotive gases	A	VSL	-	UKR	2023	1
K118.1	Natural gas	C	VSL	-	BAM, VSL, KRISS	2023	1
K93.2023	Ethanol in nitrogen	C	NPL	*BAM*	VSL, SMU, LNE, CMI, INMETRO, NIST, NMISA, IPQ, KRISS, BFKH, UME, CERI, UKR, NIMT, NIM	2023	2
K77.2023	Refinery gas	C	VSL	*NMISA*	NPL, CMI, NIM, NMISA, INMETRO, BFKH	2023	2
P239	C and O isotope ratio (CO_2 in air)	D	BIPM	-	IAEA, INRiM, KRISS, NIM, NIST, A*Star, NMIJ, NPL, UME, VNIIM, CSIRO, BGC-ISOlab, INstAAR, RUG, ECCC	2023	2
K71.2024	Stack gases	C	VSL	tbc	IPQ, NPL, KRISS, INMETRO, SMU, CENAM, NIM, NMISA, VNIIM, LATU, NIST, NIMT, UME	2025	1
K76.2026	SO_2 in nitrogen	A	NIM	tbc	NMIA, KRISS, NPL, NIST, CENAM, INMETRO, VSL, NMISA, VNIIM, CERI, NPLI	-	2
K84.2024*	Ambient CO in air	C	NOAA	tbc	KRISS, VSL, NIST, LNE, NIM, VNIIM, NPL, FMI, NOAA, EAA, UBA(D)? NMIJ?	-	1
K15.2025*	Emissions SF_6	C	KRISS	tbc	VNIIM, NIM	-	1
K26a.2025*	Ambient NO	C	NPL	tbc	tbc	-	1
KXXX*	CCUS	C	NPL	tbc	tbc	-	1
K171	*CO in N_2*	*A*	*VNIIM*		*VSL, NPL, BAM, UKR, NMIJ, NIM, KRISS, INMETRO, CENAM, NIST, NMISA*	*2020*	*1*

Figure 1 Active CCQM-GAWG comparisons (green – draft B, yellow – draft A, orange – measurements, red – planning). *Requires approval by the CCQM.

The track A key comparison on carbon monoxide in nitrogen (CCQM-K171) is postponed until further notice due to current embargoes on the transport of cylinders from the coordinating laboratory. The working group will use BIPM.QM-K2 and CCQM.K76.2026 to support broad claims under track A. Figure 2 lists the planned comparisons in the strategic plan for 2025-2029.

Start			Track	Coordinator	Model
2007	BIPM.QM-K1	Ozone	C	BIPM	-
2022	BIPM.QM-K2	Ambient CO_2	A/C	BIPM	-
2024	BIPM.QM-K6	NO_2 in nitrogen	C	BIPM	2
2026	KXXX	VOCs	C	NIM?	-
2026	Pxxx	C and O isotope ratio from carbonates	D	BIPM	-
2026	K76.2026	SO_2 (100 µmol mol^{-1})	A	NIM	1
2026	BIPM.QM-K5	Ambient CO_2 in air scales	C	BIPM	-
2026	CCQM-K65.2026	Odorants (expanded to include H_2S COS, THT, and mercaptans)	C	VSL	1
2027	K116.2027	H_2O (1 µmol mol^{-1})	C	NPL	1
2027	CCQM-K83.2027	Halocarbons	C	-	-
2027	K90.2027	Formaldehyde (1 µmol mol^{-1})	C	-	2
2027	K137.2027	NO (30 and 70 µmol mol^{-1})	C	NMISA	2
2027	Pxxx	Particle size	C	-	-
2028	K112.2028	Biogas	C	VSL?	1
2028	BIPM.QM-K3	C and O isotope ratio in pure CO_2	C	BIPM	-
2028	K53.2028	O_2	A	-	2
2028	K117.2028	Ammonia in nitrogen	C	-	1
2029	K121.2029	Monoterpenes in nitrogen	C	-	2
2029	K119.2029	LPG	C	-	1
2029	K113.2029	Noble gases	C	-	1
2029	BIPM.QM-K4	C and O isotope ratio (CO_2in air)	C	BIPM	-

