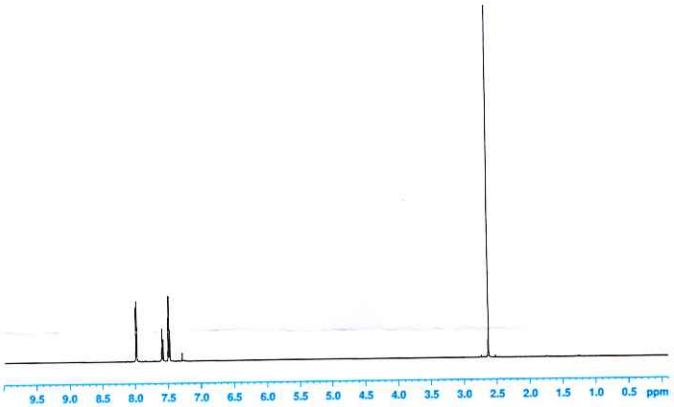
^{1}H-NMR Spectrum (600 MHz, Acetophenone in $CDCl_3$)



References:
[1] ISO Guide 31:2000, "Reference materials - Contents of certificates and labels"
[2] Eurachem/CITAC Guide, 1st Ed. (2003), "Traceability in chemical measurement"
[3] ISO Guide 35:2006, "Reference materials - General and statistical principles for certification"
[4] Eurachem/CITAC Guide, 3rd Ed. (2012), "Quantifying uncertainty in analytical measurement"
[5] Weber M, Hellriegel C, Rueck A, Sauermoser R, Wuethrich J, Accred. Qual. Assur. 18 (2013) 91-98
[6] ISO/IEC 17025:2005, "General requirements for the competence of testing and calibration laboratories"
[7] ISO Guide 34:2009, "General requirements for the competence of reference material producers"
[8] Weber M, Hellriegel C, Rueck A, Wuethrich J, Jenks P, JPBA 93 (2014) 102-110

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TraceCERT®

Traceable Certified Reference Materials

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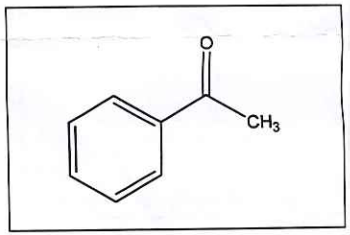
Certificate

Produced in double accredited laboratory fulfilling ISO/IEC 17025 and ISO Guide 34

This certificate is designed in accordance with ISO Guide 31 [1].

Product name: **Acetophenone**



Product no.:	63634
Lot no.:	BCBR5524V
Formula:	C_8H_8O
Molecular mass:	120.15 g/mol
Traceability [2]:	NIST SRM 350b (Benzoic acid)
Certificate issue date:	February 29, 2016
Expiry:	FEB 2020

Certified value and uncertainty according to ISO Guide 35 [3] and Eurachem/CITAC Guide [4]

Substance	Certified value as mass fraction (g/g)	Expanded uncertainty, $U = k \cdot u_c$ ($k = 2$) as mass fraction (g/g)
Acetophenone	**98.7 %**	**0.3 %**

Minimum sample: There is no recommended minimum sample weight. The substance is liquid at room-temperature and therefore homogeneous under these conditions. Potential inhomogeneity is covered by the expanded measurement uncertainty.

Intended use: Use this certified reference material (CRM) as calibrant for chromatography or any other analytical technique.

Storage and handling: The CRM should be stored in the original bottle at room-temperature (20-25°C). Shake gently before use, to ensure complete homogeneity (mp=19-20°C). After use the bottle should be tightly closed and protected from excessive moisture and light. Store under Argon.

CRM operations: A. Rück
Dr. A. Rück

Certification body:
Dr. K.D. Schmidt

ISO Guide 34 ISO/IEC 17025 ISO 9001

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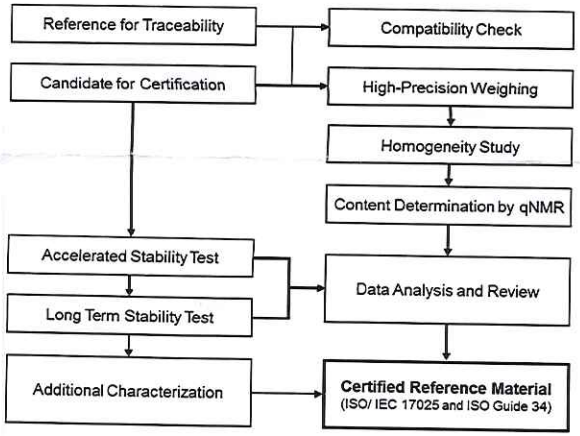
CERTIFICATION

In order to guarantee highest reliability of this *Trace***CERT** CRM a multi-component approach was applied whereby the certified value is determined by high-resolution quantitative NMR measurements (qNMR on a Bruker 600 MHz Avance III NMR spectrometer) [5]. This certified value is determined under **double-accreditation** in accordance with **ISO/IEC 17025** [6] and also **ISO Guide 34** [7]. Extensive stability and homogeneity tests are considered for certification [8].

