Innovating and networking global geochemical data resources through OneGeochemistry

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The Vision

A vision of the not-to-distant future: Imagine yourself as a researcher who is making plans for fieldwork in the Andes Mountains. You are behind your computer and load a three-dimensional visualisation of the Earth and its geology to investigate the research already done in the southern Patagonian regions. You zoom in to the mountain range of interest and select various data layers to show samples, their chemical and isotopic compositions, as well as rock ages for further reference. One area shows particularly young ages and a single click brings up an image showing the thermal and chemical evolution of the rocks, bringing to life the events experienced by that part of the Earth. Each sample and data point have all the necessary information about uncertainties in the data, and the associated description of the analytical methods enables you to verify and trust the quality of data associated with (anomalous) points. Looking back at the visualisation, you change a few parameters and, in (close to) real-time, the modelled Earth changes to display the outcomes of the selected model scenario. The model recipe and selected data are exported by another click to a standard formatted file. These data are directly usable in your chosen application and offline device. Adding your own recently collected data to the model via drag and drop makes them show up in bright colours, contrasting with the prior known data and putting them in direct context. The visualised additional data alters the prior geological understanding and confirms your suspicions regarding what information is missing. Together with a customisable visualisation of model uncertainty, this information helps you to plan the collection of new samples. You are excited to go into the field to collect and subsequently analyse samples that you know will complement existing research in the area and vastly improve the current geological understanding of this region. With this preparation in hand, you are now able to apply for the necessary funding, proposing an efficient plan that minimises cost at a high likelihood of success.

Towards Achieving a Shared Vision

This scenario envisages the streamlined handling of digital geochemical data and interoperability from various sources in the near future. This is in stark contrast to the current situation where such models must be painstakingly built by individuals based on datasets scraped together from several decades of publications, having a wide range of formats and sources (Chamberlain et al. 2021). Discipline-specific databases such as GEOROC, PetDB, PANGAEA, or AusGeochem already help considerably to find and synthesise published geochemical data; however, to achieve the above scenario, additions to legacy and future generated data are required to make them fully interoperable, such as uncertainties and metadata to enable quality assessment. Tools and simple workflows should be developed to add or combine missing data from e.g. unpublished regional or institutional data stores that may be hidden there or have never been published at all.

Our envisioned scenario requires using newly obtained data directly in the same context as previously published data enabling linkages of multiple components of geochemistry (which here always includes cosmochemistry). To establish these connections, it is essential for data collections to follow standardized procedures for reporting geochemical information, using agreed-upon terminology. For this, three major challenges need to be addressed: (i) *Standardisation of data collections and reporting:* this will enable researchers to compare and combine data from different sources; (ii) *Making data accessible online:* many data, particularly old data sets, are difficult to access and may not yet be digitally available; and (iii) *Enabling replication, verification of data quality and uncertainty*: this will allow decision making on how old and new data can be combined as a basis for new interpretations. These challenges are also known as making data Findable, Accessible, Interoperable, and Reusable for both machines and humans, in other words: FAIR (Wilkinson et al. 2016). While this has been partly achieved in other, related domains including chemistry, crystallography, seismology, and oceans science (Klöcking et al. 2023), whereas geochemistry is just getting started. We now need to harness existing initiatives and better coordinate the various community groups around the world working towards making geochemical data FAIR.

OneGeochemistry: Enabling a Shared Vision

The near-future vision and FAIR geochemical data can only be achieved in a global effort, similar to the “Editors Roundtable'' in 2007 that brought together publishers and data repository providers to discuss implementation of consistent data publication practices, which resulted in a policy statement in 2009 (Goldstein et al. 2014). The OneGeochemistry initiative aims to coordinate the development of global definitions of geochemical vocabularies, additional data reporting best practices, and their metadata requirements. OneGeochemistry currently consists of members from EarthChem, GEOROC, the Multi-scale Laboratories of the European Plate Observing System, GFZ Data Services, NFDI4Earth, and the AuScope Geochemistry Network, and represent the first governing board of the OneGeochemistry initiative (interim governance document: https://zenodo.org/record/6566075) and the newly appointed OneGeochemistry CODATA Working Group (https://codata.org/initiatives/decadal-programme2/worldfair/onegeochemistry-wg/). The ad-hoc governance represented by this group shall be replaced by a board elected by the geochemistry community in 2024.

The focus of the OneGeochemistry initiative is to better coordinate global efforts in geochemical data standardisation, facilitate communication between international groups working towards this same goal, and lessen duplication of efforts. This in order to enable development of a distributed FAIR geochemical data framework that interoperates through standard web services following the OneGeology example.

Articulating the Geochemical Data Diversity

The field of analytical geochemistry is as fascinating as it is diverse. Geochemical research starts at the beginning of our universe with the formation of the first elements, followed by the chemical and isotopic population of the periodic table and chart of nuclides during the evolution of galaxies and stars. The discipline intensively studies the formation of planetary building blocks, the Earth–Moon system, Earth's differentiation, plate tectonics, deep Earth, surface, and oceanic and atmospheric processes. Geochemistry is important for addressing questions around the future of our ecosystem and natural resources. The plethora of research fields geochemistry plays a role in naturally intersecting with many other disciplines. Similarly, the number of geochemical methods, analytical instrumentation, and laboratories is diverse and has impressively multiplied during the past few decades. These highly variable, mostly small datasets, collected by individual researchers or small teams, can be described as 'long-tail data' (Heidorn 2008) that are especially challenging to harmonise and standardise, but represent a significant number of research results. With such diversity and cross domain overlap, OneGeochemistry is focusing on the standardised reporting of chemical and isotopic data and their description. The project will thus have to be flexible evolving both with what informational demands geochemical data need to satisfy and with the emergence of new analytical methods.

