Applied Geochemistry 198 (2026) 106682

Contents lists available at ScienceDirect

Applied Geochemistry

journal homepage: www.elsevier.com/locate/apgeochem

A common ontology for stable isotope data

Nina Welti[a,*,1], Steph Hawkins[b,1], Kathryn Waltenberg[b], Cath Hughes[c], Jagoda Crawford[c], Yanfeng Shu[a], Regina Campbell[a], Alex Leslie[c], Athina Puccini[a], Christoph Gerber[a], Axel Suckow[a], Geoff Fraser[b], Lian Flick[a]

[a] CSIRO, 40 Waite Rd, Urrbrae, SA, 5064, Australia
[b] Geoscience Australia, ACT, Canberra, 2601, Australia
[c] ANSTO, Locked Bag 2001 Kirrawee, DC, NSW, 2232, Australia

ARTICLE INFO

Editorial handling by: Dr. Tao Wen

Keywords:
Stable isotope data
FAIR data
Data standards

ABSTRACT

Stable isotope data has broad applicability across multiple science domains. As more datasets are published and stable isotope data systems are built, the findability and accessibility of stable isotope data increases. However, due to a lack of a common reporting framework, the interoperability of these data systems is limited. A common ontology is needed so stable isotope data systems and published datasets can be translated into a common format without disrupting existing data models or introducing complex workflows. This common ontology for stable isotope data and associated metadata offers a methodology to achieve cross-domain interoperability of environmental stable isotope data. It functions as a straightforward data stewardship tool to enhance the findability, accessibility, interoperability, and reuse (FAIR principles) of stable isotope data across disciplines. Ultimately, this ontology aims to make existing data systems cohesive, interoperable, and discoverable across the entire measurement pipeline, encompassing publicly accessible repositories, peer-reviewed literature, and grey literature.

1. Introduction

Stable isotope data is widely used for characterising and tracing dynamic processes and fluxes within and between natural, managed, and industrial systems. However, due to the highly specialised analytical requirements, stable isotope measurements have remained nearly exclusively in the arena of research organisations. The total volume of stable isotope data is relatively modest compared to other types of scientific data (i.e. bioinformatics). Others have highlighted the utility of centralised repositories for stable isotopes (e.g. IsoBank and IsoArch) (Pauli et al., 2017; Plomp et al., 2022; Shipley et al., 2024), database systems (Suckow and Dumke, 2001), and vocabularies (Boone et al., 2022; Simons et al., 2012) to facilitate the reuse of primary research data. Given the widespread use of stable isotope data across scientific disciplines and applications (Brand and Coplen, 2012), there is a high potential for data reuse.

Harmonising data is difficult; making complex datasets comparable and compatible requires considerable effort (Cheng et al., 2024; Devaraju et al., 2021). There is a rapid uptick in tools that use big data, such as the Internet of Things, large languages models (LLM), and machine learning (ML) tools, which rely on the availability of machine-readable data in both structured and unstructured formats (Klöcking et al., 2023). Data volumes are growing at an exponential rate, with Geoscience Australia, Australia's lead agency for geoscience, responsible for providing authoritative information on Australia's geology, geography, and natural resources, seeing a 350 % increase in their minerals, energy and groundwater data holdings from July 2016 to July 2024. This highlights the need to increase the discoverability, accessibility and use of existing data, especially in the public sector (Overton et al., 2022).

Here we propose a common ontology for stable isotope data and associated metadata providing a methodology to harmonise stable isotope data across scientific domains and applications.

* Corresponding author.
E-mail address: nina.welti@csiro.au (N. Welti).
[1] co-first authors.

https://doi.org/10.1016/j.apgeochem.2026.106682
Received 12 August 2025; Received in revised form 27 November 2025; Accepted 5 January 2026
Available online 5 January 2026

2. Methods

2.1. Scope and development

An ontology is a formal way of sharing information (Washington and Lewis, 2008), a systematic format that combines attributes to give context and provide a common understanding of the data in question. Ontologies provide a common framework that can be utilised by both humans and machines (Washington and Lewis, 2008) and allow for interoperability of datasets produced at different times and places (Simons et al., 2006). By standardising nomenclature and relationships, ontologies facilitate the reuse and comparison of datasets, irrespective of their original purpose (Wilson et al., 2021). The aim of this ontology is to facilitate the harmonisation and integration of disparate stable isotope datasets while retaining data integrity.

