



National Institute of Standards & Technology

Report of Investigation

Reference Material 8554

IAEA-S-1

(Sulfur Isotopes in Silver Sulfide)

This Reference Material (RM) is an international measurement standard [1] that defines the Vienna Cañon Diablo Troilite (VCDT) scale for relative differences in sulfur (S) isotope-number ratios, $R(^{34}\text{S}/^{32}\text{S})$ [2]. Even though the value for this RM is not certified, its value is exact with no uncertainty [3,4]. The equivalent name for this RM as used by the International Atomic Energy Agency (IAEA) and the U.S. Geological Survey (USGS) is IAEA-S-1. This material was formerly called NZ-1 (New Zealand) [3]. A unit of RM 8554 consists of one bottle containing approximately 0.5 g of silver sulfide (Ag_2S).

Table 1. Reference Value for the Relative S Isotope-Number Ratio Difference of RM 8554.

| RM Number | Name | Reference Value |
|-----------|----------|--|
| 8554 | IAEA-S-1 | $10^3 \delta^{34}\text{S}_{\text{VCDT}}^{(a)}$ -0.3 exact |

^(a) The $\delta^{34}\text{S}_{\text{VCDT}}$ value is an exact value that forms the basis for the VCDT scale for S [3,4].

Reference Difference in Isotope-Number Ratio Values: The differences in measured isotope-number ratios of stable sulfur isotopes in substance P, $R(^{34}\text{S}/^{32}\text{S})_{\text{P}} = [N(^{34}\text{S})_{\text{P}} / N(^{32}\text{S})_{\text{P}}]$, are reported as $\delta^{34}\text{S}$ values [4]. The relative differences in isotope-number ratios for sulfur are referenced to VCDT where:

$$\delta^{34}\text{S} = [R(^{34}\text{S}/^{32}\text{S})_{\text{sample}} / R(^{34}\text{S}/^{32}\text{S})_{\text{VCDT}}] - 1$$

VCDT refers to the Vienna Cañon-Diablo Troilite scale, which is defined by assigning a consensus $\delta^{34}\text{S}$ value of -0.3‰ to RM 8554 [3,4], where the symbol ‰ is part per thousand and is equal to 0.001.

Expiration of Value Assignment: RM 8554 is valid until **31 December 2020**, provided the RM is handled and stored in accordance with instructions given in this Report of Investigation (see “Instructions for Handling, Storage, and Use”). This report is nullified if the RM is damaged, contaminated, or otherwise modified.

Maintenance of RM: NIST will monitor this RM over the period of its validity. If substantive technical changes occur that affect the value assignment before the expiration of this report, NIST will notify the purchaser. Registration (see attached sheet) will facilitate notification.

The technical aspects involved in the issuance of this RM were coordinated through the NIST Chemical Sciences Division by R.D. Vocke, Jr.

Support aspects involved in the issuance of this RM were coordinated through the NIST Office of Reference Materials.

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Report Issue Date: 30 January 2013
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INSTRUCTIONS FOR HANDLING, STORAGE, AND USE

Handling and Storage: RM 8554 (IAEA-S-1) is stable at room temperature. To minimize the potential for contamination, it is recommended that this RM be stored in the container in which it is supplied.

Distribution: The distribution of RM 8554 (IAEA-S-1) is limited to one unit per three-year period of time.

PREPARATION AND ANALYSIS

Preparation: RM 8554 (IAEA-S-1) was prepared and purified by B.W. Robinson, Lower Hutt, New Zealand from a sphalerite provided by S. Halas, Maria Curie-Skłodowska University, Lublin, Poland [3,5].

Analytical Methods: When $\delta^{34}\text{S}$ values of the original Cañon Diablo Troilite (CDT) were shown to be isotopically heterogeneous at a level of 0.4 ‰ [5], IAEA-S-1 was selected as a replacement reference material. Mass spectrometric measurements of SF_6 preparations of IAEA-S-1 showed that this material had a $\delta^{34}\text{S}$ value very near CDT that ranged from about -0.33 to -0.27 ‰ [3,6]. The VCDT scale was then established by assigning an exact $\delta^{34}\text{S}$ value of -0.3 ‰ (relative to VCDT) to IAEA-S-1 [3,4].

