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Preparation and Characterization of Primary Magnesium Mixtures for the *ab initio* Calibration of Absolute Magnesium Isotope Ratio Measurements – ELECTRONIC SUPPLEMENTBjörn Brandt^a, Jochen Vogl^{*a}, Janine Noordmann^b, Angela Kaltenbach^b, and Olaf Rienitz^b5 Received 15th July 2015, Accepted xx.xx.2015

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S1 Trace Levels of Ultrapure Water and Acids**Table S01** Trace Levels of Ultrapure Water and Acids. Unit: 10⁻¹² g/g.

	H ₂ O (4/2-14)	H ₂ O (11/3-14)	HNO ₃ (4/2-14)	HCl (4/2-14)
Li	2.4	5.4	1.1	1.7
Na	361	102.2	307	10·10 ³
Mg	11.4	12	19	48
Al	73	61	54	60
K	55	64	37	62
Ca	157	229	127	357
Cr	< 0.1	0.7	24	32
Mn	< 0.1	1.4	< 0.1	1.2
Fe	27	15	222	240
Co	< 0.1	0.5	2.8	3.7
Ni	< 0.1	< LOD	< 0.1	0.0
Cu	3.2	2.8	15	35
Zn	20	24	25	71
Ga	< 0.1	< LOD	< 0.1	< 0.1
Sr	0.7	2.2	6.5	1.7
Ag	< 0.1	1.1	0.1	0.1
Cd	0.2	0.8	0.2	0.5
In	< 0.1	0.3	< 0.1	n.d.
Ba	1.1	1.8	2.8	3.6
Tl	< 0.1	0.79	< 0.1	< 0.1
Pb	3.9	4.0	4.3	4.7
Bi	< 0.1	1.0	0.1	0.1

10 S2 Concentrated and Dilute Acids

Nitric acid (HNO₃) was used as solvent for all solutions in this project. It was only for IDMS column separations that a different acid (HCl) has been applied. All analytical solutions in the project have a target level of 0.02 g/g HNO₃. To achieve this level in all preparations, two HNO₃ solutions of different mass fractions had to be used: a slightly more concentrated acid was used in the digestion of magnesium (0.06 g/g HNO₃), which were always filled up later with ultra-pure water to reach the 0.02 g/g HNO₃ target level; in true dilutions, a dilute HNO₃ of 0.02 g/g were used for filling up. The following paragraphs describe the determination of the exact concentration of the concentrated acid, and its dilutions.

S2.1 Concentrated Acid (HNO₃)

Subboiling distillation alters the mass fraction and density of a concentrated acid. Since the mass fraction of the concentrated acid

is an important input parameter for calculating the acid mass fractions in diluted solutions, it had to be determined. This was done by pycnometry at BAM *via* the reference evaluation method described in the main part, using analytical balance AX-205.

30 Table S02 Determining the Density of Subboiled Concentrated HNO₃ by Pycnometry^a.

Pycnometer	W / g	s / g ^a	U (k = 2) / g	ρ / (kg/m ³)
empty	14.788609	0.000022	0.000078	-
With water	24.808470	0.002796	0.000107	1.170
With HNO ₃	28.634671	0.005268	0.000117	1.169

^a All values and standard deviations based on ten weighings (N = 10).

As the weighing values obtained with the liquids in the pycnometer showed significantly larger standard deviations than the tabulated balance measurement uncertainties (based on the calibration according to the EURAMET protocol, see main part), the standard deviations of repeated experiments were used for the uncertainty calculation. From this data the following density and its expanded uncertainty (k = 2) of the ultrapure concentrated nitric acid can be calculated as described in section 2.6 (in the main part):

$$\rho_a = (1.37839 \pm 0.00042) \frac{g}{cm^3}$$

The uncertainty is based on the formula in ref. [1], and also on a complete uncertainty budget, using either the calibration uncertainty or the standard deviation (whichever was larger, see bold values in Table S02) as the input uncertainties in the budget. For the air density, an uncertainty of 0.02 kg/m³ was assumed (for k = 2), and the uncertainty for the density of the balance calibration weight (8000 kg/m³) was chosen at 100 kg/m³.

