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PAPER

Characterization of a New Absolute Isotope Reference Material for Magnesium: *ab initio* Calibration of the Mass Spectrometers, and Determination of Isotopic Compositions and Relative Atomic Weights

– ELECTRONIC SUPPLEMENT

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S1 Preparation of Candidate Solutions

Setup calculations and the actual setup for the preparation of the three candidates ERM-AE143, -AE144 and -AE145 are shown in Table S1.

Table S1 Initial Dissolution of the magnesium IRM candidates[a].

	Cand. ERM-AE143	Cand. ERM-AE144	Cand. ERM-AE145 [d]
Mass PFA bottle / g, $N = 10$	314.38593	330.51866	67.78299
Mass of Mg metal / g, $N = 10$	2.14347825	2.019622	0.1780076
	Setup calculations		
Mg target mass fraction / (µg/g)	1000	1000	2000
Target mass of solution / g	2143.478	2019.622	89.004
HNO_3 target mass fraction / (g/g)	0.020	0.020	0.015
Required HNO_3 for dissolution / g	11.1143	10.4721	0.9230
Required HNO_3 in final sol. / g	42.8696	40.3924	0.8900
Sum required mass of HNO_3 / g	53.9839	50.8646	2.2581
Mass fraction[a] of HNO_3 / (g/g)	0.060001	0.060001	0.059979
Required mass 0.06 g/g HNO_3 / g	899.7123	847.7244	37.6482
	Actual setup, HNO_3 addition		
Mass of 0.06 g/g HNO_3 / g	900.0460	848.1654	37.698405
Mass fraction[a] of HNO_3 / (g/g)	0.060001	0.060001	0.059979
Mass of HNO_3 added / g	54.0039	50.8910	2.261113
Mass HNO_3 after digestion / g [b]	899.5104	847.8193	37.673497
Obs. total mass loss / g	0.5356	0.3461	0.0249
Expected mass loss due to H_2 / g	0.1778	0.1675	0.0148
Obs. additional mass loss / g [c]	0.3578	0.1786	0.0101
	Actual setup, fill-up with water		
Mass of water added / g	1243.6238	1170.8520	51.30
Total mass of solution / g	2145.2723	2020.7119	89.8900
Mg mass fraction / (mg/kg)	999.16	999.46	1995.80 [d]
Remaining HNO3 / g	42.8896	40.4189	1.3381
HNO_3 mass fraction / (g/g)	0.019993	0.020002	0.015003 [d]

[a] ERM-AE145 was dissolved first to test the dissolution conditions; ERM-AE143 and -AE144 were dissolved separately.

[b] Mass of solution after digestion, minus the mass of magnesium.

[c] Mass difference between acid filled in, and mass of acid determined later, minus the calculated stoichiometric mass loss due to H_2 formation.

[d] Note: this initial solution was later transferred into a solution of 0.02 g/g HNO_3 by adding 0.509 mL of conc. HNO_3 (0.65 g/g), for details see text.

S2 Raw Data

A number of individual calibration sequences were measured and evaluated. One sequence ("-1b-3", BAM) is evaluated as an example in this paper to demonstrate the procedure. Table S01 compiles the blank corrected raw data from all runs, both signal intensity as well as signal ratios.

Table S2a Blank-corrected data, sample sequence (BAM, "-1b-3").
Part a): Drift standard initial measurement and IRM candidates.

Run #	Sample (iteration)	*R*(25/24) / (V/V)	*R*(26/24) / (V/V)
		Drift standard, initial measurement	
3	Standard, 1	0.1355317	0.1593208
6	2	0.1355302	0.1593149
9	3	0.1355206	0.1592927
12	4	0.1355152	0.1592767
15	5	0.1355100	0.1592672
		Candidate 3	
18	Candidate 3, 1	0.1355250	0.1592997
21	2	0.1355243	0.1592904
24	3	0.1355214	0.1592832
27	4	0.1355139	0.1592727
30	5	0.1355114	0.1592632
		Drift standard	
33	Standard, 6	0.1354859	0.1592074
		Candidate 2	
36	Candidate 2, 1	0.1354835	0.1592040
39	2	0.1354784	0.1591979
42	3	0.1354760	0.1591918
45	4	0.1354727	0.1591848
48	5	0.1354717	0.1591828
		Drift standard	
51	Standard, 7	0.1354690	0.1591728
		Candidate 1	
54	Candidate 1, 1	0.1355822	0.1594348
57	2	0.1355762	0.1594263
60	3	0.1355803	0.1594290
63	4	0.1355738	0.1594159
66	5	0.1355712	0.1594170
		Drift standard	
69	Standard, 8	0.1354621	0.1591555

This data is the result of an outlier test, and the subtraction of blank values (after removal of outliers), from the individual cycles of the runs (50 before outlier removal, max. 11 outliers found in test sequence – typically less than 5 per cycle). The signal ratios were then drift-corrected; Table S02 compiles the results after drift correction for all runs. This data is the basis for the averaged data and standard uncertainties, which are fed into the evaluation (see table 05 in the main part)

Table S2b Blank-corrected data, sample sequence (BAM, "-1b-3"). Part b): Calibration mixtures and intermediate drift standards.

Run #	Sample (iteration)	*R*(25/24) / (V/V)	*R*(26/24) / (V/V)
		Drift standard	
69	Standard, 8	See Table 01a	
		Calibration mixtures "24"+"25"-1b	
72	"24"+"25"-1b, 1	1.009878	0.0037220
75	2	1.009846	0.0037205
78	3	1.009841	0.0037191
81	4	1.009888	0.0037107
84	5	1.009869	0.0037096
		Drift standard	
87	Standard, 9	0.1354514	0.1591328
90	Standard, 10	0.1354513	0.1591318
		Calibration mixtures "25"+"26"-1b	
93	"25"+"26"-1b, 1	46.432	51.249
96	2	46.425	51.241
99	3	46.423	51.238
102	4	46.421	51.235
105	5	46.410	51.223
		Drift standard	
108	Standard, 11	0.1354351	0.1591073
111	Standard, 12	0.1354397	0.1591071
		Calibration mixtures "24"+"26"-1b	
114	"24"+"26"-1b, 1	0.0022684	1.022096
117	2	0.0022723	1.022008
120	3	0.0022724	1.022030
123	4	0.0022693	1.021973
126	5	0.0022705	1.021986
		Drift standard	
129	Standard, 13	0.1354325	0.1590916

Table S2c Blank-corrected data, sample sequence (BAM, "-1b-3"). Part b): Isotopically enriched materials and intermediate drift standards.

Run #	Sample (iteration)	*R*(25/24) / (V/V)	*R*(26/24) / (V/V)
		Drift standard	
132	Standard, 14	0.1354370	0.1590974
		Enriched material "24"	
135	"24"-1b, 1	0.0008386	0.0007491
138	2	0.0008404	0.0007516
141	3	0.0008398	0.0007515
144	4	0.0008438	0.0007559
147	5	0.0008437	0.0007555
		Drift standard	
150	Standard, 15	0.1354268	0.1590791
153	Standard, 16	0.1354263	0.1590728
		Enriched material "25"	
156	"25"-1b, 1	56.961	0.168625
159	2	56.966	0.168628
162	3	56.966	0.168607
165	4	56.990	0.168554
168	5	56.970	0.168602
		Drift standard	
171	Standard, 17	0.1354211	0.1590654
174	Standard, 18	0.1354202	0.1590575
		Enriched material "26"	
177	"26"-1b, 1	0.38728	274.34
180	2	0.38646	273.95
183	3	0.38645	273.92
186	4	0.38638	273.71
189	5	0.38635	273.86
		Drift standard	
192	Standard, 19	0.1354154	0.1590597
195	Standard, 20	0.1354161	0.1590537

Table S3 Drift-corrected data, sample sequence (BAM, "-1b-3"), based on data in tables S1a to S1c.