Stable isotope data originates from existing data structures which were developed for other applications or purposes (Pauli et al., 2017; Plomp et al., 2022; Suckow and Dumke, 2001; Geoscience Australia, 2021). The common ontology incorporates best practice and IUPAC compliant stable isotope reporting guidelines (Brand et al., 2014; Coplen, 2011; Coplen et al., 1992, 2002a; Skrzypek, 2013; Skrzypek et al., 2022) with existing data standards (Klump et al., 2021), and models used across hydrology (Brodaric et al., 2018; Walker et al., 2009), geology (Raymond et al., 2016; Sen and Duffy, 2005; Simons et al., 2006), mineral occurrences (Urvois et al., 2022), soil information (Simons et al., 2013) and food science (Donarski et al., 2019; Eftimov et al., 2019) to harmonise best practices across scientific disciplines. Using human-readable terms, common concepts and relations were refined to create a parsimonious and flexible ontology.

Reusing existing ontologies or vocabularies is a common practice in ontology development, which not only reduces cost and time associated with the development, but also improves extensibility and interoperability of the developed ontology with other resources. We followed this practice in the development of this ontology. Specifically, we examined the W3C recommendations, the Semantic Sensor Network Ontology (SSN, https://www.w3.org/TR/vocab-ssn/), QUDT (Quantities, Units, Dimensions and DataTypes, https://github.com/qudt/qudt-public-repo), and several domain-specific dictionaries and vocabularies such as the Sedimentary Geochemistry and Paleoenvironments (SGP) attribute dictionary (Farrell et al., 2021) and the AusTraits Plant Dictionary vocabulary (Wenk et al., 2024).

2.2. Mapping between organisations

Australian Commonwealth agencies are expected to ensure the quality, integrity, security, discoverability, accessibility, and useability of data assets (Australia, 2022, 2023). As key collaboration nodes within Australia, Commonwealth Scientific and Industrial Research Organisation (CSIRO), Geoscience Australia (GA), the Australian Nuclear Science and Technology Organisation (ANSTO) and the National Measurement Institute (NMI), represent principal custodians of stable isotope data in Australia. As such, they participate in the entire chain of stable isotope data collection and curation: from study design, funding acquisition, field implementation and sample collection to the operation of analytical laboratories conducting stable isotope measurements and data interpretation, and to enable access to data collections to enable reusability and ensure the long-term preservation and persistence of data collections. Consequently, they share a common purpose to create interoperable and reusable stable isotope datasets across a wide range of scientific disciplines.

Consultation was sought throughout the development of this ontology to ensure that it was not redundant, increased accessibility, interoperability, findability (FAIR) and maintained data sovereignty. While the Commonwealth agencies are involved throughout the generation and curation of stable isotope data, they operate differently to academic research organisations. To ensure that the ontology meets the needs of industry, academic and research sectors a formal Science and Operations User Group (SOUG) was established. Members represented both stable isotope experts and potential end users, early and mid-career university researchers, industry bodies, and government policy advisors. Given the Australian cohort, an early draft version of the ontology was presented during the 13th International Conference on the Application of Stable Isotope Techniques in Ecological Studies (IsoEcol) 2024 to seek input and feedback from the wider, international academic stable isotope community.

Each organisation used different vocabularies and syntaxes, some of which were ingrained in multi-decadal systems. Creating standardization between these legacy vocabularies was the impetus to develop a common ontology. There was active consideration and discussion of all fields held by the contributing organisations to facilitate the harmonisation of existing data. The common ontology was a result of bringing together published datasets held and maintained according to each organisation's data management systems.

The contributing organisations first compared their data schemas (Miller et al., 2012; Suckow and Dumke, 2001), web service flat-file structures (Hawkins et al., 2024), and data spreadsheets to identify attributes used across all organisations. Existing stable isotope datasets (Geoscience Australia, 2021) as well as associated data standards and vocabularies (Hawkins, 2023; Hofstra et al., 2021; Raymond et al., 2016) were then used to further refine the common attributes and ensure that this ontology can translate across existing data models. To reduce complexity in the initial ontology development, only datasets from Australian continental coverage were used, with any oceanic or near-shore samples out of scope. The common attributes described the sample matrix, location of field sampling, and analytical methods. Standard, human-readable terms were chosen for these attributes and data was mapped between the organisations. The selected attributes were reviewed throughout the ontology development to ensure that they were compatible.

