

# Requirements for the Publication of Geochemical Data

## Policy Statement

Version 1.1 (January 2009)

The following policy statement was generated by the Editors' Roundtable, the participants of which are listed below. The Editors' Roundtable met 3 times (1: August 2007, 2: July 2008, 3: December 2008)<sup>1</sup>. A draft policy statement was approved in July 2008. The revised final revised version 1.1 was approved in December 2008.

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<sup>1</sup> Numbers in parentheses after individuals' names indicate which meeting(s) each one attended.

# Requirements for the Publication of Geochemical Data

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## 1. Preamble

Geochemical data, including chemical and isotopic analyses of natural and synthetic Earth and planetary materials, form the basis of the discipline of geochemistry. Yet, reporting and documenting practices of geochemical data in the scientific literature have been inconsistent or incomplete, with the effect that the original data can often not be recovered from the publications and are lost. This is not good scientific practice and is ultimately damaging to the health of the entire discipline.

Mainstream scientific journals, through a coordinated editorial policy on how geochemical data are handled, are the most effective agents to rectify these problems and implement best practices.

This policy is in part driven by the needs of digital data infrastructures for the sciences, which are a fundamental component of the emerging e-science/e-research/cyberinfrastructure. Digital data collections provide convenient and open access to the rapidly increasing pool of published data. Their quality depends critically on the consistency and completeness of data reporting.

As a first stage for generating a consistent set of criteria for geochemical data publication across disciplines, the Editors' Roundtable adopts the policy outlined below, which is designed to address both the improvement of general reporting standards and the seamless incorporation of data into scientific databases, with the overall aim of serving the scientific community.

## 2. Scope of Policy

This policy applies to geochemical compositional data (chemical abundance, isotopic) measured on natural and synthetic (experimental) samples, including rocks, sediments, fluids, and gases.

We expect this policy to be modified and extended in the future to other types of observational data (e.g. mineralogy, physical properties) for natural and synthetic samples.

### **3. Basic Requirements**

#### **3.1. Data Accessibility and Format**

*Access to the complete data, upon which new scientific discovery and knowledge is based, is a fundamental requirement for the reproducibility of scientific results.*

All NEW geochemical data used in a publication must be made available for future use by (1) submission to an accessible, persistent source such as a public database or data archive (for example, personal web sites are not persistent data archives), if it exists for the specific data type, or by (2) listing the data explicitly in a data table associated with the publication. The data must in any case be available in downloadable format.

For chemical abundance data of samples, elemental or oxide abundance data must be given unless a compelling reason can be provided; elemental abundance *ratios* are acceptable *only* if the compositional data do not exist. Isotope ratios are, of course, acceptable.

#### **3.2. Data Quality Information**

*Proper documentation of data quality is fundamental for comparison of research results and estimation of uncertainty.*

Authors must provide sufficient information (metadata) about the analytical process and reproducibility of measurements in order that the data quality can be properly evaluated. Correction procedures need to be clearly presented. This information is necessary to allow for scholarly reproduction of the results.

Basic metadata such as analytical technique, lab, and values measured on reference materials need to accompany the data. If possible, metadata should be provided in standardized tabular format to facilitate access to this information for editors, reviewers, readers, and data managers.

#### **3.3. Sample Information**

*The geochemical data addressed in this policy are tied to samples. Essential information about the samples must be provided in order to allow for proper identification of their origin and type, and to trace their analytical history.*

All natural samples for which data are reported require, if applicable, information about the sample location. In addition and if applicable, samples should be classified (e.g. lithology for rocks and sediments, species for minerals and fossils). Samples should have global unique identifiers so that data can be unambiguously referenced to a sample. This allows a complete analytical profile of a sample to be established that includes data generated at different times or in different labs, and reported in different publications.

## 4. Specific Guidelines

### *for Compositional Data Measured on Natural and Synthetic Samples*

#### **4.1. Data Accessibility and Format**

Data should be reported in tabular format. Data must always be available as a downloadable file in a format that can be easily converted into spreadsheet format (for example, .csv, .txt). The file should include units for the listed measured values.

This means that if a publication contains a data table in the main text or a pdf or image version of the data table as an electronic supplement, the data in the table(s) must also be available in a downloadable form that can be easily converted to spreadsheet format.

#### **4.2. Data Quality Information**

Information about the analytical procedure must be provided for each measured parameter. If a parameter has been analyzed by more than one method, each method must be documented separately. If possible, this information should be provided in tabular format.