Run #	Sample (iteration)	*R*(25/24) / (V/V)	*R*(26/24) / (V/V)
		Candidate 3	
18	Candidate 3, 1	0.1355406	0.1593370
21	2	0.1355439	0.1593377
24	3	0.1355450	0.1593404
27	4	0.1355415	0.1593399
30	5	0.1355430	0.1593403
		Candidate 2	
36	Candidate 2, 1	0.13552192	0.15929689
39	2	0.13551970	0.15929653
42	3	0.13552012	0.15929617
45	4	0.13551963	0.15929497
48	5	0.13552145	0.15929869
		Candidate 1	
54	Candidate 1, 1	0.1356359	0.1595596
57	2	0.1356311	0.1595539
60	3	0.1356363	0.1595595
63	4	0.1356310	0.1595494
66	5	0.1356295	0.1595533
		Calibration mixtures "24"+"25"-1b	
72	"24"+"25"-1b, 1	1.010334	0.0037254
75	2	1.010315	0.0037239
78	3	1.010323	0.0037227
81	4	1.010384	0.0037143
84	5	1.010378	0.0037132
		Calibration mixtures "25"+"26"-1b	
93	"25"+"26"-1b, 1	46.4571	51.3029
96	2	46.4511	51.2959
99	3	46.4502	51.2945
102	4	46.4486	51.2929
105	5	46.4383	51.2817
		Calibration mixtures "24"+"26"-1b	
114	"24"+"26"-1b, 1	0.0022698	1.023316
117	2	0.0022737	1.023245
120	3	0.0022738	1.023283
123	4	0.0022707	1.023244
126	5	0.0022719	1.023273
		Enriched material "24"	
135	"24"-1b, 1	0.0008391	0.0007500
138	2	0.0008410	0.0007526
141	3	0.0008403	0.0007525
144	4	0.0008443	0.0007569
147	5	0.0008443	0.0007565
		Enriched material "25"	
156	"25"-1b, 1	57.0012	0.168862
159	2	57.0069	0.168865
162	3	57.0072	0.168846
165	4	57.0315	0.168794
168	5	57.0120	0.168843
		Enriched material "26"	
177	"26"-1b, 1	0.38757	274.74
180	2	0.38675	274.36
183	3	0.38675	274.32
186	4	0.38668	274.11
189	5	0.38665	274.27

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S3 Evaluation Equations

The analytical solution to the underlying system of calibration equations allowed to set up an uncertainty budget using GUM Workbench, and to directly obtain uncertainty results for the evaluations of the experiments. The system of calibration equations as well as its analytical solution(s) can be obtained in the following way. Tables S4 and S5 compile all necessary symbols.

Table S4: Symbols of quantities needed to derive the evaluation equations

Symbol	Unit	Quantity
$R_{j,i}$	mol/mol	isotope amount ratio, i^{th} isotope divided by 1st isotope (^{24}Mg), in material *j*
R^{m}	V/V	measured signal intensity ratio
I	V	signal intensity (voltage)
n	mol	amount of substance
m	g	mass
M	g/mol	molar mass
x	mol/mol	amount-of-substance fraction
K	(mol/mol)/(V/V)	calibration factor

Table S5: Subscripts used throughout the derivation of the evaluation equations

Subscript	Meaning
1	isotope ^{24}Mg
2	isotope ^{25}Mg
3	isotope ^{26}Mg
A	Mg material enriched with respect to ^{24}Mg
B	Mg material enriched with respect to ^{25}Mg
C	Mg material enriched with respect to ^{26}Mg
AB	mixture prepared from materials A and B
BC	mixture prepared from materials B and C
AC	mixture prepared from materials A and C

The mixing scheme (Fig. S1) shows that up to 12 signal intensity ratios R^{m} in total could be measured, which represent the two independent isotope amount ratios $R_{j,2} = n(^{25}\text{Mg})/n(^{24}\text{Mg})$ and $R_{j,3} = n(^{26}\text{Mg})/n(^{24}\text{Mg})$ in the three parent materials and in the three mixtures. To be able to determine the 2 calibration factors (mass discrimination correction factors) K from the measurement(s), only 2 out of the 3 mixtures and a set of merely 8 signal intensity ratios R^{m} and 4 masses m are required. But even when focusing on 2 mixtures, 4 mathematically equivalent solutions can be obtained, because apart from the 6 signal intensity ratios in the parent materials A, B, and C only 1 intensity ratio in each of the 2 mixtures is necessary. Fig. S2 shows how this leads to 4 possible combinations and in turn to 4 mathematically equivalent solutions.

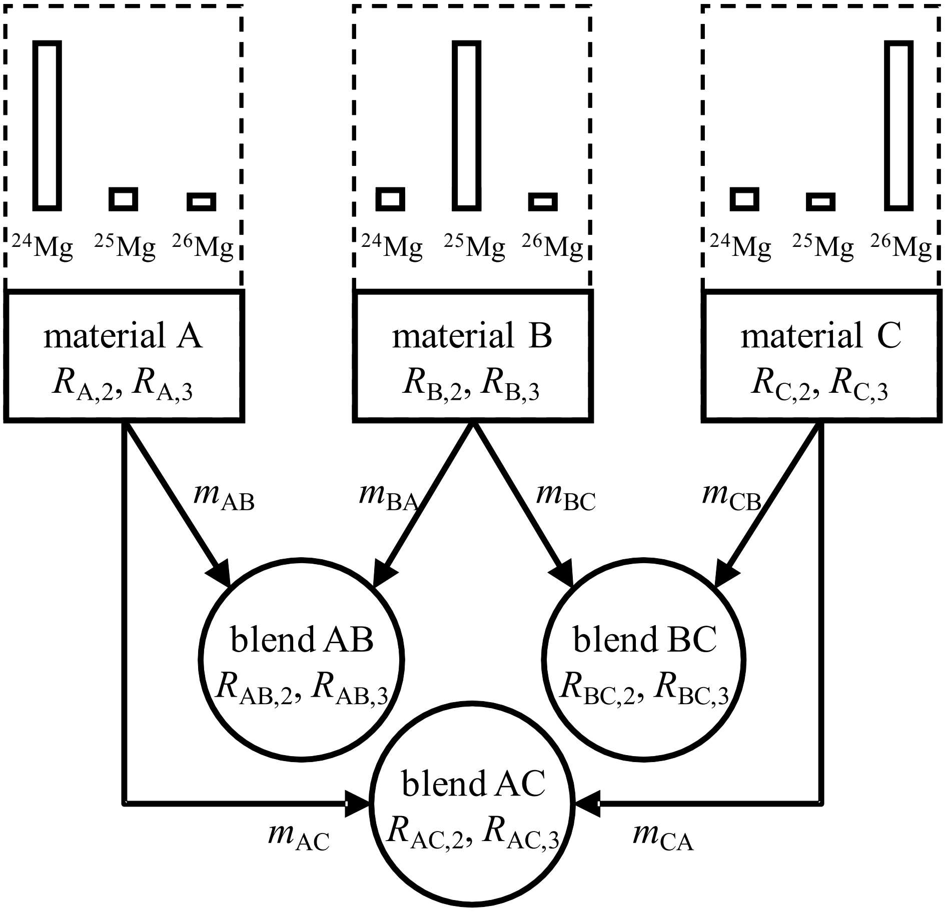

Fig. S1: Preparation of the three isotope mixtures AB ("^{24}Mg" plus "^{25}Mg"), BC ("^{25}Mg" plus "^{26}Mg"), and AC ("^{24}Mg" plus "^{26}Mg") from the isotopically enriched so-called parent materials A ("^{24}Mg"), B ("^{25}Mg"), and C ("^{26}Mg"). Suitable masses like e.g. m_{AB}, mass of solid material A mixed with material B to yield mixture AB, or m_{BA}, mass of solid material B mixed with material A to yield mixture AB, were blended via masses of their respective solutions.