Hydrogen (H), oxygen (O), carbon (C), nitrogen (N), and strontium (Sr) stable isotopes were used as a basis for mapping, as they represented the common stable isotope systems held by the contributing organisations. Tritium (3H) was included to ensure flexibility within the ontology, to facilitate the potential future inclusion of radioisotopes. However, the ontology is not exclusive to these five stable isotope systems. It is designed to be inclusive for all stable isotope systems (Meija et al., 2016) including radiogenic and compound specific stable isotope data. Lead (Pb) and sulphur (S) isotopes were considered, though not used to develop the initial version. The regolith dataset (de Caritat and Cooper, 2011) included within Geoscience Australia (2021) which was used to map Sr also includes Pb (Desem et al., 2023) and bioavailable Sr (de Caritat et al., 2022, 2023, 2025). The Geoscience Australia hydrochemistry database that was mapped through Hawkins et al., 2022 contains S, Pb, and argon (Ar) isotope data (Trihey and HarrisPascal, 2021; Schroder et al., 2020) indicating potential use of the ontology. As the available stable isotope data was originally collected for a variety of purposes such as environmental monitoring, soil science and water applications, the ontology is widely applicable across domains beyond environmental science.

3. Results

The common vocabulary attributes that describe stable isotope metadata are represented by the stable isotope ontology. The design of the stable isotope ontology is heavily influenced by the specific and unique attributes associated with hydrochemistry, geochemistry and environmental monitoring.

3.1. Main concepts and relations

The stable isotope ontology contains sixclasses – Site, Sample, Method, Measurement, Agent, Traceability (Fig. 1), distilled from

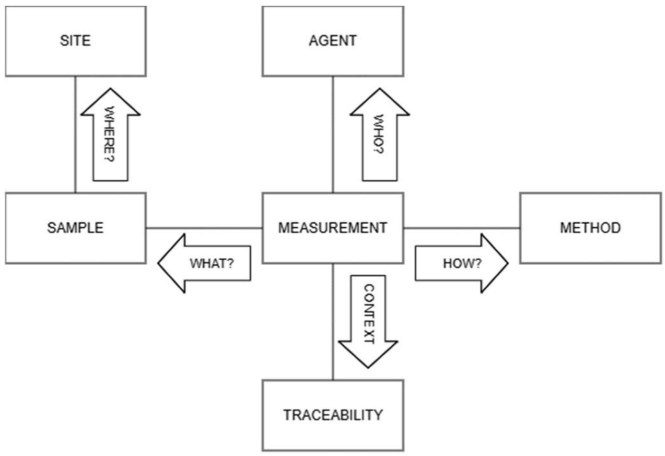

Fig. 1. Top-level view of the stable isotope ontology.

63attributes. A full description of the data attributes and object properties can be found in Tables 1 and 2, respectively. Of these attributes, 15 are required to facilitate a minimal level of interoperability (Table 3). Simple metadata attributes including a citation and contributing organisation were included to enable associated data not included within the ontology to be found.

- **Site** — contains 10attributes that describe where the sample was collected, including site names and description, site type, location coordinates, elevation and datum.
- **Sample** — contains 22 attributes that describe the sample itself, including sample IDs, sample types, and persistent identifier (PID) information for the samples.
- **Method** — contains 5 attributes that describe how the sample was collected and analysed, including pretreatment and storage metadata.
- **Measurement** — contains 8 attributes that describe the stable isotope analytical results including the measured isotope, results, units, scale and analytical uncertainty.
- **Agent** — contains 6 attributes that describe the provenance of the data, including contact details for sample collection, analytical laboratory, and citation references for sample and related results.
- **Traceability** — contains 9 attributes that describe data quality assurance and compliance information such as data processing, reference materials and procedure information.

