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Certificate of Analysis – Certified Reference Material

Bromide Standard for IC

TraceCERT® Traceable Certified Reference Materials

Product no.:	43147
Lot no.:	BCCF8024
Description of CRM:	Sodium bromide (pure material) in high-purity water (18.2 MΩ·cm, 0.22 µm filtered).
Expiry date:	MAR 2024
Storage:	Store at 5°C-25°C
Density (certified) at 20°C:	999.2 kg m^{-3} ± 0.5 kg m^{-3}

Constituent	Certified values at 20°C and expanded uncertainties, $U = k \cdot u$ (k = 2) [1][2]	
Bromide	**1001 mg kg^{-1} ± 4 mg kg^{-1}**	**1000 mg L^{-1} ± 4 mg L^{-1}**

Metrological traceability:	Certified values are traceable to the International System of units (SI) through a metrologically valid weighing process. Details see "Details on metrological traceability".[3]
Measurement method:	The certified value is determined by high-precision weighing of thoroughly characterized starting materials and verified by measurement against NIST SRMs or similar CRMs
Intended use:	Calibration of ion chromatography or any other analytical technique.
Instructions for handling and correct use:	The bottle's temperature must be 20°C. Shake well before every use. If storage of a partially used bottle is necessary (at the user`s risk), the cap should be tightly sealed and the bottle should be stored at reduced temperature (e.g. refrigerator) to minimize transpiration rate.
Health and safety information:	Please refer to the Safety Data Sheet for detailed information about the nature of any hazard and appropriate precautions to be taken.
Packaging:	100 mL HDPE bottle
Accreditation:	Sigma-Aldrich Production GmbH is accredited by the Swiss accreditation authority SAS as registered reference material producer SRMS 0001 in accordance with ISO 17034 and registered testing laboratory STS 0490 according to ISO/IEC 17025.[4][5]
Certificate issue date:	07 MAY 2021

ISO 17034 SRMS 0001

ISO / IEC 17025 STS 0490

ISO 9001 005356 QM08

S. Matt – CRM Operations

Dr. P. Zell – Approving Officer

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Certification process details:

To guarantee top reliability of the values for this *Trace***CERT®** certified reference material, three independent procedures were followed. The values have to agree in the range of their uncertainties, but the value from the gravimetric preparation has been chosen as certified value [3]:

1. Gravimetric preparation using pure materials is a practical realization of concentration units, through conversion of mass to amount of substance [3]. If the purity of the materials is demonstrated and if contamination and loss of material is strictly prevented this approach allows highest accuracy and small uncertainties. The certified value of this *Trace***CERT®** reference material is based on this approach and directly traceable to the SI unit kilogram. Therefore comprehensively characterized materials of high purity are used. All balances are calibrated annually by an ISO/IEC 17025 accredited laboratory and certified according to DKD guidelines. Calibration is checked daily with OIML Class E2 or F2 weights.
2. The starting material is measured against a certified reference material (i.e. NIST or BAM) followed by gravimetric preparation using balances calibrated with SI-traceable weights. Consequently the value calculated by this unbroken chain of comparisons is traceable to the reference to which the starting material is compared.
3. Whenever applicable the bottled *Trace***CERT®** calibration solution is compared to a second reference which is independent from the first reference.

Details on metrological traceability:

Only internationally accepted reference materials e.g. from NIST (USA) or BAM (Germany) have been carefully selected to provide the basis for traceability to the SI unit mole. When no such reference is available, an elemental metal or an adequate salt of highest available purity is used to confirm traceability to this pure material (and therefore to the SI unit kg).

To underpin the certified gravimetric value all traceability measurements are performed with the most accurate and precise analytical technique available. Therefore titrimetry measurement series are applied whenever possible (corrected for trace impurities). When no titrimetric technique is available, the traceability measurements are performed with another analytical technique, e.g. ICP-OES or AAS.

Reference and applied technique used for traceability measurements of the

starting material: NIST SRM 999 / argentometric

bottled solution: Sodium chloride, certified by BAM (Sigma-Aldrich No. 71387) / argentometric titration

Details on starting materials:

For high purity materials (P >99.9%) the most appropriate way of purity determination is to quantify the impurities (w_i) and to subtract the sum from 100%. Impurities below the detection limit are considered with a contribution of half of the detection limit (DL_j).

$$P = 100\% - \sum_i w_i - \sum_j \left(\frac{DL_j}{2}\right)$$

Water containing materials were dried to absolute dryness by individual drying conditions (up to 600°C). When drying is impossible due to decomposition water was determined by high-precision KF-titration.