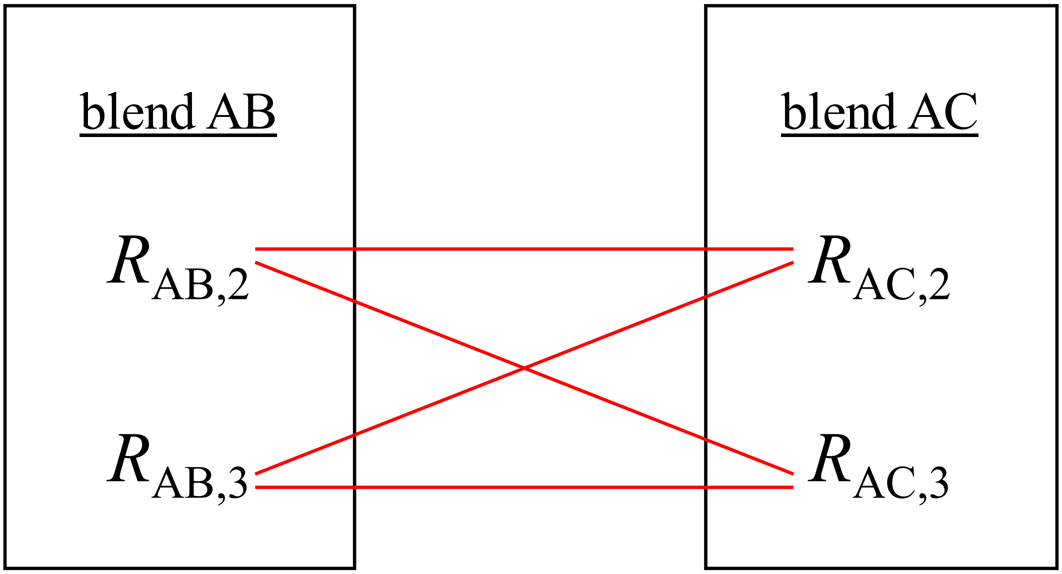

Fig. S2: Selecting 1 signal intensity ratio from each of the 2 mixtures AB and AC, leads to 4 possible (and entirely equivalent) combinations required to obtain a mathematical solution for the calibration factors.

Since 3 pairs of mixtures can be selected (AB + AC, AB + BC, and BC + AC), each enabling 4 mathematical solutions, all in all 12 mathematically entirely equivalent solutions to determine/calculate the calibration factors are available. These solutions along with their assigned index (to distinguish between them) are listed in Table S6.

Table S6: Possible combination of pairs of mixtures and selection of signal intensity ratios within these mixtures yields 12 equivalent mathematical solutions to determine/calculate the calibration factors. Numbers in the first column have the following meaning: 2 = $I(^{25}\mathrm{Mg})/I(^{24}\mathrm{Mg})$ and 3 = $I(^{26}\mathrm{Mg})/I(^{24}\mathrm{Mg})$. Numbers assigned to a specific combination will be used in the following as indices to distinguish between these solutions.

	AB + AC	**AB + BC**	**BC + AC**
2 + 2	01	05	09
2 + 3	02	06	10
3 + 2	03	07	11
3 + 3	04	08	12

The isotope amount ratio $R_{\mathrm{AB},2}$ in mixture AB is connected to the respective measured signal intensity ratio via the calibration factor K_2. It simply is the amount-of-substance ratio of the isotopes 2 (^{25}Mg) and 1 (^{24}Mg). This in turn can be expressed as the respective sums of amounts of the isotopes from the parent materials A and B. The amount of substance $n_{\mathrm{A},2}$ of ^{25}Mg from parent material A is the product of the respective amount-of-substance fraction $x_{\mathrm{A},2}$ and the total amount of substance n_A brought into the mixture AB from material A (Eqn. S1).

$$R_{\mathrm{AB},2} = K_2 \cdot R^{\mathrm{m}}_{\mathrm{AB},2} = \frac{n_{\mathrm{AB},2}}{n_{\mathrm{AB},1}} = \frac{n_{\mathrm{A},2} + n_{\mathrm{B},2}}{n_{\mathrm{A},1} + n_{\mathrm{B},1}} = \frac{x_{\mathrm{A},2} \cdot n_\mathrm{A} + x_{\mathrm{B},2} \cdot n_\mathrm{B}}{x_{\mathrm{A},1} \cdot n_\mathrm{A} + x_{\mathrm{B},1} \cdot n_\mathrm{B}} \tag{S1}$$

The amount-of-substance fractions can be replaced with the respective amount ratios (Eqn. S2).

$$K_2 \cdot R^{\mathrm{m}}_{\mathrm{AB},2} = \frac{x_{\mathrm{A},2} \cdot n_\mathrm{A} + x_{\mathrm{B},2} \cdot n_\mathrm{B}}{x_{\mathrm{A},1} \cdot n_\mathrm{A} + x_{\mathrm{B},1} \cdot n_\mathrm{B}} = \frac{\frac{R_{\mathrm{A},2}}{1 + R_{\mathrm{A},2} + R_{\mathrm{A},3}} \cdot n_\mathrm{A} + \frac{R_{\mathrm{B},2}}{1 + R_{\mathrm{B},2} + R_{\mathrm{B},3}} \cdot n_\mathrm{B}}{\frac{1}{1 + R_{\mathrm{A},2} + R_{\mathrm{A},3}} \cdot n_\mathrm{A} + \frac{1}{1 + R_{\mathrm{B},2} + R_{\mathrm{B},3}} \cdot n_\mathrm{B}} \tag{S2}$$

On the right-hand side of Eqn. S2, since they are unknown, the amount ratios should be expressed as measured signal intensity ratios (Eqn. S3). Calibration factor K_3 is introduced into the equation the same way.

$$K_2 \cdot R^{\mathrm{m}}_{\mathrm{AB},2} = \frac{\frac{K_2 \cdot R^{\mathrm{m}}_{\mathrm{A},2}}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{A},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{A},3}} \cdot n_\mathrm{A} + \frac{K_2 \cdot R^{\mathrm{m}}_{\mathrm{B},2}}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{B},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{B},3}} \cdot n_\mathrm{B}}{\frac{1}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{A},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{A},3}} \cdot n_\mathrm{A} + \frac{1}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{B},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{B},3}} \cdot n_\mathrm{B}} \tag{S3}$$

Dividing eqn. S3 by K_2 yields eqn. S4:

$$R^{\mathrm{m}}_{\mathrm{AB},2} = \frac{\frac{R^{\mathrm{m}}_{\mathrm{A},2}}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{A},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{A},3}} \cdot n_\mathrm{A} + \frac{R^{\mathrm{m}}_{\mathrm{B},2}}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{B},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{B},3}} \cdot n_\mathrm{B}}{\frac{1}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{A},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{A},3}} \cdot n_\mathrm{A} + \frac{1}{1 + K_2 \cdot R^{\mathrm{m}}_{\mathrm{B},2} + K_3 \cdot R^{\mathrm{m}}_{\mathrm{B},3}} \cdot n_\mathrm{B}} \tag{S4}$$

In the next step the amounts n_A and n_B should be replaced yielding expressions based on the signal intensity ratios and masses (Eqns. S5 and S6).

$$n_{\mathrm{A}}=\frac{m_{\mathrm{A}}}{M_{\mathrm{A}}}=\frac{m_{\mathrm{A}}}{x_{\mathrm{A},1}\cdot M_1+x_{\mathrm{A},2}\cdot M_2+x_{\mathrm{A},3}\cdot M_3}$$

$$n_{\mathrm{A}}=\frac{m_{\mathrm{A}}}{\frac{1}{1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}}\cdot M_1+\frac{K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}}{1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}}\cdot M_2+\frac{K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}}{1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}}\cdot M_3}$$

$$n_{\mathrm{A}}=\frac{m_{\mathrm{A}}}{\frac{1}{1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}}\cdot\left(M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\cdot M_3\right)}$$

$$n_{\mathrm{A}}=\frac{m_{\mathrm{A}}\cdot\left(1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\right)}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\cdot M_3} \tag{S5}$$

$$n_{\mathrm{B}}=\frac{m_{\mathrm{B}}\cdot\left(1+K_2\cdot R^{\mathrm{m}}_{\mathrm{B},2}+K_3\cdot R^{\mathrm{m}}_{\mathrm{B},3}\right)}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{B},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{B},3}\cdot M_3} \tag{S6}$$

Replacing n_{A} and n_{B} in Eqn. S4 with these expression yields Eqn. S7.

$$R^{\mathrm{m}}_{\mathrm{AB},2}=\frac{\frac{m_{\mathrm{A}}\cdot R^{\mathrm{m}}_{\mathrm{A},2}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\cdot M_3}+\frac{m_{\mathrm{B}}\cdot R^{\mathrm{m}}_{\mathrm{B},2}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{B},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{B},3}\cdot M_3}}{\frac{m_{\mathrm{A}}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\cdot M_3}+\frac{m_{\mathrm{B}}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{B},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{B},3}\cdot M_3}} \tag{S7}$$