Using the experimental density, ρ_a , and its uncertainty, the mass fraction and amount-of-substance concentration can be obtained from interpolation of tabulated data [2] (uncertainties for k = 2):

$$w_a = (62.376 \pm 0.085) \frac{g}{100 g}$$

$$c_a = (13.643 \pm 0.023) \frac{mol}{L}$$

S2.2 Dilute Acids

Dilute acids with two different acid mass fractions were used in this project. The dilution was carried out under full gravimetric control including buoyancy correction, so that the mass fraction could be calculated from the previously determined mass fraction of the concentrated acid. After that the solution was homogenized by shaking, and it was left for equilibration (typically for a few hours). The density of the dilute acid was determined by interpolation of the data available in reference [2].

For all analytical solutions in this project a target mass fraction of 0.02 g/g HNO₃ was chosen. Typically 0.02 g/g HNO₃ was prepared in 2 L and 5 L batches using a 2 L or 5 L PFA bottle and the balances LC-5101S and FCB12K0.1B.

The dissolution of Mg metal, however, requires a slightly more concentrated acid, as the metallic magnesium reacts with protons in the acid, and the acid strength decreases. Therefore, 0.06 g/g were chosen, which allows the resulting solution to be filled up with water to achieve the target mass fractions of magnesium and acid. The resulting mass fractions of the diluted acids and their associated uncertainties are listed in Table S03b.

Table S03 Preparation of Dilute Acids.

	0.06 g/g	0.02 g/g, 1 st	0.02 g/g, 2 nd
Empty PFA Bottle			
<i>W</i> (PFA, Empty), <i>N</i> = 10 / g	121.4453	308.0259	655.34
2 <i>s</i> / g	0.0010	0.0067	0.10
ρ_{air} / (kg/m ³)	1.17030	1.19819	1.17658
Correction Factor PFA	1.0003983	1.0004078	1.0004004
<i>m</i> (PFA, Empty) / g	121.4937	308.1514	655.60
Water			
<i>W</i> (PFA+Water) / g	532.0898	2261.5701	5539.20
(<i>N</i> = 5)		(<i>N</i> = 10)	(<i>N</i> = 10)
2 <i>s</i> / g	0.0009	0.0055	0.13
ρ_{air} / (kg/m ³)	1.17030	1.19513	1.17762
Correction Factor PFA	1.0003983	1.0004067	1.0004007
ρ_{water} / (kg/m ³)	997.882	998.141	997.442
Correction Factor Water	1.0010277	1.0010492	1.0010347
<i>m</i> (Water) / g	411.0665	1955.5935	4888.91
Concentrated Acid			
<i>W</i> (Acid by Difference) / g	49.600	64.708	161.783
(<i>N</i> = 1)		(<i>N</i> = 1)	(<i>N</i> = 1)
ρ_{air} / (kg/m ³)	1.17030	1.19513	1.17988
Correction Factor Acid	1.0007033	1.0007183	1.0007091
<i>m</i> (Acid) / g	49.6349	64.754	161.898
Total Mass			
<i>W</i> (PFA+Solution) / g	581.6960	2326.2851	5700.93
(<i>N</i> = 5)		(<i>N</i> = 10)	(<i>N</i> = 10)
2 <i>s</i> / g	0.0014	0.0074	0.13
ρ_{air} / (kg/m ³)	1.16936	1.18297	1.18589
Correction Factor PFA	1.0003979	1.0004026	1.0004036
Correction Factor Solution	1.0009793 ^a	1.0010256	1.0010282
<i>m</i> (Solution) / g	460.7014	2020.3272	5050.78
Total Mass After Additional Water Added			
<i>W</i> (PFA+Solution) / g	637.1254	-	-
2 <i>s</i> / g	0.0011	-	-
ρ_{air} / (kg/m ³)	1.164747	-	-
Correction Factor PFA	1.0003964	-	-
Correction Factor Solution	1.0009850	-	-
<i>m</i> (Solution)	516.1877	-	-
Mass Fraction, Dilute HNO ₃			
<i>m</i> (Concentrated Acid) / g	49.6349	64.7338 ^b	161.898
<i>m</i> (Total) / g	516.1877	2020.3272	5050.78
<i>w</i>	5.9979	1.9987	1.9991

^a Note that at this stage, the preparation of the 0.06 g/g acid has not been completed; the mass fraction was calculated, and density interpolated.

^b This value is calculated from the difference between the total mass, and the amount of water added; compare with the direct weighing cited in line "mass of concentrated acid".

