Bureau International des Poids et Mesures

# Change in the value of the UV ozone absorption cross section Recommendations for metadata provision

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## **RAPPORT BIPM – 2024/01**

#### Summary

- The international gas measurement community will adopt a new value for the ozone absorption cross section for calculating surface measurements made by Ultraviolet (UV) photometers.
- The new value enables ozone measurements with less uncertainty and higher accuracy than the current absorption cross section value.
- The implementation of the new value will start on 1 January 2025 and should be accomplished before 1 January 2026.
- It is recommended to use flags or metadata to note which absorption cross section value you used to generate your data. This will help the community to know how to interpret the data reported around the time of the change. Therefore, before 1 January 2025, you should flag individual data entries or use metadata for a time series to show which value you used for your measurements.
  - *Hearn*.1961 for the currently accepted absorption cross section
  - CCQM.O3.2019 for the new absorption cross section

## Background

Surface ozone measurements are mainly made using UV photometric techniques, which follow Beer-Lambert law dependence of UV absorption on the ozone amount fraction. In most cases, the Hartely UV band near 255 nm is used due to its strong absorption signatures. Mercury-vapour lamps that emit incoherent light in the UV and VIS regions with the most intense emission occurring at a wavelength of 253.65 nm are used in most ozone analysers. The absorption cross section at this wavelength was reported by Hearn [1] with a value of  $1.1476 \times 10^{-17}$  cm<sup>2</sup> [2] and a standard uncertainty of  $0.024 \times 10^{-17}$  cm<sup>2</sup> per molecule. It is used by most analysers and is also implemented in the NIST Standard Reference Photometers (SRP) [3], which serve as a reference to calibrate ozone instruments in the field.

The Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM) recommended in 2020 [4] to use the absorption cross section of  $1.1329 \times 10^{-17}$  cm<sup>2</sup> with a standard uncertainty of  $0.0035 \times 10^{-17}$  cm<sup>2</sup> published by Hodges et al. [5]. The new value is referred to as CCQM.O3.2019 as a unique shorthand identifier. The change to the CCQM.O3.2019 value will increase all SRP traceable ozone amount fractions by a factor of 1.01293 [6]. It should be noted that this conversion factor<sup>1</sup> is slightly larger than the

<sup>&</sup>lt;sup>1</sup> Historically, slightly different values for the absorption coefficient have been used in the literature, with a maximum relative difference of 0.12 %. The majority of users world-wide used the specific value of 308.32 atm<sup>-1</sup> cm<sup>-1</sup>. This corresponds to a conversion factor of 1.01293.

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ratio of the CCQM.O3.2019 value and the value reported by Hearn [1] due to rounding effects in the value of the linear absorption coefficient, equal to 308.32 cm<sup>-1</sup>, used in the NIST Standard Reference Photometers (see [6] for details).

The current timeline is for the new value to be implemented in the ongoing key comparison for ozone standards (BIPM.QM-K1) in January 2025. The implementation of the new value will have an impact on all ozone photometers with traceability to an SRP. Consequently, information on the absorption cross section that is used is crucial, and the following recommendations are made.

#### Recommendation for metadata provision of ozone time series

In order to facilitate the change of the ozone absorption cross section, surface ozone measurement networks, data centres, instrument manufacturers, research communities and metrology institutes shall supply their ozone amount fraction data with the absorption -cross-section value used for the measurement (Hearn.1961 or CCQM.O3.2019). This can be done either in the metadata of a time series, or as a flag for individual data entries in a time series.

It is important that the implementation of the flagging/metadata is made before the change to the new cross section value becomes effective (1 January 2025). Flagging or providing metadata, stating the ozone cross section value of existing data series, should start in 2024. It is recommended to provide information on the ozone cross-section value in the metadata or as a data flag for all future ozone amount fraction measurements at the latest from January 2025 onwards.

## **Contacts / Questions**

Questions on this guidance document, such as how to identify which ozone absorption cross-section is implemented in ozone analysers based on UV photometry, or how to flag values which differ from Hearn.1961, can be addressed to the Executive Secretary of the <u>Task</u> <u>Group on ozone absorption cross-section change management</u>.

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#### References

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