

**IRMM**

Institute for Reference Materials and Measurements

CERTIFICATE**ISOTOPIC REFERENCE MATERIAL (SPIKE) IRMM-620**

$$(1.733\,5 \pm 0.001\,6) \cdot 10^{-4} \text{ mol } ^{57}\text{Fe} \cdot \text{kg}^{-1} \text{ of solution}$$

The Isotopic Reference Material (Spike) is supplied with an amount concentration of ^{57}Fe certified as above.

Other iron isotopes present are related to the ^{57}Fe concentration through the following certified amount ratios :

$$\begin{aligned} n(^{54}\text{Fe})/n(^{57}\text{Fe}) &: < 0.000\,1 \\ n(^{56}\text{Fe})/n(^{57}\text{Fe}) &: 0.025\,39 \pm 0.000\,31 \\ n(^{58}\text{Fe})/n(^{57}\text{Fe}) &: 0.025\,16 \pm 0.000\,18 \end{aligned}$$

This corresponds to an isotopic composition with following abundances :

	Mole %	Mass %	Uncertainty
^{54}Fe	< 0.01	< 0.01	
^{56}Fe	2.417	2.374	± 0.028
^{57}Fe	95.188	95.189	± 0.033
^{58}Fe	2.395	2.437	± 0.017

The molar mass of the iron is $(56.935\,12 \pm 0.000\,44) \text{ g} \cdot \text{mol}^{-1}$

From the certified values, the following element concentrations are derived :

$$\begin{aligned} &(9.868\,8 \pm 0.007\,1) \cdot 10^{-6} \text{ kg } ^{57}\text{Fe} \cdot \text{kg}^{-1} \text{ of solution} \\ &(10.368\,3 \pm 0.006\,2) \cdot 10^{-6} \text{ kg } \text{Fe} \cdot \text{kg}^{-1} \text{ of solution} \\ &(1.821\,1 \pm 0.001\,1) \cdot 10^{-4} \text{ mol } \text{Fe} \cdot \text{kg}^{-1} \text{ of solution} \end{aligned}$$

NOTES

1. All uncertainties indicated are levels of possible inaccuracies, computed on a 2s basis for all components. These include : measurement reproducibility, reproducibilities of measurements of correction factors for known systematic errors and possible uncertainties of systematic nature estimated on a 2s equivalence basis.
2. IRMM-620 consists of flame-sealed quartz glass ampoules containing about 4 ml of a chemically stable solution of iron in hydrochloric acid. The molality is about 4 m HCl (i.e. 4 mol HCl \cdot kg⁻¹ of solvent); the molarity is about 4.5 M HCl (i.e. 4.5 mol HCl \cdot L⁻¹ of solution). The ampoule should preferably be opened using a diamond-edged glass-cutter, so as to avoid contamination.
3. The Avogadro constant used is $(6.022\ 136 \pm 0.000\ 012) \cdot 10^{23}$ mol⁻¹.
4. The molar masses, used in the calculations, are

⁵⁴Fe (53.939 612 7 \pm 0.000 001 5) g \cdot mol⁻¹

⁵⁶Fe (55.934 939 3 \pm 0.000 001 6) g \cdot mol⁻¹

⁵⁷Fe (56.935 395 8 \pm 0.000 001 6) g \cdot mol⁻¹

⁵⁸Fe (57.933 277 3 \pm 0.000 001 6) g \cdot mol⁻¹

5. Using this Spike Reference Material (Spike), ⁵⁶Fe (also applies to ⁵⁴Fe, ⁵⁸Fe) and Fe concentrations in unknown samples can be determined by Isotope Dilution Mass Spectrometry, through a measurement of the molar isotope dilution ratio $R_B = n(^{56}\text{Fe})/n(^{57}\text{Fe})$ in the blend. They should be computed with the aid of the following formula which allows an easy identification of the sources of the uncertainties in the procedure :

$$c(^{56}\text{Fe})_X = \frac{R_Y - R_B}{R_B - R_X} \cdot R_X \cdot \frac{m_Y}{m_X} \cdot c(^{57}\text{Fe})_Y$$

$$c(\text{Fe})_X = \frac{R_Y - R_B}{R_B - R_X} \cdot \frac{\sum (R_X)_i}{\sum (R_Y)_i} \cdot \frac{m_Y}{m_X} \cdot c(\text{Fe})_Y$$

where

- R_X = molar ratio $n(^{56}\text{Fe})/n(^{57}\text{Fe})$ in the unknown sample material
 R_Y = molar abundance ratio $n(^{56}\text{Fe})/n(^{57}\text{Fe})$ in the spike material
 m_X = mass of the unknown sample
 m_Y = mass of the sample of spike solution used

$c(^{56}\text{Fe})_X$ = number of moles $^{56}\text{Fe} \cdot \text{kg}^{-1}$ unknown material
 $c(^{57}\text{Fe})_Y$ = number of moles $^{57}\text{Fe} \cdot \text{kg}^{-1}$ spike solution
 $\Sigma(R_X)_i$ = sum of all molar abundance ratios in the unknown sample material
 $\Sigma(R_Y)_i$ = sum of all molar abundance ratios in the spike material
 $c(\text{Fe})_X$ = number of moles $\text{Fe} \cdot \text{kg}^{-1}$ unknown material
 $c(\text{Fe})_Y$ = number of moles $\text{Fe} \cdot \text{kg}^{-1}$ spike solution.

6. This Isotopic Reference Material (Spike) is traceable to the international SI unit for amount of substance - the mole - in the shortest possible way. The values for this Spike IRM are calibrated against synthetically prepared isotope mixtures. Measurements calibrated against this Isotopic Reference Material will, therefore, also be traceable to the SI unit system.

The isotopic measurements by Thermal Ionisation Mass Spectrometry were performed by A. Kynaston.

Chemical preparation of the samples (purification) was performed by K. Van Bakel and P. Taylor.

The purity was determined by ICP-MS by P. Taylor.

Metrological aspects involved in the preparation and certification were performed by F. Hendrickx. The ampoulation of this Isotopic Reference Material (Spike) was accomplished by K. Van Bakel, P. Taylor and G. Van Baelen.

The overall coordination leading to the establishment, certification and issuance of this Isotopic Reference Material (Spike), was performed by P. Taylor.

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P. DE BIEVRE
Head
EC-IRMM Mass Spectrometry