A completely analogue expression can be derived in the case of the amount-of-substance ratio of the isotopes 3 (^{26}Mg) and 1 (^{24}Mg) to be found in mixture AC.

$$R^{\mathrm{m}}_{\mathrm{AC},3}=\frac{\frac{m_{\mathrm{A}}\cdot R^{\mathrm{m}}_{\mathrm{A},3}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\cdot M_3}+\frac{m_{\mathrm{C}}\cdot R^{\mathrm{m}}_{\mathrm{C},3}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{C},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{C},3}\cdot M_3}}{\frac{m_{\mathrm{A}}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{A},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{A},3}\cdot M_3}+\frac{m_{\mathrm{C}}}{M_1+K_2\cdot R^{\mathrm{m}}_{\mathrm{C},2}\cdot M_2+K_3\cdot R^{\mathrm{m}}_{\mathrm{C},3}\cdot M_3}} \tag{S8}$$

Apart from measured signal intensity ratios and masses as well as published molar masses of all Mg isotopes, Eqns. S7 and S8 contain merely the two unknown calibration factors K_2 and K_3. Therefore, after several rearrangement steps [1] the equations expressing the calibration factors can be written down explicitly.

$$K_2=\frac{M_1\cdot N_2}{M_2\cdot D}$$

$$K_3=-\frac{M_1\cdot N_3}{M_3\cdot D}$$

While both factors share D, N_i is different. D and N_i are different for each of the 12 combinations listed in Table S5 [2]. All these combinations are mathematically entirely equivalent and yield exactly the same result. In practice, when used with experimental data and its associated uncertainties, they each can yield significantly different results with quite different associated uncertainties. Since all results agree within the limits of their uncertainties, the uncertainties associated with a particular set of K factors are therefore already the criterions to decide which is the most suitable set. In the case of the Mg measurements described here, combination 02 yielded the smallest uncertainties of all sets, which is in perfect agreement with the theoretical prediction, that measuring in the mixture AB of "^{25}Mg" and "^{24}Mg" the signal intensity ratio "2" = $I(^{25}\mathrm{Mg})/I(^{24}\mathrm{Mg})$ and in mixture AC of "^{26}Mg" and "^{24}Mg" the signal intensity ratio "3" = $I(^{26}\mathrm{Mg})/I(^{24}\mathrm{Mg})$ would be preferable, since the mixtures were prepared in a way that these ratios were adjusted close to unity.

Combination 01:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},2}, R^{\mathrm{m}}_{\mathrm{AC},2}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)
\end{aligned}$$

Combination 02:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},2}, R^{\mathrm{m}}_{\mathrm{AC},3}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)
\end{aligned}$$

Combination 03:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},3}, R^{\mathrm{m}}_{\mathrm{AC},2}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)
\end{aligned}$$

Combination 04:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},3}, R^{\mathrm{m}}_{\mathrm{AC},3}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{AB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{AB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{AC}} m_{\mathrm{BA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)
\end{aligned}$$

Combination 05:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},2}, R^{\mathrm{m}}_{\mathrm{BC},2}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)
\end{aligned}$$

Combination 06:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},2}, R^{\mathrm{m}}_{\mathrm{BC},3}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{AB},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)
\end{aligned}$$

Combination 07:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},3}, R^{\mathrm{m}}_{\mathrm{BC},2}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)
\end{aligned}$$

Combination 08:

$$\underline{R^{\mathrm{m}}_{\mathrm{AB},3}, R^{\mathrm{m}}_{\mathrm{BC},3}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{A},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3} R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{AB},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{BA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{BA}} m_{\mathrm{CB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{BC}} m_{\mathrm{AB}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AB},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)
\end{aligned}$$

Combination 09:

$$\underline{R^{\mathrm{m}}_{\mathrm{BC},2}, R^{\mathrm{m}}_{\mathrm{AC},2}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{BC},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{BC},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{BC},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{A},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\
& + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)
\end{aligned}$$

Combination 10:

$$\underline{R^{\mathrm{m}}_{\mathrm{BC},2}, R^{\mathrm{m}}_{\mathrm{AC},3}}$$

$$\begin{aligned}
D = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{BC},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2}\right) \\
& + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{BC},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\
& + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{BC},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{A},2}\right)
\end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned}
N_2 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)
\end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned}
N_3 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\
& + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\
& + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)
\end{aligned}$$

Combination 11:

$$\underline{R^{\mathrm{m}}_{\mathrm{BC},3}, R^{\mathrm{m}}_{\mathrm{AC},2}}$$

$$\begin{aligned} D = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{BC},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2}\right) \\ & + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{BC},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right)\left(R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\ & + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{BC},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{A},2}\right) \end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned} N_2 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\ & + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\ & + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned} N_3 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \\ & + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{A},2}\right) \\ & + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right) \end{aligned}$$

Combination 12:

$$\underline{R^{\mathrm{m}}_{\mathrm{BC},3}, R^{\mathrm{m}}_{\mathrm{AC},3}}$$

$$\begin{aligned} D = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{BC},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{B},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3} R^{\mathrm{m}}_{\mathrm{A},2}\right) \\ & + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{BC},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right)\left(R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{B},2} - R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{B},3}\right) \\ & + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{B},3} - R^{\mathrm{m}}_{\mathrm{BC},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{C},2} R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3} R^{\mathrm{m}}_{\mathrm{A},2}\right) \end{aligned}$$

$$\underline{K_2}$$

$$\begin{aligned} N_2 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\ & + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\ & + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \end{aligned}$$

$$\underline{K_3}$$

$$\begin{aligned} N_3 = {} & m_{\mathrm{CB}} m_{\mathrm{CA}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \\ & + m_{\mathrm{CB}} m_{\mathrm{AC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{C},2} - R^{\mathrm{m}}_{\mathrm{B},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{A},3}\right) \\ & + m_{\mathrm{CA}} m_{\mathrm{BC}} \cdot \left(R^{\mathrm{m}}_{\mathrm{A},2} - R^{\mathrm{m}}_{\mathrm{C},2}\right)\left(R^{\mathrm{m}}_{\mathrm{BC},3} - R^{\mathrm{m}}_{\mathrm{B},3}\right)\left(R^{\mathrm{m}}_{\mathrm{AC},3} - R^{\mathrm{m}}_{\mathrm{C},3}\right) \end{aligned}$$

S4 Results of All Sequences

The data compiled in tables S6 to S8 show all results for the isotopic composition of the three IRM candidates measured with the calibrated mass spectrometers with associated expanded uncertainties (for $k = 2$) based on the uncertainty budgets; there is one table per laboratory (S6 shows data from LGC, S7 shows PTB data, and S8 data from BAM). Those data are also represented in graphical form in Fig. 7 in the main part of this publication. There are three sets of calibration mixtures, denoted 1b, 2b, and 3b (b denotes the fact that this is the second setup of calibration solutions; data from the first setup are only shown in one part of this paper, see Fig. 6 in the main part and the discussion). Only one set of calibration solutions was used per sequence. PTB measured three sequences per set of calibration mixture, which resulted in nine measured sequences in each of those labs; BAM measured one additional sequence, resulting in 10 measured sequences; LGC has measured one sequence per set of calibration mixtures, which resulted in three total sequences measured.

Table S7 All values (3 sequences) for absolute isotopic composition of the three IRM candidates measured at LGC, with expanded uncertainties ($k = 2$).