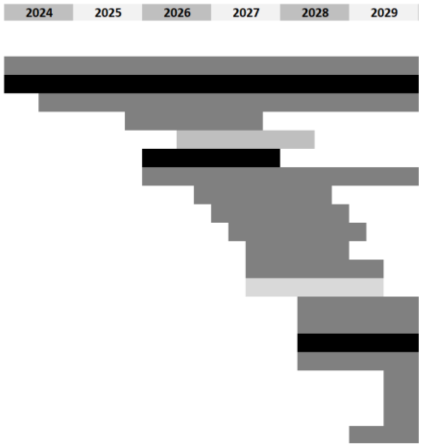


Figure 2 Planned comparisons for the period 2024 – 2028 (black – track A, dark grey – track C, light grey – track D).

3. Working group activities progressing the state of the art in measurement science

A session to present research developments on enabling confidence in breath analysis for disease detection was held at the 50th CCQM-GAWG meeting at KRISS. The analysis of volatile organic compounds in exhaled human breath is a novel non-invasive diagnostic tool that has the potential to revolutionise the early detection of diseases, the monitoring of disease progression and personalised medicine both in and out of the clinical environment improving patient outcomes while reducing costs. However, poor data comparability is currently limiting clinical confidence in data inhibiting the translation of breath analysis research into routine clinical practice. There are several requirements from stakeholder that depend on the intervention of metrology. In particular:

- Breath is a challenging matrix to measure with the biomarkers of interest typically being present at low concentrations relative to VOCs commonly found as background components in almost all exhaled breath.
- Patient to patient variability and contamination from exogeneous sources make identifying and quantifying biomarkers relevant to specific diseases very challenging.
- Regulatory bodies often do not know what criteria is needed to certify new breath analysis technology because it is so novel.
- There is a lack of breath-specific reference materials available commercially.

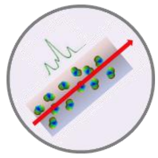
Research activities at NIST, KRISS and NPL were presented along with opportunities for future collaboration.

A pilot study (CCQM-P229) on absolute line intensities of selected $^{12}C^{16}O$ transitions has been completed by the task group on advanced spectroscopy and published. It is the first of its kind and involves distinct primary measurements of amount fraction based on linear absorption spectroscopy. Participants each chose a specific spectroscopic technique and measured the overlapping sets of rotation-vibration transitions within the 3-0 vibrational band of the $^{12}C^{16}O$ isotopologue of carbon monoxide. Pure carbon monoxide was used at near natural isotopic abundance measured near room temperature and corrected to a reference temperature of 296 K using the known partition function of $^{12}C^{16}O$ and lower-state energy for each transition. CO was chosen as a nearly ideal candidate for this study given the relatively low density of transitions, its low affinity to adhere to chamber walls, and the accuracy with which intensities of this diatomic molecule can be determined from semi-empirical potential energy determinations and quantum-chemical calculations of transition moments. The pilot study investigated the systematic biases between the different experimental techniques and made direct comparisons with theory. It demonstrated the feasibility of making exceptionally accurate determinations of molecular line intensities (<1‰ relative uncertainty level) through coordinated experiments that leveraged complementary and independent primary measurements from participating laboratories. This work discussed serves as a reference case to which experimentalists using a variety of independent spectroscopic methods can compare their results and establish confidence in their assigned measurement uncertainties. Extension to other bands of carbon monoxide as well as other molecular bands that are amenable to line-by-line analysis should make possible continued advances in primary spectroscopic measurements of amount fraction, partial pressure, temperature, and isotopologue ratios.