Table S03b Mass Fractions of Dilute Acids and Their Expanded Uncertainties.

Nitric Acid (HNO ₃)	<i>w</i> / (g/(100 g))	<i>U</i> (<i>k</i> = 2) / (g/(100 g))	<i>U</i> _{rel} (<i>k</i> = 2) / %
0.06 g/g, digestion	5.9979	0.0082	0.14
0.02 g/g, 2 L batch	1.9987	0.0031	0.15
0.02 g/g, 5 L batch	1.999	0.017 ^a	0.85

^a For balance FCB12K0.1B an uncertainty of 1 g has been used (*k* = 2).

General: uncertainties for the water densities were set to 2 · 10⁻⁷ kg/m³ based on the assumption that the uncertainty of the temperature is 1 °C.

S3 Determination of Densities

S3.1 Determination of Liquid Densities

The density of elemental solutions changes slightly non-linearly with concentration. Therefore – to obtain best results –, the densities of Mg solutions (0.02 g/g HNO₃) were determined by pycnometry covering the range of Mg mass fractions (2 mg/kg to 1000 mg/kg) applied within this project. Uncertainties were expressly calculated only for two of the four values using GUM Workbench. To obtain values for all target mass fractions, the measured values were subjected to regression analysis. The measured and fitted densities are displayed in Table S04 with their associated uncertainties. For Mg solutions with mass fractions below 20 mg/kg the density is nearly constant, while for 100 mg/kg a slight increase can be observed, which is still covered by the expanded uncertainty. For a Mg mass fraction of 1000 mg/kg, however, the density is significantly different by 0.6 %, pointing out that for higher concentrated elemental solutions the change in density has to be considered.

Table S04 Densities Determined by Pycnometry and Inter- and Extrapolated Densities for Solutions with Different Mg Mass Fractions.

Mg mass fraction in mg/kg	Measured density in kg/m ³ Value	<i>U</i> (<i>k</i> = 2)	Fitted density in kg/m ³ Value	<i>U</i> (<i>k</i> = 2)
0	-	-	1008.44	1.01
2	1008.30	0.40	1008.45	0.40 ^a
10	1008.74	-	1008.50	0.40 ^a
20	-	-	1008.57	0.40 ^a
100	1008.99	-	1009.08	0.40 ^a
1000	1014.88	0.41	1014.87	0.41 ^a

^a Uncertainties were later expanded to 0.1 % rel. to account for additional sources of uncertainty (text).

The density of the 0.02 g/g HNO₃ was determined from the linear regression calculated for a Mg mass fraction of 0, which yielded a value of 1008.44 kg/m³. An uncertainty of 0.1 % was assigned for this value, to account for the fact that this is an extrapolated value (outside the initial calibration region), and that the uncertainty of the Mg mass fraction, or other systematic effects such as temperature offset or drift were not considered before. Due to the same reasons, this increased uncertainty of 0.1 % was also assigned to all other values resulting from the regression fit.

S3.2 Determination of Magnesium Isotope Solid Densities

The densities of three disks of magnesium, singly sublimated from high purity Mg (purity > 0.99 g/g) with natural-like isotopic composition were measured with high accuracy at PTB using hydrostatic weighing. After sublimation, the purity of this material will have improved; most impurities, excepting Zn, will have reduced close to or even below 1 mg/kg. Oxygen will be present in form of an oxide layer, as the density measurements could not be carried out immediately after the sublimation. However, all those factors are not expected to increase the uncertainty of the determined density.

The density of the three magnesium sublimate disks was determined as 1730 kg/m³ at 20 °C. This value is in excellent agreement with literature values for bulk magnesium (1738 kg/m³, [3]). The expanded uncertainty was conservatively estimated to be 1 % (for $k = 2$) based on previous experiences.

Due to the limited amounts and high costs of magnesium isotopes, direct determinations of their solid densities was prohibited; instead, the value determined for native Mg sublimate disk was recalculated into an expected value for the isotope – assuming that in the isotopically enriched materials only the atomic mass is changed, and all other parameters such as lattice constants remain the same; for this purpose, published high-accuracy isotope masses [4] were used. Additionally, the isotopic compositions of the enriched materials as provided by ORNL were used to calculate the average molar mass of the enriched materials, as they were sufficiently accurate for this purpose. This was verified later with the accurate isotopic compositions measured. For the natural-like Mg, the IUPAC atomic weight was used [4]. Small differences in the isotopic composition of natural Mg, and also the remaining impurities in the enriched isotopes were considered negligible. The densities calculated for the three isotopically enriched materials in this way are listed in Table S05 together with their expanded uncertainties ($k = 2$).