	Candidate		
Parameter	ERM-AE143	ERM-AE144	ERM-AE145
Isotope amount fractions			
	$x(^{24}\text{Mg})$ / (mol/mol)		
Solutions -1b	0.789931(18)	0.790132(19)	0.790065(19)
Solutions -2b	0.789972(19)	0.790167(19)	0.790079(24)
Solutions -3b	0.789967(20)	0.790165(26)	0.790066(27)
Average	0.789957(19)	0.790155(22)	0.790070(24)
$s(x(^{24}\text{Mg}))$/(mol/mol)	0.000022	0.000020	0.0000078
	$x(^{25}\text{Mg})$ / (mol/mol)		
Solutions -1b	0.099989(11)	0.099933(13)	0.099955(12)
Solutions -2b	0.099982(13)	0.099927(11)	0.099957(15)
Solutions -3b	0.099982(12)	0.099926(17)	0.099959(17)
Average	0.099984(12)	0.099929(14)	0.099957(15)
$s(x(^{25}\text{Mg}))$/(mol/mol)	0.0000039	0.0000038	0.0000021
	$x(^{26}\text{Mg})$ / (mol/mol)		
Solutions -1b	0.110080(16)	0.109935(16)	0.109980(17)
Solutions -2b	0.110045(17)	0.109906(18)	0.109963(22)
Solutions -3b	0.110052(18)	0.109909(23)	0.109975(25)
Average	0.110059(17)	0.109917(19)	0.109973(22)
$s(x(^{26}\text{Mg}))$/(mol/mol)	0.000018	0.000016	0.0000084
Isotope amount ratios			
	$n(^{25}\text{Mg})/n(^{24}\text{Mg})$ / (mol/mol)		
Solutions -1b	0.126579(16)	0.126477(18)	0.126514(16)
Solutions -2b	0.126564(18)	0.126464(15)	0.126515(21)
Solutions -3b	0.126565(17)	0.126462(24)	0.126520(24)
Average	0.126569(17)	0.126468(19)	0.126518(21)
$s(n(^{25}\text{Mg})/n(^{24}\text{Mg}))$	0.0000084	0.0000079	0.0000028
	$n(^{26}\text{Mg})/n(^{24}\text{Mg})$ / (mol/mol)		
Solutions -1b	0.139354(23)	0.139135(23)	0.139203(24)
Solutions -2b	0.139303(25)	0.139092(25)	0.139180(31)
Solutions -3b	0.139312(26)	0.139096(32)	0.139197(36)
Average	0.139323(25)	0.139108(27)	0.139193(31)
$s(n(^{26}\text{Mg})/n(^{24}\text{Mg}))$	0.000027	0.000024	0.000012
Relative atomic weights	$A_r(\text{Mg})$		
Solutions -1b	24.305001(32)	24.304655(32)	24.304766(34)
Solutions -2b	24.304925(35)	24.304591(35)	24.304736(43)
Solutions -3b	24.304937(37)	24.304597(45)	24.304760(49)
Average	24.304954(35)	24.304614(38)	24.304754(42)
$s(A_r(\text{Mg}))$	0.000041	0.000035	0.000016

Table S8 All values (9 sequences) for absolute isotopic composition of the three IRM candidates measured at PTB, with expanded uncertainties ($k = 2$).

	Candidate		
Parameter	ERM-AE143	ERM-AE144	ERM-AE145
Isotope amount fractions			
	$x(^{24}Mg)$ / (mol/mol)		
(Solutions -1b) 1	0.789958(18)	0.790166(18)	0.790109(19)
2	0.7899021(91)	0.7901089(91)	0.7900653(91)
3	0.7899100(92)	0.7901136(91)	0.7900719(93)
(Solutions -2b) 4	0.789900(10)	0.790102(10)	0.790066(10)
5	0.789912(13)	0.790115(13)	0.790077(13)
6	0.789907(10)	0.7901128(93)	0.7900714(92)
(Solutions -3b) 7	0.789912(11)	0.790116(10)	0.790073(11)
8	0.789941(26)	0.790138(41)	0.790114(25)
9	0.789967(11)	0.790160(10)	0.790124(11)
Average	0.789923(14)	0.790126(17)	0.790086(14)
$s(x(^{24}Mg))$/(mol/mol)	0.000025	0.000023	0.000023
	$x(^{25}Mg)$ / (mol/mol)		
(Solutions -1b) 1	0.099980(12)	0.099924(12)	0.099941(13)
2	0.1000030(55)	0.0999462(55)	0.0999622(56)
3	0.0999920(55)	0.0999358(55)	0.0999518(56)
(Solutions -2b) 4	0.1000080(67)	0.0999520(69)	0.0999660(66)
5	0.1000025(63)	0.0999454(62)	0.0999610(63)
6	0.1000037(55)	0.0999477(55)	0.0999624(54)
(Solutions -3b) 7	0.0999903(75)	0.0999353(74)	0.0999498(76)
8	0.099988(12)	0.099933(19)	0.099943(11)
9	0.0999752(63)	0.0999187(62)	0.0999367(65)
Average	0.0999936(79)	0.0999375(93)	0.0999527(79)
$s(x(^{25}Mg))$/(mol/mol)	0.000011	0.000011	0.000011
	$x(^{26}Mg)$ / (mol/mol)		
(Solutions -1b) 1	0.110062(16)	0.109911(16)	0.109949(17)
2	0.1100948(66)	0.1099449(66)	0.1099725(65)
3	0.1100980(66)	0.1099506(65)	0.1099762(67)
(Solutions -2b) 4	0.1100917(72)	0.1099460(72)	0.1099681(71)
5	0.110085(11)	0.109939(11)	0.109962(11)
6	0.1100891(72)	0.1099395(69)	0.1099662(68)
(Solutions -3b) 7	0.1100979(71)	0.1099490(68)	0.1099768(72)
8	0.110072(20)	0.109929(37)	0.109943(19)
9	0.1100575(86)	0.1099209(76)	0.1099389(77)
Average	0.110083(11)	0.109937(15)	0.109961(11)
$s(x(^{26}Mg))$/(mol/mol)	0.000016	0.000014	0.000014
Isotope amount ratios			
	$n(^{25}Mg)/n(^{24}Mg)$ / (mol/mol)		
(Solutions -1b) 1	0.126564(17)	0.126459(17)	0.126490(18)
2	0.1266018(80)	0.1264967(80)	0.1265240(82)
3	0.1265865(81)	0.1264829(81)	0.1265098(82)
(Solutions -2b) 4	0.126608(10)	0.126505(10)	0.126529(10)
5	0.1265995(91)	0.1264947(89)	0.1265207(92)
6	0.1266019(81)	0.1264980(80)	0.1265233(79)
(Solutions -3b) 7	0.126584(11)	0.126482(11)	0.126507(11)
8	0.126576(18)	0.126476(28)	0.126492(17)
9	0.1265561(92)	0.1264537(90)	0.126482(10)
Average	0.126586(12)	0.126483(14)	0.126509(12)
$s(n(^{25}Mg)/n(^{24}Mg))$	0.000018	0.000018	0.000017
	$n(^{26}Mg)/n(^{24}Mg)$ / (mol/mol)		
(Solutions -1b) 1	0.139326(23)	0.139098(23)	0.139157(24)
2	0.139378(10)	0.139152(10)	0.139194(10)
3	0.139380(10)	0.139158(10)	0.139198(10)
(Solutions -2b) 4	0.139374(11)	0.139154(10)	0.139189/10)
5	0.139364(16)	0.139143(16)	0.139179(16)
6	0.139370(11)	0.139144(10)	0.139185(10)
(Solutions -3b) 7	0.139380(10)	0.139156(10)	0.139198(10)
8	0.139342(30)	0.139127(54)	0.139148(28)
9	0.139319(13)	0.139112(11)	0.139141(11)
Average	0.139359(16)	0.139138(22)	0.139177(16)
$s(n(^{26}Mg)/n(^{24}Mg))$	0.000024	0.000021	0.000022
Relative atomic weights	$A_r(Mg)$		
(Solutions -1b) 1	24.304955(32)	24.304597(32)	24.304692(34)
2	24.305044(15)	24.304688(15)	24.304759(15)
3	24.305040(15)	24.304689(15)	24.304756(15)
(Solutions -2b) 4	24.305043(16)	24.304696(16)	24.304754(16)
5	24.305025(23)	24.304676(23)	24.304738(23)
6	24.305034(16)	24.304679(15)	24.304747(15)
(Solutions -3b) 7	24.305038(16)	24.304685(16)	24.304755(16)
8	24.304983(45)	24.304643(76)	24.304680(44)
9	24.304942(19)	24.304612(17)	24.304666(17)
Average	24.305011(24)	24.304663(31)	24.304728(24)
$s(A_r(Mg))$	0.000040	0.000036	0.000037

Table S9 All values (10 sequences) for the absolute isotopic composition of the three IRM candidates measured at BAM, with expanded uncertainties ($k = 2$).

