

Editorial

Standards for publication of isotope ratio and chemical data in *Chemical Geology*

Abstract

In an International Journal such as *Chemical Geology*, it is vitally important to include a reasonable assessment of precision and accuracy, and appropriate information regarding analytical methodologies so that data can be compared between different laboratories. The policy of the Journal to insure adequate documentation is outlined below.

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1. Major and trace element data

Any paper that reports major and/or trace element concentration data will need to quote both precision and accuracy for the analytical technique used to procure these data. The manuscript must report the type of instrument used and the lab where the measurements were made. Ascertaining the accuracy of elemental analyses requires reporting data for international standards that were analyzed in the same laboratory, using the same techniques as the “unknowns” reported in the paper. Ideally, such analyses should be carried out during the analytical session in which the unknowns were measured. However, lacking this, it is also acceptable to quote an internationally accessible publication in which such data are reported for the laboratory in question. If such analyses are not previously published, they must be provided in the paper under consideration.

For major and trace elements, there are a large number of reasonably well-characterized whole rock standards from a variety of sources. Examples are given in Govindaraju (1994) and Eggins et al. (1997). Standards for in situ trace element analyses (e.g., SIMS or LA-ICP-MS) range from the relatively well-documented and widely used NIST glasses (summarized by Pearce et al., 1997) to a series of USGS

and MPI-DING glasses that have been synthesized specifically as standards for in situ work (e.g., Jochum et al., 2000). Unfortunately, there is still a lack of good international mineral standards for in situ work. Estimates of accuracy for LA-ICP-MS need to be based on replicate analyses of a standard, *other than the calibration standard*, that was analyzed as an unknown during the course of the analyses. In addition, the values used for the calibration standard (e.g., NIST glasses) must be quoted or referenced.

The manuscript must also contain an adequate description of sample processing procedures, and a statement about blanks. If sample dissolution is required by the method employed (e.g., solution ICP-MS), then the authors need to provide explicit details of how this was accomplished (e.g., by acid attack in screw-top Teflon beakers, by bomb dissolution, flux fusions, etc.).

2. Radiogenic isotope data

In order for radiogenic isotope data (e.g., Sr, Nd, Pb, Hf, U-series) to be published, a manuscript must report the data relative to an internationally used standard, with adequate documentation of the lab’s analyses of the standard and the external reproducibil-

ity. If the laboratory regularly measures standards that are internal to that lab, then adequate information on intercalibration of the internal lab standard to an international standard is required.

Some of the acceptable international standards include, but are not restricted to: (1) Sr isotopes: Eimer and Amend, NBS987; (2) Nd isotopes: La Jolla, JNdi-1; (3) Pb isotopes: NBS981, NBS982; (4) Hf isotopes: JMC-475; (5) U-series: Table Mountain Latite, ATHO, NBS U500 or U960.

If no internationally recognized standards exist, such as for Pt–Re–Os isotopes, a description of the manner in which the lab controls data quality must be included.

The report must include the mean measured value of the standard, its external reproducibility (2σ , where σ is the standard deviation of the standard results), and the number of analyses of the standard. The external reproducibility is not given by the standard error of the mean ($2\sigma_m = 2\sigma/n^{0.5}$, where n is the number of analyses), which estimates the uncertainty of the average value measured based on the replicate analyses. In many manuscripts, we have found that the $2\sigma_m$ is confused with external reproducibility.

If the data are further corrected to a “defined value” of the standard (e.g., if $^{87}\text{Sr}/^{86}\text{Sr}$ ratios are corrected to a value of 0.70800 for the Eimer and Amend Standard), it must be clearly stated and the value used must be explicitly stated. If the data are not corrected, this should also be stated.

In the usual case that the internal measurement errors of samples are smaller than the 2σ external reproducibility of the standard, then the 2σ external reproducibility, rather than the sample measurement error, represents the estimate of sample error. Authors are encouraged nevertheless to report the sample measurement errors in the data table. If the measurement error of the sample is larger than the external reproducibility of the replicated standards, then the measurement error represents the estimate of the sample error.

The manuscript must report the type of instrument used and the lab where the measurements were made. If the reported isotope ratio is corrected for instrumental mass fractionation using stable isotope ratios, then the normalizing ratio used must be identified (e.g., $^{87}\text{Sr}/^{86}\text{Sr}$ ratios are normalized

to $^{86}\text{Sr}/^{88}\text{Sr}=0.1194$). If the element used to correct for instrumental mass fractionation is different from the one being reported, as is often the case for multiple collection ICPMS, the element, the isotopes and the value of the normalizing ratio must also be identified. Other important information on analytical procedure, such as single or multiple collection, static or dynamic multicollection, whether isotopes are measured as metal or oxide, or as positive or negative ions, must also be stated.

