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COMMISSION ON ATOMIC WEIGHTS AND
ISOTOPIC ABUNDANCES*

**REPORTING OF RELATIVE SULFUR
ISOTOPE-RATIO DATA**

(Technical Report)

Prepared for publication by

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Reporting of relative sulfur isotope-ratio data

Abstract: To eliminate possible confusion in the reporting of sulfur isotope-ratio data, the Commission on Atomic Weights and Isotopic Abundances recommends that relative $^{34}\text{S}/^{32}\text{S}$ ratios of all sulfur-bearing substances be expressed on the VCDT scale, defined by assigning a $\delta^{34}\text{S}$ value of -0.3‰ exactly (relative to VCDT) to the silver sulfide reference material IAEA-S-1. Reporting of sulfur isotope-ratio analyses relative to CDT should be discontinued.

COMMENT

Relative sulfur isotope-ratio data in geochemical and environmental studies are traditionally reported as $\delta^{34}\text{S}$ values in parts per thousand (‰ or per mill) difference from a standard. The standard may be real or hypothetical. In the latter case, it is defined in terms of an existing internationally distributed reference material. For several decades troilite (FeS) from the Cañon Diablo meteorite, CDT, has been employed as the standard (ref. 1). Thus, for the sulfur isotopic composition of a sample x , we have

$$\delta^{34}\text{S} \text{ (in ‰)} = \left[\frac{\left[\frac{^{34}\text{S}}{^{32}\text{S}} \right]_x}{\left[\frac{^{34}\text{S}}{^{32}\text{S}} \right]_{\text{CDT}}} - 1 \right] 1000.$$

Similarly defined $\delta^{33}\text{S}$ and $\delta^{36}\text{S}$ scales have also been used to examine non-mass dependent isotopic fractionation.

Use of a nonterrestrial material as a reference can present problems. The material may not fit the mass dependent isotopic trends of terrestrial specimens if the nucleosynthetic histories and (or) subsequent exposure to nuclear radiation differ. Thus, excess ^{33}S and ^{36}S have been reported for some meteorites (refs. 2 & 3).

The choice of CDT as the standard was historically influenced by the remarkable consistency of $\delta^{34}\text{S}$ values among meteorites (refs. 4, 5 & 6), in contrast to most terrestrial specimens. However, it was also recognized very early in sulfur isotope-ratio investigations that measured $\delta^{34}\text{S}$ values of CDT varied by 1‰ (ref. 1). There was a question as to the extent that the measured variations reflected chemical extraction techniques (H_2S evolution by HCl, chemical or Parr Bomb oxidation, *etc.*) or inhomogeneity (ref. 7). Recently, high precision sulfur isotope-ratio analyses using SF_6 , have established a range of $\delta^{34}\text{S}$ values for CDT of 0.4‰ with an analytical uncertainty of 0.05‰ (ref. 8).

At the "Consultants' Meeting on Stable Isotope Standards and Intercomparison Materials" sponsored by the International Atomic Energy Agency and held in Vienna in December 1993, it was noted that $\delta^{34}\text{S}$ values reported for SF_6 prepared from the reference material IAEA-S-1 silver sulfide (previously called IAEA-NZ1) ranged from about -0.33 to -0.27‰ (ref. 9). This group recommended (ref. 9) that a VCDT scale be established and defined by assigning a $\delta^{34}\text{S}$ value of -0.3‰ exactly (relative to VCDT) to IAEA-S-1. The Subcommittee for Natural Isotopic Fractionation met July 31, 1995 in Geel, Belgium, and reported to the Commission on Atomic Weight and Isotopic Abundances, meeting in Guildford, U.K., in August 1995, that they were in agreement with the recommendation of the IAEA consultants and that the Commission should adopt this recommendation. Furthermore, because CDT has been shown to be isotopically inhomogeneous (ref. 8), the Subcommittee recommended that the use of CDT for reporting of $\delta^{34}\text{S}$ data be discontinued. The Commission agreed and requested that this document be prepared.

The reference material IAEA-S-1 is available from the sources listed in the appendix.

REFERENCES

1. W. U. Ault and M. L. Jensen, in "Summary of Sulfur Standards," *Biogeochemistry of Sulfur Isotopes* (Editor: M. L. Jensen), Proceedings of National Science Foundation Symposium, Yale University, New Haven, Connecticut, 16–29 (1962).
2. C. E. Rees and H. G. Thode, *Geochim. Cosmochim. Acta* 41, 1679–1682 (1977).
3. X. Gao and M. H. Thiemens, *Geochim. Cosmochim. Acta* 55, 2671–2679 (1991).
4. J. Macnamara and H. G. Thode, *Phys. Rev.* 78, 307–308 (1950).
5. I. R. Kaplan and J. R. Hulston, *Geochim. Cosmochim. Acta* 30, 479–496 (1966).
6. J. Hulston and H. G. Thode, *Jour. Geophys. Res.* 70, 3475–3484 (1965).
7. M. L. Jensen and N. Nakai, in "Sulfur isotope meteorite standards results and recommendations," *Biogeochemistry of Sulfur Isotopes* (Editor: M. L. Jensen), Proceedings of National Science Foundation Symposium, Yale University, New Haven, Connecticut, 30–35 (1962).
8. G. Beaudoin, B. E. Taylor, D. Rumble III, and M. Thiemens, *Geochim. Cosmochim. Acta* 58, 4253–4255 (1994).
9. B. W. Robinson, in "Sulphur Isotope Standards," *Reference and intercomparison materials for stable isotopes of light elements*, IAEA-TECDOC-825, International Atomic Energy Agency, Vienna, 39–45 (1995).

APPENDIX A: SOURCES OF REFERENCE MATERIALS

Reference material IAEA-S-1 (previously known as IAEA-NZ1) may be obtained from

National Institute of Standards and Technology
Standard Reference Materials Program
Room 204, Building 202
Gaithersburg, Maryland 20899-0001
USA
Fax: +1 301 948 3730
Phone: +1 301 975 6776
Email: SRMINFO@enh.nist.gov
Request RM8554 for IAEA-S-1 silver sulfide

or from

International Atomic Energy Agency
Section of Isotope Hydrology
Wagramerstr. 5, PO Box 100
A-1400 Vienna
Austria
Fax: +43 1 20607
Phone: +43 1 206021735
Email: IAEA@iaea1.iaea.or.at