Parameter	Candidate ERM-AE143	 ERM-AE144	 ERM-AE145
Isotope amount fractions			
	$x(^{24}\mathrm{Mg})$ / (mol/mol)		
(Solutions -1b) 1	0.789894(18)	0.790104(18)	0.790059(19)
2	0.789889(10)	0.790102(10)	0.7900632(98)
3	0.789880(11)	0.790087(10)	0.790051(10)
(Solutions -2b) 4	0.7899146(95)	0.7901237(96)	0.7900834(96)
5	0.789913(12)	0.790124(12)	0.790081(12)
6	0.789910(11)	0.790118(10)	0.7900787(98)
7	0.789921(10)	0.790126(10)	0.790083(10)
(Solutions -3b) 8	0.789913(12)	0.790121(12)	0.790084(12)
9	0.7899079(98)	0.790115(10)	0.7900698(98)
10	0.7899113(99)	0.790118(10)	0.7900731(97)
Average	0.789905(12)	0.790114(11)	0.790073(12)
$s(x(^{24}\mathrm{Mg}))$/(mol/mol)	0.000013	0.000013	0.000012
	$x(^{25}\mathrm{Mg})$ / (mol/mol)		
(Solutions -1b) 1	0.099999(13)	0.099941(13)	0.099957(13)
2	0.1000021(61)	0.0999450(58)	0.0999579(59)
3	0.1000066(72)	0.0999500(67)	0.0999618(69)
(Solutions -2b) 4	0.1000035(58)	0.0999459(57)	0.0999595(58)
5	0.1000004(71)	0.0999425(70)	0.0999570(70)
6	0.1000101(60)	0.0999528(59)	0.0999655(58)
7	0.1000009(57)	0.0999448(57)	0.0999582(57)
(Solutions -3b) 8	0.0999952(65)	0.0999378(61)	0.0999498(62)
9	0.0999943(56)	0.0999387(61)	0.0999541(56)
10	0.0999989(63)	0.0999435(64)	0.0999570(60)
Average	0.1000011(72)	0.0999442(72)	0.0999577(71)
$s(x(^{25}\mathrm{Mg}))$/(mol/mol)	0.0000048	0.0000046	0.0000042
	$x(^{26}\mathrm{Mg})$ / (mol/mol)		
(Solutions -1b) 1	0.110107(15)	0.109955(15)	0.109985(15)
2	0.1101085(76)	0.1099534(79)	0.1099789(74)
3	0.1101129(83)	0.1099633(76)	0.1099875(76)
(Solutions -2b) 4	0.1100820(70)	0.1099305(72)	0.1099570(72)
5	0.1100866(88)	0.1099337(89)	0.1099615(89)
6	0.1100804(84)	0.1099292(78)	0.1099558(74)
7	0.1100783(82)	0.1099288(85)	0.1099585(82)
(Solutions -3b) 8	0.110092(10)	0.109941(10)	0.109966(10)
9	0.1100978(76)	0.1099465(77)	0.1099760(76)
10	0.1100897(73)	0.1099382(80)	0.1099699(71)
Average	0.1100936(91)	0.1099419(91)	0.1099696(91)
$s(x(^{26}\mathrm{Mg}))$/(mol/mol)	0.000012	0.000012	0.000012
Isotope amount ratios			
	$n(^{25}\mathrm{Mg})/n(^{24}\mathrm{Mg})$ / (mol/mol)		
(Solutions -1b) 1	0.126597(19)	0.126491(19)	0.126518(19)
2	0.1266027(89)	0.1264964(84)	0.1265189(86)
3	0.126610(10)	0.1265050(97)	0.1265258(99)
(Solutions -2b) 4	0.1266004(85)	0.1264939(83)	0.1265177(84)
5	0.126597(10)	0.126490(10)	0.126515(10)
6	0.1266095(87)	0.1265036(86)	0.1265260(84)
7	0.1265961(83)	0.1264922(83)	0.1265161(83)
(Solutions -3b) 8	0.1265902(93)	0.1264841(88)	0.1265053(88)
9	0.1265898(81)	0.1264863(88)	0.1265130(82)
10	0.1265951(91)	0.1264919(93)	0.1265161(88)
Average	0.126599(10)	0.126493(10)	0.126517(10)
$s(n(^{25}\mathrm{Mg})/n(^{24}\mathrm{Mg}))$	0.0000070	0.0000067	0.0000060
Isotope amount ratios			
	$n(^{26}\mathrm{Mg})/n(^{24}\mathrm{Mg})$ / (mol/mol)		
(Solutions -1b) 1	0.139395(21)	0.139165(21)	0.139211(22)
2	0.139397(11)	0.139164(11)	0.139203(11)
3	0.139405(12)	0.139179(11)	0.139216(11)
(Solutions -2b) 4	0.139359(10)	0.139131(10)	0.139171(11)
5	0.139365(13)	0.139135(13)	0.139177(13)
6	0.139358(12)	0.139130(11)	0.139171(11)
7	0.139354(12)	0.139128(12)	0.139173(12)
(Solutions -3b) 8	0.139373(15)	0.139144(15)	0.139183(15)
9	0.139381(11)	0.139153(11)	0.139198(11)
10	0.139370(11)	0.139141(12)	0.139190(10)
Average	0.139376(13)	0.139147(13)	0.139189(13)
$s(n(^{26}\mathrm{Mg})/n(^{24}\mathrm{Mg}))$	0.000018	0.000017	0.000017
Relative atomic weights	$A_r(\mathrm{Mg})$		
(Solutions -1b) 1	24.305064(31)	24.304703(30)	24.304778(31)
2	24.305071(17)	24.304704(17)	24.304768(16)
3	24.305084(18)	24.304728(17)	24.304789(17)
(Solutions -2b) 4	24.305019(16)	24.304659(16)	24.304726(16)
5	24.305025(20)	24.304662(20)	24.304732(20)
6	24.305023(18)	24.304663(17)	24.304729(16)
7	24.305009(18)	24.304654(18)	24.304727(18)
(Solutions -3b) 8	24.305031(21)	24.304671(21)	24.304734(22)
9	24.305042(17)	24.304684(17)	24.304758(17)
10	24.305030(16)	24.304672(17)	24.304749(16)
Average	24.305040(20)	24.304680(19)	24.304749(19)
$s(A_r(\mathrm{Mg}))$	0.000025	0.000024	0.000023

S5 Discussion

Published fractionation laws and their conversion into equations of the same systematic:

$$R_i = \frac{x_i}{x_1}$$

Linear Law 1 (Taylor *et al.* [3]):

$$\frac{R_2^{true}}{R_2^{meas}} = 1 + \Delta M_2 \times \varepsilon = 1 + (M_1 - M_2) \times \varepsilon$$

$$\frac{R_3^{true}}{R_3^{meas}} = 1 + \Delta M_3 \times \varepsilon = 1 + (M_1 - M_3) \times \varepsilon$$

$$\varepsilon = \frac{\frac{R_2^{true}}{R_2^{meas}} - 1}{M_1 - M_2}$$

$$\frac{R_3^{true}}{R_3^{meas}} = 1 + (M_1 - M_3) \times \frac{\frac{R_2^{true}}{R_2^{meas}} - 1}{M_1 - M_2}$$

$$\frac{R_3^{true}}{R_3^{meas}} = 1 + \frac{M_1 - M_3}{M_1 - M_2} \times \left(\frac{R_2^{true}}{R_2^{meas}} - 1 \right)$$

$$\frac{R_3^{true}}{R_3^{meas}} = 1 + \frac{M_3 - M_1}{M_2 - M_1} \times \left(\frac{R_2^{true}}{R_2^{meas}} - 1 \right)$$

$$R_3^{true} = R_3^{meas} \times \left[\underbrace{1 + \gamma \times \left(\underbrace{\frac{R_2^{true}}{R_2^{meas}}}_{=K_2} - 1 \right)}_{=K_3} \right]$$