The manuscript must also contain an adequate description of sample processing procedures and a statement about blanks.

3. Noble gas isotope and concentration data

All noble gas isotope data (He, Ne, Ar, Kr, Xe) should be reported as absolute values (presumed to be corrected for mass discrimination and blanks) with the exception of helium where the isotopic ratio can be reported relative to air. For example, the notation R/R_A can be used where R =sample $^3\text{He}/^4\text{He}$ and R_A =air $^3\text{He}/^4\text{He}$. If the absolute value of the $^3\text{He}/^4\text{He}$ (or $^4\text{He}/^3\text{He}$) ratio is reported, then the value adopted for air (e.g., 1.4×10^{-6}) to calculate this value must be given. The type of standard used by the laboratory (e.g., air) must be given. If another standard is used (e.g., one with a $^3\text{He}/^4\text{He}$ ratio greater than air), then details of the calibration of such a standard relative to air (i.e., its accuracy) must be included. An analysis of the error propagation is encouraged and it must be explicitly stated if the quoted errors on isotope ratios (in tables and plots) are at the 1σ or 2σ level.

In the case of helium, $^3\text{He}/^4\text{He}$ ratios are sometimes further corrected for air or air-saturated water. The initial (sometimes referred to as ‘measured’) $^3\text{He}/^4\text{He}$ value *must* be given, irrespective of whether air-corrected or air-saturated water values are also included in the data table. In the case of correcting for air-saturated water helium, the assumed $^4\text{He}/^{20}\text{Ne}$ ratio used and the conditions of equilibration should be stated (e.g., temperature, salinity and amount of excess air).

The concentration of noble gases in a specific medium (water, glass, phenocryst) should be reported in stated units (atoms, moles or cm^3

STP) per unit mass (usually grams) of that medium. For example, the concentration of ^4He in groundwater could be reported as $4.2 \times 10^{-6} \text{ cm}^3 \text{ STP g}^{-1} \text{ H}_2\text{O}$, or the concentration of cosmogenic ^{21}Ne in a quartz crystal as $500 \times 10^6 \text{ atoms g}^{-1} \text{ quartz}$. Prefixes such as ‘n’ (nano)—in the form $\text{ncm}^3 \text{ STP}$ (i.e., meaning $\times 10^{-9} \text{ cm}^3 \text{ STP}$)—are not to be used in this manner. It is important to include the mass of sample processed to obtain the reported data (in order for readers to gauge total amounts of noble gases undergoing analysis).

Details of the analytical procedure used to produce noble gas data should be reported. This should include, where necessary, sample collection procedure and analytical (preparation) protocols—this includes preparation protocols that may have taken place ‘off-line’ prior to sample introduction to the mass spectrometer system. It is useful to include details of the extraction device and how it was used, for example, on-line crushers with incremental steps of 2-min crushes, Bieri-type furnace with samples heated prior to analysis. It should be stated explicitly whether a cryogenic system was used to isolate the noble gas of interest or if noble gases were not separated prior to analysis. Relevant mass spectrometer details (analytical lab, model of the mass spectrometer) plus measurement routines (dynamic or static multicollection) should be included. Procedural blanks (and details how they were produced) must be included together with an assessment of their variance.

4. Stable isotope data

Reporting of the stable isotopic composition variations of the light elements should follow the guidelines proposed by Coplen et al. (2002). Suitable reference materials are available from National Institute of Standards and Technology; information about them can be accessed at the NIST site: http://patapsco.nist.gov/srmcatalog/tables/view_table.cfm?table=104_10.htm. Detailed information about measurements on many of these reference materials is compiled by Hut (1987).

The details of the sample preparation procedures must be outlined in the experimental section of the paper and all relevant fractionation factors used to report the data must be stated and referenced.

If stable isotope ratios are reported for elements for which there is not yet internationally available reference material in use by the geoscience community, wherever feasible, measurement results for the isotope reference materials cited in the most recent compilation of the International Union of Pure and Applied Chemistry should be included in the data set (e.g., Rosman and Taylor, 1997).

5. Other general policies

For any category of analyses, the Editor may request additional information.

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