The certified values are confirmed by extended analytical data including impurity determination. These data are not covered by the scope of accreditation but extended analytical data are determined following best practices in analytical measurements.



Candidate substances are checked for suitability in terms of purity. Only materials of highest available purity are accepted. 2D-NMR (H-H COSY) measurements are applied to guarantee that no impurities underlie to a peak of interest. Detection limit usually is below 0.1%.

Compatibility check guarantees that the candidate substance does not react neither with the solvent nor with the internal qNMR reference (t=0 and t=24h comparison).

High precision weighing is performed under ISO/IEC 17025 accreditation with ultra-micro balances certified by DKD and calibrated with OIML Class E2 weights.

Accelerated stability test is performed with samples which are stored above the recommended storage temperature. The material is tested by qNMR after 1, 3, 9 and 18 months.

Long term stability test is performed with samples which are stored at the recommended storage temperature and qNMR double determination after 24 and 48 months.

Homogeneity of the material is tested by qNMR measurements using 5-10 subsamples which are taken from different positions in the entire bulk material. The recommended minimal sample size is taken for all the homogeneity test samples. Analysis of variance (ANOVA) results are included into the calculation of content uncertainty of this CRM.

Absolute content determination by qNMR is performed using 5-10 separate samples of the candidate substance which are each spiked with an adequate amount of internal reference and then immediately dissolved in deuterated solvent. In most cases 16-32 scans are recorded for every sample with a ^{1}H relaxation time of d1= 60 seconds. Quantification of the candidate content is directly calculated from the ^{1}H-NMR peak areas and the initial weights of the candidate and reference substance. After ANOVA the resulting standard deviation is included into the uncertainty calculation of the certified value.

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UNCERTAINTY CALCULATION

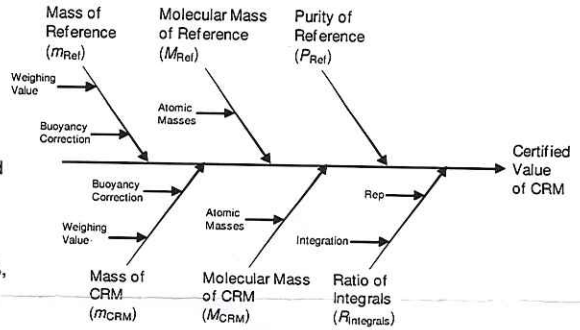
All uncertainties are calculated according to Eurachem/CITAC Guide and reported as combined expanded uncertainties. The uncertainty contributions are illustrated by the following cause-effect diagram.

Typical relative contributions are:

$u(P_{Ref})$	< 0.10 %
$u(m_{Ref})$	< 0.03 %
$u(m_{CRM})$	< 0.03 %
$u(M_{Ref})$	< 0.003 %
$u(M_{CRM})$	< 0.003 %
$u(R_{Integrals})$	<0.15 %

The combined uncertainty is calculated by combination of the squared contribution values.

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



INFORMATIONAL VALUES

mp	19-20 °C (lit.)
bp	202 °C (lit.)
refractive index n20/D	1.534 (lit.)

Cation traces

Al: ≤0.5 mg/kg	Li: ≤0.1 mg/kg
Ba: ≤0.1mg/kg	Mg: ≤0.1 mg/kg
Bi: ≤0.1 mg/kg	Mn: ≤0.02 mg/kg
Ca: ≤0.5 mg/kg	Mo: ≤0.1 mg/kg
Cd: ≤0.05 mg/kg	Na: ≤0.5 mg/kg
Co: ≤0.02 mg/kg	Ni: ≤0.02 mg/kg
Cr: ≤0.02 mg/kg	Pb: ≤0.1 mg/kg
Cu: ≤0.02 mg/kg	Sr: ≤0.1 mg/kg
Fe: ≤0.1 mg/kg	Zn: ≤0.1 mg/kg
K: ≤0.5 mg/kg	

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