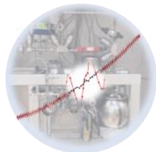
4. Working group stakeholder engagement activities

Work has continued with stakeholders via five task groups:

1 - Ozone Cross-Section Change Management to develop a plan and timetable to allow a globally coordinated and universal implementation of the new consensus value of ozone absorption cross-section at 254 nm, CCQM.O3.2019 (J T Hodges *et al.*, Metrologia, 56 034001, (2019)).



2 - Advanced Spectroscopy to develop and validate accurate spectroscopic measurements of analyte number density and isotopic abundance to provide fit-for-purpose alternatives to traditional mass and manometric-based measurement techniques, which can be limited by the availability of consumable reference materials, sensitivity, portability, selectivity and dynamic response.

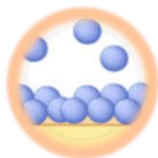


3 - Greenhouse Gas Scale Comparisons to meet the future demand for gas reference materials that are traceable to the WMO scale, because of the requirement for multiple measurement sites for greenhouse gases around the world for evaluating a robust economic system based on their mitigation.

4 - Isotope Ratio Metrology to build on current research advances, formalise the collaboration between NMIs and expert laboratories and provide a measurement infrastructure to underpin global measurements of source apportionment that will have enduring value.

5- Aerosol Metrology to engage with stakeholders to identify the metrology gaps, provide a framework to demonstrate capability required to meet future legislative and end user requirements.

In addition, a new task groups have been established:



6- Passivation Chemistry In response to the BIPM-WMO climate workshop recommendations to collate knowledge related to adsorption and reactive losses of greenhouse gas and other important components in high pressure gas cylinders and sampling systems. Connect to modelling and explanations for new knowledge and develop and study innovative cylinder passivation chemistries towards reference materials with enhanced stability.

Dissemination activities:

The new reference value for ozone absorption cross section was implemented on January 1^{st} 2025 and the CMC review process is underway. A guidance document on updating CMCs for ozone amount fraction with the new reference value (CCQM.O3.2019) has been published (GAWG/25-01).

The 27th ISO/TC158 plenary meeting and working group meetings were held in Hangzhou, China in October 2024. A workshop on the applications of gas analysis for industry followed and featured lectures from members of the CCQM-GAWG.

Representation at the 1st CIPM Sectorial Task Group on Environment Stakeholder meeting at the BIPM in September 2024. Presentations and contributions were made by members of the CCQM-GAWG in response to the recommendations from the BIPM-WMO Workshop on Metrology for Climate Action in 2022.

5. Additional items from the working group meetings

Christina Cecelski (NIST) has been appointed as CCQM-GAWG representative on the CCQM-KCWG.

Following the decision at the 48th CCQM-GAWG meeting on archiving key comparison, those older than 15 years where a replacement is available are under review. The strategic plan is being developed to ensure repeat key comparisons are in place within 15 years of the previous study.

In collaboration with the RMOs, the CCQM-GAWG has developed a strategy to ensure the removal of CMCs from the KCDB with insufficient or obsolete evidence. This involves two processes:

i) Continue the process of archiving key comparisons using the principles agreed by the CCQM-GAWG on a 1 year rolling basis. When key comparisons are archived, CMCs are reviewed which use this evidence and laboratories are identified that have not updated their CMCs.

ii) Continue the process of reviewing CMCs on a 1 year rolling basis as proposed at the 50th CCQM-GAWG meeting. This will start with comparisons completed in 2022-2023 for the current review cycle and then focus on the previous year moving forward. We will identify laboratories that did not participate or have not updated their CMCs based on this evidence.

The CCQM-GAWG Strategy 2025 – 2030+ has been prepared and is a revision of the document published in 2021. It includes information on the gap analysis performed by the working group for archiving CMCs and the agreed principles, an update to the strategic plan for comparisons, an update to the data for laboratories who have coordinated key comparisons and pilot studies, information on task groups, updates to research activities and changes in strategic direction from CCQM workshops and new impact case studies.

The 52nd meeting of the CCQM-GAWG and a stakeholder workshop on passivation chemistry will be hosted by INRiM from 21st – 24th October 2025.