Table S05 Densities as Determined for Natural-Like Mg and as Calculated for the Enriched Magnesium Isotopes with their Expanded Uncertainties U ($k = 2$).

Material	Measured Density / (kg/m ³)	Calculated Density / (kg/m ³)
Mg (native)	1730 ± 17	-
²⁴ Mg ^a	-	1707 ± 17
²⁵ Mg ^a	-	1777 ± 17
²⁶ Mg ^a	-	1849 ± 18

40 S4 Purification of Magnesium Isotopes

Table S06 Allotments of Isotopically Enriched Materials, and Recoveries During the Five Sublimation Cycles for Purification.

step	²⁴ Mg ^a	²⁵ Mg ^a	²⁶ Mg ^a
ORNL delivered	200.45 mg	200.46 mg	200.69 mg
Redirected for analysis	4.12 mg	4.68 mg	5.79 mg
Redirected for analysis	2.1 %	2.3 %	2.9 %
Introduced into 1 st cycle	196.33 mg	195.78 mg	194.90 mg
Recovered from 1 st cycle	191.89 mg	188.12 mg	190.21 mg
Recovery over 1 st cycle	97.7 %	96.1 %	97.6 %
Introduced into 2 nd cycle	192.68 mg ^a	187.92 mg	190.21 mg
Recovered from 2 nd cycle	186.00 mg	183.71 mg	188.28 mg
Recovery over 2 nd cycle	96.5 %	97.8 %	99.0 %
Introduced into 3 rd cycle	185.86 mg	183.45 mg	188.14 mg
Recovered from 3 rd cycle	182.23 mg	181.07 mg	185.85 mg
Recovery over 3 rd cycle	98.1 %	98.7 %	98.5 %
Introduced into 4 th cycle	182.14 mg	180.95 mg	185.74 mg
Recovered from 4 th cycle	180.32 mg	178.75 mg	183.70 mg
Recovery over 4 th cycle	99.0 %	98.8 %	98.9 %
Introduced into 5 th cycle	180.32 mg	176.03 mg ^b	183.69 mg
Recovered from 5 th cycle	177.39488 mg	173.25404 mg	181.81282 mg
Recovery over 5 th cycle	98.4 %	98.4 %	99.0 %
Recovery over all cycles	90.4 %	88.5 %	93.3 %

^a Additional residue from the lid's border area was recovered and combined later with the body, causing a higher starting mass of cycle 2.

^b The first approach for the 5th cycle was incomplete and had to be repeated, resulting in a loss of 2 mg between 4th and 5th cycle.

The five sublimation cycles used for the purification of the isotopically enriched Mg materials cause only minor fractionation which is less than 0.2 ‰ per amu; more details will be given in the follow-up paper, which describes the mass spectrometric measurements. This is not significant and additionally it does not contribute to the results, because the isotopically enriched materials were characterised after purification.

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S5 Determination of Purity

After digestion of the isotopically enriched magnesium materials (after their purification by sublimation), the mass fractions of impurities were determined using ICPMS; Zn (as the known major impurity) was determined specifically using IDMS. Tables S07 and S08 reflect the determined values. See main text for details on the analysis.

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Table S07 Trace Levels of Enriched Magnesium Isotopes after Purification, Stated as Mass Fractions in the Solid Matrix ^a. Unit: 10⁻⁶ g/g.