Linear Law 2 (Zindler and Hart [4]):

$$R_3^{true} = R_3^{meas} \cdot \frac{\left(\frac{R_2^{true}}{R_2^{meas}} \right)}{\gamma + \left(\frac{R_2^{true}}{R_2^{meas}} \right) \cdot (1 - \gamma)}$$

$$\gamma = \frac{M_3 - M_1}{M_2 - M_1}$$

$$R_3^{true} = R_3^{meas} \cdot \frac{K_2}{\underbrace{\gamma + K_2 \cdot (1 - \gamma)}_{=K_3}}$$

$$R_3^{true} = R_3^{meas} \cdot \frac{K_2}{\frac{M_3 - M_1}{M_2 - M_1} + K_2 \cdot \left(1 - \frac{M_3 - M_1}{M_2 - M_1} \right)}$$

or

$$R_3^{true} = R_3^{meas} \cdot \frac{1}{\underbrace{1 + \gamma \cdot \frac{R_2^{meas} - R_2^{true}}{R_2^{true}}}_{=K_3}}$$

$$R_3^{true} = R_3^{meas} \cdot \frac{1}{1 + \frac{M_3 - M_1}{M_2 - M_1} \cdot \frac{R_2^{meas} - R_2^{true}}{R_2^{true}}}$$

Power Law (Zindler and Hart [4])

$$R_3^{true} = R_3^{meas} \cdot \underbrace{\underbrace{\left(\frac{R_2^{true}}{R_2^{meas}} \right)}_{=K_2}^{\gamma}}_{=K_3}$$

$$\gamma = \frac{M_3 - M_1}{M_2 - M_1}$$

$$R_3^{true} = R_3^{meas} \cdot \left(\frac{R_2^{true}}{R_2^{meas}} \right)^{\left(\frac{M_3 - M_1}{M_2 - M_1} \right)}$$

Power Law (Taylor *et al.* [3])

$$\frac{R_2^{true}}{R_2^{meas}} = (1 + \varepsilon)^{\Delta M_2} = (1 + \varepsilon)^{(M_1 - M_2)}$$

$$\left(\frac{R_2^{true}}{R_2^{meas}} \right)^{\frac{1}{M_1 - M_2}} = 1 + \varepsilon$$

$$\varepsilon = \left(\frac{R_2^{true}}{R_2^{meas}} \right)^{\frac{1}{M_1 - M_2}} - 1$$

$$\frac{R_3^{true}}{R_3^{meas}} = (1 + \varepsilon)^{(M_1 - M_3)}$$

$$\frac{R_3^{true}}{R_3^{meas}} = \left(1 + \left(\frac{R_2^{true}}{R_2^{meas}} \right)^{\frac{1}{M_1 - M_2}} - 1 \right)^{(M_1 - M_3)}$$

$$\frac{R_3^{true}}{R_3^{meas}} = \left(\frac{R_2^{true}}{R_2^{meas}} \right)^{\frac{M_1 - M_3}{M_1 - M_2}}$$

$$\frac{R_3^{true}}{R_3^{meas}} = \left(\frac{R_2^{true}}{R_2^{meas}} \right)^{\frac{M_3 - M_1}{M_2 - M_1}}$$

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Exponential Law (Taylor *et al.* [3]):

$$\frac{R_2^{true}}{R_2^{meas}} = e^{\varepsilon\times\Delta M_2} = e^{\varepsilon\times(M_1-M_2)}$$

$$\frac{R_2^{true}}{R_2^{meas}} = \left(e^{\varepsilon}\right)^{(M_1-M_2)}$$

$$\left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{1}{M_1-M_2}} = e^{\varepsilon}$$

$$\ln\left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{1}{M_1-M_2}} = \ln e^{\varepsilon} = \varepsilon\times\ln e = \varepsilon$$

$$\frac{R_3^{true}}{R_3^{meas}} = e^{\varepsilon\times(M_1-M_3)}$$

$$\frac{R_3^{true}}{R_3^{meas}} = e^{(M_1-M_3)\times\ln\left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{1}{M_1-M_2}}}$$

$$\frac{R_3^{true}}{R_3^{meas}} = e^{\ln\left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{M_1-M_3}{M_1-M_2}}}$$

$$\frac{R_3^{true}}{R_3^{meas}} = \left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{M_1-M_3}{M_1-M_2}}$$

$$\frac{R_3^{true}}{R_3^{meas}} = \left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{M_3-M_1}{M_2-M_1}}$$

Rayleigh Law (Zindler and Hart [4])

$$R_3^{true} = R_3^{meas}\cdot\underbrace{\frac{\beta_2^{\gamma}}{\beta_3}\cdot\left(\underbrace{\frac{R_2^{true}}{R_2^{meas}}}_{=K_2}\right)^{\gamma}}_{=K_3}$$

$$\beta_3 = \sqrt{\frac{M_1}{M_3}} \qquad \beta_2 = \sqrt{\frac{M_1}{M_2}}$$

$$\gamma = \frac{1-\beta_3}{1-\beta_2} = \frac{1-\sqrt{\frac{M_1}{M_3}}}{1-\sqrt{\frac{M_1}{M_2}}}$$

$$R_3^{true} = R_3^{meas}\cdot\frac{\left(\sqrt{\frac{M_1}{M_2}}\right)^{\frac{1-\sqrt{\frac{M_1}{M_3}}}{1-\sqrt{\frac{M_1}{M_2}}}}}{\sqrt{\frac{M_1}{M_3}}}\cdot\left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{1-\sqrt{\frac{M_1}{M_3}}}{1-\sqrt{\frac{M_1}{M_2}}}}$$

Exponential Law (Zindler and Hart [4])

$$R_3^{true} = R_3^{meas}\cdot\underbrace{\left(\underbrace{\frac{R_2^{true}}{R_2^{meas}}}_{=K_2}\right)^{\gamma}}_{=K_3}$$

$$\gamma = \frac{\ln\left(\frac{M_3}{M_1}\right)}{\ln\left(\frac{M_2}{M_1}\right)}$$

$$R_3^{true} = R_3^{meas}\cdot\left(\frac{R_2^{true}}{R_2^{meas}}\right)^{\frac{\ln\left(\frac{M_3}{M_1}\right)}{\ln\left(\frac{M_2}{M_1}\right)}}$$

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Russel's Law [5]:

$$\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}} = \left(\frac{M_2}{M_1}\right)^{\varepsilon}$$

$$\ln\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}} = \ln\left(\frac{M_2}{M_1}\right)^{\varepsilon} = \varepsilon \times \ln\left(\frac{M_2}{M_1}\right)$$

$$\varepsilon = \frac{\ln\left(\dfrac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)}{\ln\left(\dfrac{M_2}{M_1}\right)}$$

$$\frac{R_3^{\mathrm{true}}}{R_3^{\mathrm{meas}}} = \left(\frac{M_3}{M_1}\right)^{\varepsilon}$$

$$\frac{R_3^{\mathrm{true}}}{R_3^{\mathrm{meas}}} = \left(\frac{M_3}{M_1}\right)^{\frac{\ln\left(\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)}{\ln\left(\frac{M_2}{M_1}\right)}}$$

$$\ln\left(\frac{R_3^{\mathrm{true}}}{R_3^{\mathrm{meas}}}\right) = \ln\left[\left(\frac{M_3}{M_1}\right)^{\frac{\ln\left(\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)}{\ln\left(\frac{M_2}{M_1}\right)}}\right] = \frac{\ln\left(\dfrac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)}{\ln\left(\dfrac{M_2}{M_1}\right)} \times \ln\left(\frac{M_3}{M_1}\right)$$

$$\ln\left(\frac{R_3^{\mathrm{true}}}{R_3^{\mathrm{meas}}}\right) = \frac{\ln\left(\dfrac{M_3}{M_1}\right)}{\ln\left(\dfrac{M_2}{M_1}\right)} \times \ln\left(\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)$$

$$\ln\left(\frac{R_3^{\mathrm{true}}}{R_3^{\mathrm{meas}}}\right) = \ln\left[\left(\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)^{\frac{\ln\left(\frac{M_3}{M_1}\right)}{\ln\left(\frac{M_2}{M_1}\right)}}\right]$$

$$\frac{R_3^{\mathrm{true}}}{R_3^{\mathrm{meas}}} = \left(\frac{R_2^{\mathrm{true}}}{R_2^{\mathrm{meas}}}\right)^{\frac{\ln\left(\frac{M_3}{M_1}\right)}{\ln\left(\frac{M_2}{M_1}\right)}}$$

Table S10 *K*-factor $K_{26/24}$ calculated for different fractionation laws by using $K_{2\text{-}02}$ ($^{25}Mg/^{24}Mg$) as the input quantity and comparison with the reference *K*-factor $K_{3\text{-}02}$ ($^{26}Mg/^{24}Mg$) determined by using the synthetic isotope mixtures; expanded uncertainties ($k = 2$) are given in brackets. The Δ values reflect the difference between the *K*-factor calculated by using a specific fractionation law and the reference *K*-factor $K_{3\text{-}02}$ expressed in ‰. The uncertainty of the Δ values contain the uncertainties of the input quantity $K_{2\text{-}02}$ ($^{25}Mg/^{24}Mg$) and the uncertainty contributions deriving from the calculation by using the fractionation laws. Calculations were made for all sequences measured at three different institutes using three different MC-ICPMS instruments.

