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Toward Consistent, Comprehensive, and Meaningful Documentation of Analytical Methods in Geochemistry: The Data Repository Perspective

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The deposition of geochemical data in trusted, open data repositories is increasingly recommended and adopted in the geochemistry community as a best practice (e.g. Klöcking et al. 2023). Repositories make data openly accessible to anybody interested, independently of a scientific article that may be only accessible via a journal subscription. But this practice it separates the data in the repository from the detailed description of the analytical method and procedures described in the article. Repositories, specifically those that archive and curate geochemical data such as the EarthChem Library and the Astromaterials Data System, therefore make it part of their curation process to ensure that researchers submit comprehensive method information along with the data. But what information can the repositories make mandatory and what is optional? Globally endorsed and governed community standards for describing analytical methods and data quality are still missing,and the large diversity of analytical methods does not allow for a single, easy solution that fits all.

EarthChem started to work with the geochemistry community two decades ago to establish guidelines for the reporting of geochemical data. These guidelines were refined and endorsed by the Editors Roundtable in 2009 (Goldstein et al. 2014) and have informed the design of the EarthChem Data Submission Templates (https://earthchem.org/ecl/templates). But these templates do not accommodate all relevant metadata for the large and growing variety of analytical methods used by geochemists. The Astromaterials Data System (Astromat) has used metadata schemas that the OSIRIS-REx Sample Analysis Team developed for the large number of methods used to analyze samples from asteroid Bennu. Neither EarthChem's nor Astromat's metadata schemas are true international standards. In order to advance convergence toward globally standardized documentation of analytical methods and data quality in geochemistry, EarthChem and Astromat are now collaborating with the Australian Geochemistry Network and through the OneGeochemistry initiative to develop initial versions of Method Metadata Profiles that will be reviewed by the community and refined.

Klöcking, M et al. (2023): Community recommendations for geochemical data, services and analytical capabilities in the 21st century. https://doi.org/10.1016/j.gca.2023.04.024

Goldstein, S L et al. (2014): Requirements for the Publication of Geochemical Data. https://doi.org/10.1594/IEDA/100426.