El.	" ²⁴ Mg"	" ²⁵ Mg"	" ²⁶ Mg"	LOD	LOQ
Li		< LOD		0.0050	0.015
Be		< LOD		0.017	0.050
B	2.9±0.87	3.0±0.89	2.8±0.84	0.89	2.7
C	not expected (good separation)			N.A.	
N	3±3 (estimate of upper bound)			N.A.	
O	15±15 (estimate of upper bound)			N.A.	
F	not expected (good CI separation)			N.A.	
Na	3.6±1.1	8.6±2.6	< LOD	0.76	2.3
Mg	Matrix (see below in summary).			N.A.	
Al	0.61±0.18	0.69±0.21	3.2±0.97	0.079	0.24
Si		< LOD		0.50	1.5
P		< LOD		0.52	1.5
S		< LOD		9.5	28.6
Cl	not expected (based on GDMS)			N.A.	
K		< LOD		0.88	2.7
Ca	(1.3±0.77)	3.0±0.91	(0.26±0.26)	0.51	1.5
Sc		< LOD		0.0027	0.0081
Ti	0.054±0.016		< LOD	0.027	0.080
V		< LOD		0.0012	0.0037
Cr	0.028±0.014	0.13±0.040	0.043±0.013	0.010	0.029
Mn		< LOD		0.027	0.082
Fe	1.2±0.37	1.0±0.30	0.73±0.22	0.067	0.20
Co		< LOD		0.028	0.084
Ni		< LOD		0.20	0.61
Cu	(0.049±0.037)	0.14±0.041	0.081±0.025	0.025	0.075
Zn	52.20±0.20	194.98±0.71	957.4±3.1	IDMS Results	
Ga		< LOD		0.0036	0.011
Ge		< LOD		0.20	0.60
As		< LOD		0.092	0.28
Se		< LOD		0.73	2.2
Br	not expected (based on GDMS)			N.A.	
Rb	(0.0010±0.0007)	< LOD		0.0005	0.0014
Sr	0.0060±0.0018	0.0082±0.0025	0.0072±0.0022	0.0015	0.0046
Y	Used as internal standard.			N.A.	
Zr		< LOD		0.29	0.87
Nb		< LOD		0.00027	0.00080
Mo		< LOD		0.095	0.29
Tc	Not expected (no stable isotope).			N.A.	
Ru		< LOD		0.00028	0.00084
Rh		< LOD		0.00058	0.0017
Pd		< LOD		0.21	0.62
Ag	< LOD	0.013±0.0040	0.016±0.0047	0.0029	0.0086
Cd	6.5±2.0	22.5±6.7	56.8±17.0	0.0010	0.0031
In		< LOD		0.0011	0.0034
Sn	(0.086±0.048)		< LOD	0.032	0.096
Sb		< LOD		0.0018	0.0054
Te		< LOD		0.046	0.14
I	not expected (based on GDMS)			N.A.	
Cs		< LOD		0.00011	0.00034
Ba	(0.029±0.0086)	(0.019±0.0057)	(0.024±0.0071)	0.0011	0.0034
La	< LOD	(0.00046±0.00027)	< LOD	0.00018	0.00054
	Lanthanoids, see separate table				
Hf		< LOD		0.25	0.76
Ta		< LOD		0.00019	0.00057
W		< LOD		0.0036	0.011
Re		< LOD		0.00058	0.0017
Os		< LOD		0.011	0.033
Ir		< LOD		0.00084	0.0025
Pt		< LOD		0.0041	0.012
Au		< LOD		0.0043	0.013
Hg	0.087±0.026	< LOD	(0.023±0.023)	0.015	0.046
Tl	< LOD		0.067±0.020	0.013	0.039
Pb	0.029±0.0087	0.089±0.027	0.041±0.012	0.00088	0.0027
Bi		< LOD		0.26	0.78
	Po, At, Rn, Fr, Ra, Actinides not expected				
Th		< LOD		0.0028	0.0084
U		< LOD		0.00021	0.00064

^a See text in main part of paper for details.

5 Table S08 Trace Levels of Enriched Magnesium Isotopes after Purification – Lanthanoids. Unit: 10⁻⁶ g/g.

	" ²⁴ Mg"	" ²⁵ Mg"	" ²⁶ Mg"	LOD	LOQ
Ce	(0.0013±0.0008)	(0.0033±0.0010)	< LOD	0.00050	0.0015
Pr		< LOD		0.00083	0.0025
Nd	< LOD	0.0029±0.0009	< LOD	0.00058	0.0018
Pm	Not expected (no stable isotope).			N.A.	
Sm		< LOD		0.00035	0.0011
Eu		< LOD		0.000057	0.00017
Gd		< LOD		0.00030	0.00089
Tb		< LOD		0.00014	0.00041
Dy		< LOD		0.00017	0.00052
Ho		< LOD		0.000067	0.00020
Er		< LOD		0.00015	0.00044
Tm		< LOD		0.000061	0.00018
Yb		< LOD		0.00018	0.00054
Lu		< LOD		0.00062	0.0019

S6 Mixing of the Solutions of Isotopically Enriched Materials

Table S09 Preparation of Intermediate Dilutions at 100 mg/kg Level.