Homogeneity assessment:

Due to the production process, a homogeneous solution derives. Nevertheless a small homogeneity contribution is included into the calculation of content uncertainty of this CRM.

Density Measurement:

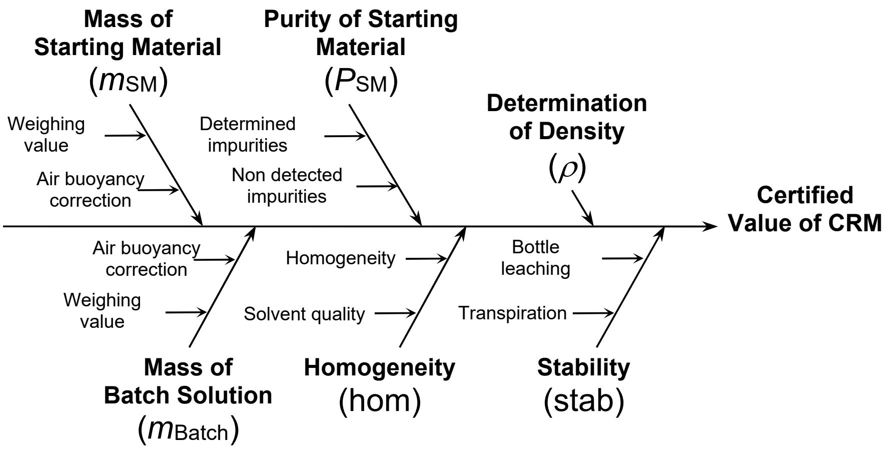
The density measurement is carried out under the scope of the ISO/IEC 17025 accreditation according to ISO 15212-1 [6] and using the digital density meter DMA 4500M from Anton Paar with an oscillating U-tube installed. The measurement uncertainty is calculated according to Eurachem/CITAC Guide and reported as combined expanded uncertainty at the 95% confidence level, using a coverage factor of k = 2.

Uncertainty evaluation:

The uncertainty contributions are illustrated by the following cause-effect diagram [7]:

Typical relative contributions are:

$u(m_{SM})$	< 0.01 %
$u(m_{Batch})$	< 0.01 %
$u(P_{SM})$	< 0.05 %
u_{hom}	< 0.03 %
u_{stab}	< 0.20 %
$u(\rho)$	< 0.05 %



The combined standard uncertainty is calculated by combination of the standard uncertainties of the input estimates according to Eurachem/CITAC Guide "Quantifying Uncertainty in Analytical Measurement" and ISO 17034.[2][4]

Expanded uncertainty is then calculated to a confidence level of 95%, typically by multiplying with a confidence level factor of k=2.

Trace Impurities in bottled solution:

The following anions were measured as possible impurities (in µg kg^{-1}, <X = below detection limit, m = matrix):

Bromide	Chloride	Fluoride	Iodide	Nitrite	Phosphate	Sulfate
m	1196.6	< 12.5	< 12.5	< 12.5	< 12.5	19.1

References:

[1] ISO Guide 35:2017, "Reference materials - Guidance for characterization and assessment of homogeneity and stability"
[2] Eurachem/CITAC Guide, 3rd Ed. (2012), "Quantifying uncertainty in analytical measurement"
[3] Eurachem/CITAC Guide, 2nd Ed. (2019), "Metrological Traceability in chemical measurement"
[4] ISO 17034:2016, "General requirements for the competence of reference material producers"
[5] ISO/IEC 17025:2017, "General requirements for the competence of testing and calibration laboratories"
[6] DIN EN ISO 15212-1:1998, Oscillation-type density meters - Part 1: Laboratory instruments
[7] Reichmuth, A., Wunderli, S., Weber, M., Meyer, V. R. (2004), "The uncertainty of weighing data obtained with electronic analytical balances", Microchimica Acta 148: 133-141.

Certificate of analysis revision history:

Certificate version	**Certificate issue date**	**Reason for version**
01	07 MAY 2021	Initial version

Disclaimer:

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