The $\delta^{34}\text{S}$ value reported in Table 1 for RM 8554 (IAEA-S-1) is the value accepted by the Commission on Isotopic Abundances and Atomic Weights of the International Union of Pure and Applied Chemistry (IUPAC) (<http://ciaaw.org/Sulfur.htm>) and the IAEA as of the date of this report.

Isotopic Homogeneity: Data from an inter-laboratory comparison of IAEA-S-1 suggests that there is no evidence of isotopic heterogeneity in this reference material [3].

Normalization: The $\delta^{34}\text{S}$ values in samples should be normalized to the VCDT δ -scale by calibrating the measurement with respect to the δ -value for IAEA-S-1 (RM 8554) and the δ -value from the appropriate ^{34}S -enriched or ^{34}S -depleted anchor RMs. IAEA-S-2 (RM 8555) should be used as the anchor for the ^{34}S -enriched end while IAEA-S-3 (RM 8529) is appropriate for the ^{34}S -depleted end of the scale. A general formula for normalizing measured sulfur isotope number ratios using two laboratory standards LS1 (e.g. IAEA-S-1, RM 8554) and LS2 (e.g. IAEA-S-2, RM 8555) can be expressed as:

$$\delta^{34}\text{S}_{\text{sample,cal}} = \delta^{34}\text{S}_{\text{LS1,cal}} + (\delta^{34}\text{S}_{\text{sample,WS}} - \delta^{34}\text{S}_{\text{LS1,WS}}) \times f \quad (1)$$

where the normalization factor f is:

$$f = \frac{(\delta^{34}\text{S}_{\text{LS2,cal}} - \delta^{34}\text{S}_{\text{LS1,cal}})}{(\delta^{34}\text{S}_{\text{LS2,WS}} - \delta^{34}\text{S}_{\text{LS1,WS}})} \quad (2)$$

Note: In the formulas above, cal denotes calibrated measurements made versus the VCDT scale, and $\delta^{34}\text{S}_{\text{LS1,cal}}$ and $\delta^{34}\text{S}_{\text{LS2,cal}}$ are the conventionally fixed $\delta^{34}\text{S}$ values for IAEA-S-1 (RM 8554) and IAEA-S-2 (RM 8555). WS denotes measurements made versus a transfer gas (working standard), and $\delta^{34}\text{S}_{\text{LS1,WS}}$ and $\delta^{34}\text{S}_{\text{LS2,WS}}$ are the $\delta^{34}\text{S}$ values for calibrated laboratory working standards.

Reporting of Sulfur Stable Isotope δ -values: The following recommendations from IUPAC are provided for reporting $\delta^{34}\text{S}$ values [4]. It is recommended that:

- the use of meteoritic troilite and the reporting of $\delta^{34}\text{S}$ data relative to CDT be discontinued;
- all relative sulfur isotopic compositions be reported relative to VCDT;
- the VCDT scale be realized through the use of IAEA-S-1, silver sulfide (RM 8554).

In addition, researchers are encouraged to report the isotopic composition of any internationally distributed sulfur isotopic reference materials [7] in their publications, as appropriate to the method, as though they have been interspersed among unknowns.

Current Reports of Investigation (ROI) for all light stable isotopic Reference Materials mentioned in this report are available on the NIST Standard Reference Materials web site [8].

REFERENCES

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- [8] *Light Stable Isotopic Materials (gas, liquid and solid forms)*; NIST SRM Order Request System; National Institute of Standards and Technology; U.S. Department of Commerce: Gaithersburg, MD 20899; available at <https://www-s.nist.gov/srmors/viewTableV.cfm?tableid=42> (accessed Dec 2012).

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| Report Revision History: 30 January 2013 (Expiration date assigned; editorial changes); 22 June 1992 (Original report issue date). |
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Users of this RM should ensure that the Report of Investigation in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srminfo@nist.gov; or via the Internet at <http://www.nist.gov/srm>.