Parameter	²⁴ Mg ^a	<i>U</i> (<i>k</i> = 2)	Type ^a	source
Weighing, Empty PFA Bottle				
<i>W</i> (PFA Bottle) / g, <i>N</i> = 5	44.633036	0.000132 ^d	A	AX-205
Temperature <i>θ</i> / °C	23.9	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	51.2	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1007.9	10	B(n)	upper bound
Density PFA / (kg/m ³)	2150	100	B(r)	upper bound
Density balance / (kg/m ³)	8000	100	B(r)	upper bound
Air density / (kg/m ³)	1.175	0.015	R	Equation 3
Buoyancy cor. <i>K</i> / (g/g)	1.000400	0.000030	R	Equation 2
<i>m</i> (PFA Bottle) / g	44.6509	0.0013	R	Equation 1
Weighing, Parent Solution ²⁴ Mg ^a Material				
Mg mass fraction / (mg/kg) ^b	999.414	0.040	R	Equation 5
<i>W</i> (container full) / g, <i>N</i> = 2 ^c	29.335745	0.000095 ^d	A	AX-205
<i>W</i> (container empty) / g, <i>N</i> = 2	19.020680	0.000071 ^d	A	AX-205
<i>W</i> (solution, net value) / g	10.31507	0.00012	R	difference
Temperature <i>θ</i> / °C	24.8	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	44.8	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1010.6	10	B(n)	upper bound
Density solution <i>ρ</i> _{sol} / (kg/m ³)	1014.9	1.0	B(r)	pycnometer
Density balance / (kg/m ³)	8000	100	B(r)	upper bound
Air density / (kg/m ³)	1.176	0.015	R	Equation 3
Buoyancy cor. <i>K</i> / (g/g)	1.001013	0.000013	R	Equation 2
<i>m</i> (solution, net value) / g	10.32551	0.00018	R	Equation 1
Total Mass of Solution Before 1 st Use				
<i>W</i> _{total} (Bottle+Sol.) / g, <i>N</i> = 3	147.883330	0.000376 ^d	A	AX-205
Temperature <i>θ</i> / °C	24.0	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	48.3	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1003.2	10	B(n)	upper bound
Density solution <i>ρ</i> _{sol} / (kg/m ³)	1009.08	0.1 %	B(r)	pycnometer
Density balance / (kg/m ³)	8000	100 kg/m ³	B(r)	upper bound
Air density / (kg/m ³)	1.170	0.015	R	Equation 3
Net <i>W</i> (Solution) / g	103.250213	0.00051	R	Difference
Buoyancy cor. <i>K</i> / (g/g)	1.001014	0.000013	R	Equation 2
<i>m</i> (Solution) / g	103.35496	0.00018	R	Equation 1
Mass Fraction of Intermediate Dilution				
Mg mass fraction / (mg/kg)	99.8448	0.0042	R	Dilution ^e

^a Type A (observation), Type B: “n” denoting normal distribution, “r” denoting rectangular distribution. Type “R”: intermediate or final result.

5 ^b This mass fraction is based on new weighing data directly prior to dilution, and reflects evaporation loss of water since the preparation of the parent solution; compare the difference to values in table 04 (main part).

10 ^c The parent solution was transferred to the dilution container via a PFA bottle. The amount of solution was determined by difference weighing of the flask filled, and after quantitative transfer of the parent solution into the container of the dilution.

15 ^d Based on the balance calibration report according to EURAMET guide cg-18, and represents the uncertainty of the weighing values. It is one input parameter for the uncertainty budget. In the uncertainty budget, the uncertainty introduced into the buoyancy correction based on the weather data⁷ uncertainty is independently calculated.

^e Based on the simple dilution formula:

$$W_{Mg} = W_{Mg,parent} \frac{m_{parent\ solution}}{m_{total\ solution}} = 999.432\ mg/kg \cdot \frac{10.32551\ g}{103.35496\ g}$$

20 **Table S10** Preparation of a Binary Mixture at the 2 x 10 mg/kg Level for the Example of Mixture “24”+“26”-1b. Annotations: see Table S09.