1. GENERAL ANALYTICAL METADATA must include:
  - a. Analytical technique (e.g. ICP, XRF, EMP)
  - b. Laboratory (name of department/lab & institution)
  - c. Analytical accuracy & reproducibility
    - i. Name(s) and measured value(s) of (internationally recognized) reference standard(s) measured as unknown sample
    - ii. Estimated uncertainty of reference standard measurement, and, if applicable, number of measurements
2. METHOD SPECIFIC METADATA must include, *as appropriate to the method* (see Appendix):
  - a. Fractionation correction
  - b. Standardization (Normalization)
  - c. Total procedural blank
  - d. Detection limit
  - e. Calibration

### 4.3. Sample Information

- a. Metadata: All samples for which data are reported require, if applicable, information about sample location including, if possible *latitude and longitude* (if these are unknown, approximate coordinates obtained by using Google Earth would suffice). Marine samples require a *depth below sea level*. If applicable, the *position of a sample within a stratigraphic section or within a core* should be reported. Other critical sample metadata include *lithological classification and age*.
- b. Unique Identification: The problem of non-unique sample names needs to be addressed by the global earth science community. Currently, the only available system where individuals can obtain global unique identifiers for their samples is the sample registry SESAR (System for Earth Sample Registration, [www.geosamples.org](http://www.geosamples.org)). The unique identifier provided and administered by SESAR is the 9-digit alphanumeric International Geo Sample Number (IGSN), which is used together with a person's or institution's sample name to ensure unambiguous identification of a sample. IGSNs can be obtained from SESAR by submitting the information about a sample that is required for publication through this policy.

## 5. Appendix I: Required Metadata

### 5.1. Method Specific Analytical Metadata

The list below identifies metadata sets that are relevant for different types of analytical techniques, which may vary depending upon the specific analysis:

#### A. Bulk Elemental Analyses (e.g. AAS, HPLC, ICPAES, ICPMS, INAA, XRF)

- a. Standardization (Normalization)
- b. Total procedural blank
- c. Detection limit

#### B. In-situ Elemental Analyses (e.g. EMP, SIMS, LA-ICPMS)

- a. Standardization (Normalization)
- b. Detection limit
- c. Calibration

#### C. Bulk Isotopic Analyses (e.g. TIMS, MC-ICPMS)

- a. Standardization (Normalization)
- b. Fractionation correction
- c. Total procedural blank
- d. Detection limit

#### D. In-situ Isotope Analyses (e.g. SIMS, LA-MC-ICPMS, LA-ICPMS)

- a. Standardization (Normalization)
- b. Detection limit
- c. Normalization
- d. Fractionation correction

## 5.2. Sample Metadata

The list below identifies which metadata should be provided for samples (if applicable).

- a. Sample name
- b. Geospatial coordinates (latitude, longitude, possibly even utilizing Google Earth for an approximate value if otherwise unknown)
- c. Unique Identifier (e.g. International GeoSample Number, IGSN)
- d. Classification (e.g. lithology)
- e. Age
- f. Depth in core or position within a stratigraphic section (if applicable)
- g. Cruise or field program (if applicable)

## 6. Appendix II: Checklist for Authors and Editors

A checklist has been created to help authors and editors ensure completeness of metadata (see page 9). The checklist can be downloaded from the EarthChem web site at <http://www.earthchem.org/earthchemWeb/roundtable.jsp>. This web site also lists a series of spreadsheets that provide examples for various data types (e.g. major oxides measured by microprobe, trace elements measured by ICP-MS, radiogenic isotope ratios measured by TIMS) how data and metadata should be reported.

# CHECK LIST

## For the Publication of Geochemical Data

Author(s):
Title:
Manuscript Number:

### Data

- All data listed in data tables *or*
- Reference to an accessible, persistent source such as a public database or data archive (*NOTE: personal web sites are not persistent data archives*)
- Downloadable format

*Comment*

### Sample Information

- Sample name<sup>1</sup>:  Yes  No  N/A
- Location (lat/long):  Yes  No  N/A
- Depth below sea level:  Yes  No  N/A
- Depth in core/strat section:  Yes  No  N/A
- Classification:  Yes  No  N/A
- Age:  Yes  No  N/A

*Comment*

### Data Table

- Units:  Yes  No  N/A
- Technique:  Yes  No  N/A
- Laboratory:  Yes  No  N/A
- Reference material(s):
  - Name:  Yes  No  N/A
  - Measured value(s):  Yes  No  N/A
  - Number of measurem.:  Yes  No  N/A
  - Reproducibility:  Yes  No  N/A

*Comment*

<sup>1</sup> Sample names should be unambiguous. Use of the International Geo Sample Numbers (IGSN) is recommended (can be obtained at [www.geosamples.org](http://www.geosamples.org)).