Standardising Geochemical Data

Technological, sociological, and organisational leaps come from agreements on rules for how things are done: standard containers revolutionised shipping, the internet protocol our modern world, and SI units the basic exchange of scientific knowledge. Standardising geochemical data reporting has a similar potential to revolutionise how we will access and work with geochemical data. Regarding the standardisation efforts for this specific discipline, much can be learned from other communities such as crystallography, genomics, climate, and seismology, having established similar organisations to OneGeochemistry (Stall et al. 2020; Klöcking et al. 2023). As a community, we should strive to make geochemical data easily accessible to all online and accelerate interdisciplinary data integration.

Based on input from all stakeholders (FIG. 1), best practices will allow users to re-use datasets and validify their quality. Numerous suggestions on how to best report geochemical data have been published but are not yet widely adopted (e.g., Schaen et al. 2021; Flowers et al. 2022; Wallace et al. 2022). Adoption of reporting best practices is about to change with the increasing requirement from journals to publish data in domain-specific repositories such as EarthChem, DIGIS, Astromat, or AusGeochem. This improves access to these data, and makes the data FAIR, as these repositories require and facilitate the use of best practices via templates and discipline specific data models e.g., EarthChem XML schema or EarthChem Data Submission Templates. OneGeochemistry aims to structure, publicise, and promulgate these existing efforts in a community built, global system of FAIR geochemical data reporting. The aim is to make best practices available in a machine-actionable form following the 10 rules for FAIR vocabularies (Cox et al. 2021) by a OneGeochemistry technical expert committee. The collective outcomes of this initiative will be published through the International Union of Pure and Applied Chemistry's (IUPAC) colour book series. The IUPAC has offered the geochemistry community a new 'brown book', dedicated to geo- and cosmochemical data standards, nomenclature, terminology, and symbols; a book to be used and implemented by researchers, repositories, publishers, service providers, laboratories, and companies, etc. (FIG. 1).

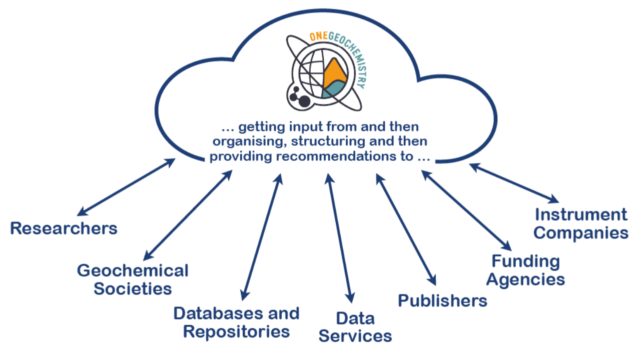

Figure 1; The proposed structure for OneGeochemistry; where it receives input for standards and best practices from various stakeholders working with geochemical data. Expert committees within OneGeochemistry formally check and accept these with goal to making them available in machine actionable formats as well as publications in the IUPAC brown book and on the OneGeochemistry webpage as recommendations for the various stakeholders to be implemented.

Figure 1: The OneGeochemistry logo

OneGeochemistry as an International Organisation of Communities and Agreements

Predominantly a voluntary effort, the OneGeochemistry initiative (FIG. 2) is currently run through a working group of the International Science Council's Committee on DATA (CODATA), providing the initiative an initial operational structure. Strong community engagement, interaction, and feedback are essential for the success of the OneGeochemistry initiative for which it has already sought endorsement from societies and unions. Currently, the initiative is endorsed by the Geochemical Society, the European Association of Geochemistry, the Association of Applied Geochemists, the International Association of Geochemistry, and the Meteoritical Society. The IUGS commission on Global Geochemical Baselines endorses the OneGeochemistry CODATA Working Group.

The current OneGeochemistry initiative members — largely similar to the authors of this article — are active in the community through the organisation of sessions and town hall meetings at international conferences such as the EGU General Assembly, Goldschmidt, and AGU Fall Meeting, where we encourage readers to engage with this initiative. OneGeochemistry is still very much developing and we want you to get involved in deciding on its governance, formal and legal structure, help make decisions, and participate in the process of defining community-led guidelines for geochemical data handling and preservation. As part of this, you can make yourself electable for the board, and join or lead scientific and technical expert committees to advise on and help coordinate development of standard data reporting methods, method specific vocabularies, as well as metadata profiles (e.g., Klöcking et al. 2023). OneGeochemistry also welcomes any suggestions and reviews of project outcomes and progress via our Slack workspace (https://onegeochemistry.slack.com) or email address (onegeochemistry@codata.org).

The OneGeochemistry initiative invites you, other researchers, data groups, and initiatives to help make the introductory vision come true, by making geochemical data more standardised and interoperable between institutions and nations, **creating a global network of geochemical data resources**. For more information, please visit the OneGeochemistry website at www.onegeochemistry.org. Please join OneGeochemistry using the above-mentioned channels or by getting in touch with Alexander Prent at onegeochemistry@codata.org.

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