Parameter	²⁴ Mg ^a	<i>U</i> (<i>k</i> = 2)	Type ^a	source
Weighing, Empty PFA Bottle				
<i>W</i> (PFA Bottle) / g, <i>N</i> = 5	45.256666	0.000133 ^d	A	AX-205
Temperature <i>θ</i> / °C	24.5	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	49.5	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1009.7	10	B(n)	upper bound
Density PFA / (kg/m ³)	2150	100	B(r)	upper bound
Density balance / (kg/m ³)	8000	100	B(r)	upper bound
Air density / (kg/m ³)	1.175	0.015	R	Equation 3
Buoyancy cor. <i>K</i> / (g/g)	1.000400	0.000030	R	Equation 2
<i>m</i> (PFA Bottle) / g	45.2748	0.0014	R	Equation 1
Weighing, Intermediate Solution ²⁴ Mg ^a Material				
Mg mass fraction / (mg/kg) ^b	99.8448	0.0042	R	Equation 5
<i>W</i> (container full) / g, <i>N</i> = 2 ^c	31.171450	0.000100 ^d	A	AX-205
<i>W</i> (container empty) / g, <i>N</i> = 2	20.842525	0.000075 ^d	A	AX-205
<i>W</i> (solution, net value) / g	10.32893	0.00012	R	difference
Temperature <i>θ</i> / °C	24.2	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	48.4	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1003.2	10	B(n)	upper bound
Density solution <i>ρ</i> _{sol} / (kg/m ³)	1009.1	1.0	B(r)	pycnometer
Density balance / (kg/m ³)	8000	100	B(r)	upper bound
Air density / (kg/m ³)	1.169	0.015	R	Equation 3
Buoyancy cor. <i>K</i> / (g/g)	1.001014	0.000013	R	Equation 2
<i>m</i> (solution, net value) / g	10.33939	0.00018	R	Equation 1
Weighing, Intermediate Solution ²⁶ Mg ^a Material				
Mg mass fraction / (mg/kg) ^b	99.6533	0.0053	R	Equation 5
<i>W</i> (container full) / g, <i>N</i> = 2 ^c	41.920915	0.000125 ^d	A	AX-205
<i>W</i> (container empty) / g, <i>N</i> = 2	31.830175	0.000101 ^d	A	AX-205
<i>W</i> (solution, net value) / g	10.09074	0.00016	R	difference
Temperature <i>θ</i> / °C	24.5	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	51.8	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1002.0	10	B(n)	upper bound
Density solution <i>ρ</i> _{sol} / (kg/m ³)	1009.1	1.0	B(r)	pycnometer
Air density / (kg/m ³)	1.166	0.015	R	Equation 3
Buoyancy cor. <i>K</i> / (g/g)	1.001011	0.000013	R	Equation 2
<i>m</i> (solution, net value) / g	10.10094	0.00021	R	Equation 1
Total Mass of Solution Before 1 st Use				
<i>W</i> _{total} (Bottle+Sol.) / g, <i>N</i> = 3	148.987533	0.000380 ^d	A	AX-205
Temperature <i>θ</i> / °C	24.5	2	B(n)	upper bound
Rel. Humidity <i>φ</i> / %	49.7	6	B(n)	upper bound
Abs. Pressure <i>p</i> / hPa	1002.7	10	B(n)	upper bound
Density solution <i>ρ</i> _{sol} / (kg/m ³)	1008.6	1.0	B(r)	pycnometer
Air density / (kg/m ³)	1.167	0.015	R	Equation 3
Net <i>W</i> (Solution) / g	103.73074	0.00051	R	Difference
Buoyancy cor. <i>K</i> / (g/g)	1.001012	0.000013	R	Equation 2
<i>m</i> (Solution) / g	103.8357	0.0016	R	Equation 1
Masses, Binary Mixture “24”+“26”-1b				
²⁴ Mg ^a in solution / mg	1.032335	0.000043	R	Calculated
²⁶ Mg ^a in solution / mg	1.006593	0.000054	R	Calculated

Notes and references

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‡ Note that only absolute mass (in kg) is defined by the SI system, and that it is a desirable quantity since it allows to determine amount of substance.

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