Sequence	$K_{2\text{-}02}$(25/24) / (V/V/mol/mol)	$K_{3\text{-}02}$(26/24) / (V/V/mol/mol)	K_{lin1}(26/24) / (V/V/mol/mol)	$\Delta_{\text{lin1-ref}}$ / ‰	K_{lin2}(26/24) / (V/V/mol/mol)	$\Delta_{\text{lin2-ref}}$ / ‰	K_{pow}(26/24) / (V/V/mol/mol)	$\Delta_{\text{pow-ref}}$ / ‰	K_{ray}(26/24) / (V/V/mol/mol)	$\Delta_{\text{ray-ref}}$ / ‰	K_{exp}(26/24) / (V/V/mol/mol)	$\Delta_{\text{exp-ref}}$ / ‰
LGC 01	0.926828(86)	0.86170(10)	0.85395(17)	-9.0(2.1)	0.86387(15)	2.52(53)	0.85927(16)	-2.82(62)	0.86340(16)	1.97(43)	0.86183(16)	0.149(33)
LGC 02	0.927411(81)	0.86260(12)	0.85511(16)	-8.7(2.0)	0.86488(14)	2.64(56)	0.86035(15)	-2.61(58)	0.86446(15)	2.16(48)	0.86289(15)	0.336(75)
LGC 03	0.928081(93)	0.86386(13)	0.85645(19)	-8.6(2.3)	0.86605(16)	2.54(60)	0.86159(17)	-2.63(65)	0.86567(17)	2.10(52)	0.86411(17)	0.289(72)
PTB 01	0.93339(13)	0.87349(14)	0.86705(26)	-7.4(2.5)	0.87532(23)	2.10(65)	0.87146(24)	-2.32(74)	0.87529(24)	2.06(65)	0.87381(24)	0.37(12)
PTB 02	0.934042(59)	0.874594(60)	0.86835(12)	-7.1(1.1)	0.87647(10)	2.15(29)	0.87267(11)	-2.20(32)	0.87647(11)	2.15(31)	0.87500(11)	0.464(67)
PTB 03	0.933638(59)	0.873914(60)	0.86754(12)	-7.3(1.1)	0.87576(10)	2.11(28)	0.87192(11)	-2.28(33)	0.87574(11)	2.09(30)	0.87426(11)	0.396(57)
PTB 04	0.935489(71)	0.877024(66)	0.87124(14)	-6.6(1.2)	0.87901(13)	2.26(38)	0.87538(13)	-1.87(31)	0.87911(13)	2.38(39)	0.87766(13)	0.73(12)
PTB 05	0.935638(66)	0.87739(10)	0.87154(13)	-6.7(1.2)	0.87927(12)	2.15(38)	0.87565(12)	-1.98(35)	0.87938(12)	2.27(40)	0.87793(12)	0.62(11)
PTB 06	0.935528(58)	0.877377(62)	0.87132(12)	-6.9(1.1)	0.87908(10)	1.94(26)	0.87545(11)	-2.20(32)	0.87918(11)	2.06(30)	0.87773(11)	0.403(58)
PTB 07	0.935311(78)	0.877123(63)	0.87088(16)	-7.1(1.4)	0.87870(14)	1.80(31)	0.87504(15)	-2.38(44)	0.87878(14)	1.89(33)	0.87733(14)	0.236(41)
PTB 08	0.93524(12)	0.87697(15)	0.87074(24)	-7.1(2.3)	0.87857(21)	1.83(54)	0.87491(22)	-2.35(71)	0.87865(22)	1.92(58)	0.87720(22)	0.264(80)
PTB 09	0.934954(66)	0.876394(67)	0.87017(13)	-7.1(1.2)	0.87807(12)	1.91(30)	0.87438(12)	-2.30(36)	0.87813(12)	1.98(31)	0.87668(12)	0.326(51)
BAM 01	0.93436(14)	0.87544(13)	0.86898(28)	-7.4(2.6)	0.87702(25)	1.80(58)	0.87327(26)	-2.48(82)	0.87705(25)	1.84(59)	0.87559(26)	0.171(57)
BAM 02	0.934198(61)	0.875066(63)	0.86866(12)	-7.3(1.1)	0.87674(11)	1.91(28)	0.87297(11)	-2.40(35)	0.87676(11)	1.94(28)	0.87529(11)	0.256(37)
BAM 03	0.933474(71)	0.873705(69)	0.86722(14)	-7.4(1.3)	0.87547(12)	2.02(32)	0.87162(13)	-2.39(40)	0.87544(13)	1.99(33)	0.87396(13)	0.292(49)
BAM 04	0.934165(60)	0.874802(64)	0.86860(12)	-7.1(1.1)	0.87668(11)	2.15(31)	0.87290(11)	-2.17(32)	0.87670(11)	2.17(32)	0.87523(11)	0.489(71)
BAM 05	0.934635(75)	0.875780(80)	0.86953(15)	-7.1(1.4)	0.87751(13)	1.98(34)	0.87378(14)	-2.28(42)	0.87755(14)	2.02(37)	0.87609(14)	0.354(65)
BAM 06	0.934772(62)	0.875843(66)	0.86981(12)	-6.9(1.1)	0.87775(11)	2.18(32)	0.87404(12)	-2.06(32)	0.87780(11)	2.23(33)	0.87634(11)	0.567(83)
BAM 07	0.935150(60)	0.876656(73)	0.87056(12)	-7.0(1.1)	0.87841(11)	2.00(30)	0.87474(11)	-2.19(33)	0.87849(11)	2.09(31)	0.87704(11)	0.438(66)
BAM 08	0.934933(64)	0.876466(91)	0.87013(13)	-7.2(1.3)	0.87803(11)	1.78(29)	0.87434(12)	-2.43(42)	0.87810(12)	1.86(32)	0.87664(12)	0.199(34)
BAM 09	0.935103(60)	0.876809(68)	0.87047(12)	-7.2(1.1)	0.87833(11)	1.73(26)	0.87465(11)	-2.46(36)	0.87840(11)	1.81(27)	0.87695(11)	0.161(24)
BAM 10	0.935268(64)	0.876997(65)	0.87080(13)	-7.1(1.2)	0.87862(11)	1.85(27)	0.87496(12)	-2.32(36)	0.87871(12)	1.95(30)	0.87725(12)	0.288(45)

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1 G. Mana and O. Rienitz, *Int. J. Mass Spectrom.*, 2010, **291**, 55.
2 A. Pramann, O. Rienitz, J. Noordmann, B. Güttler and D. Detlef Schiel, *Zeitschrift für Physikalische Chemie*, 2014, **228**, 405.
3 P. D. P Taylor, P. Debievre, A. J. Walder, A. Entwistle, *J. Anal. At. Spectrom.*, 1995, **10**, 395.
4 S. R. Hart, A. Zindler, A., *Int. J. Mass Spectrom. Ion Proc.*, 1989, **89**, 287.
5 J. Meija, L. Yang, Z. Mester and R. Sturgeon, "Correction of Instrumental Mass Discrimination for Isotope Ratio Determination with Multi-Collector Inductively Coupled Plasma Mass Spectrometry," in Isotopic Analysis, Weinheim, Wiley-VCH Verlag & Co KGaA, 2012, pp. 113-138.