Based on the concepts identified (Fig. 1), we developed the stable isotope ontology. In the development we reused the Semantic Sensor Network Ontology (SSN), which is a W3C recommendation for describing sensors and their observations, the involved procedures, the features of interest, the samples used, and the observed properties, as well as actuators. SSN includes a lightweight but self-contained core ontology called SOSA (Sensor, Observation, Sample, and Actuator) for its elementary classes and properties. We reused "sosa:Sample" and "sosa:FeatureOfInterest for describing samples and their features of interest (e.g., sites). Specifically, we defined "Sample" and "Site" as subclasses of "sosa:FeatureOfInterest", as both can be the features of interest that samples come from. "Sample" was also defined as a subclass of "sosa:Sample", which has its own properties like type and amount, and links to "sosa:FeatureOfInterest" via "sosa:isSampleOf". Fig. 2 shows the main classes and relations of the ontology, as described in Table 2. Noting that the ontology was designed to be adaptable and modular the classes can be expanded, e.g. "Sample" can be further extended to include specific sample types, such as "WaterSample".

3.2. Structure

A key criterion is to reduce barriers for reporting data in a unified format, enabling contributors with all experience levels to use the stable isotope ontology to report their results. As a result, we created a structured, formatted output for ontology implementation that simplifies sharing data and facilitates a simple user-experience. The flat (denormalised) table structure can be used as an Excel spreadsheet, comma-separated value (.csv) file or to translate between relational databases and user-friendly output. Users retain control of their data management, be that spreadsheet or relational database, effectively decentralising data management and maintaining data sovereignty. The defined structure can be expanded as needed ensuring the stable isotope ontology is flexible and adaptable to a variety of specific applications, while maintaining interoperability. An example of how the stable isotope ontology maps between organisations (as described in 2.2) using the Geoscience Australia web services can be found in Table 4. The flat structure also allows the stable isotope ontology to be implemented as a modular add-on to larger ontologies, in the same way as the Geoscience Australia's hydrochemistry and isotope database incorporate GeoSciML to include borehole, field site or stratigraphic unit information for groundwater metadata when delivered via web service (Geoscience Australia, 2021; Hawkins, 2023). These services do not share all attributes captured in the Geoscience Australia data systems and are subject to change.

3.3. Syntax

The SITE, SAMPLE, and METHOD attributes follow a general syntax of attribute class and name separated with an underscore. Examples of this are as follows: SAMPLE_ID, SITE_NAME, METHOD_SAMPLE_CONTAINER, TRACEABILITY_UNCERTAINTY. The remaining attribute classes do not follow this syntax, instead using IUPAC recommendations to create naming conventions for MEASURMENT and TRACEABILITY (Skrzypek et al., 2022).

The stable isotope ontology uses human readable terms to ensure easier engagement. Attribute names were simplified where possible. These terms can be converted to semantic standards with persistent identifiers but are presented here as a less formal flat-structure to increase adoption and adaption.

3.4. Reporting requirements

The mapping across organisations identified the common data attributes, which resulted in three tiers of reporting requirements. Required, recommended, and optional attribute fields are delineated within the stable isotope ontology to improve data quality control and provide guidance to those intending to follow the ontology for their own data management needs (Table 3). Required and recommended attributes were distinguished to strike a balance between adopting IUPAC recommendations (Coplen, 2011; Coplen et al., 2002a; Skrzypek et al., 2022) and accommodating legacy data with limited metadata. Delineating between required, recommended, and optional attributes aims to increase access and interoperability between imperfect datasets. Using a three-tiered approach, the aim is to reduce barriers to entry and inclusion, promoting best practices that uplift data robustness and quality of metadata provided. As such, if the mandatory field (e.g. UNCERTAINTY_KIND and SAMPLE_DATE_START) cannot be supplied, a set of default values can be used (e.g. "Not Provided" and January 01, 3000).

There are 15 required attributes, describing the basic information needed to make any data collection re-useable. These attributes include a unique sample name, sample type description, sample acquisition date and location, and publication references allowing users to be redirected to source datasets and/or publications. The mandatory fields also cover analysis information – analyte, isotope, values, units and scale. A minimum of one isotope measurement is required for a sample to be

Table 1
Main attributes (data properties) of the stable isotope ontology.

Attribute	Description	Class	Format	Reporting	Reference
PUBLICATION	Publication details in which this data was first published.	Agent	String	Required	
SAMPLE_PROJECT_IDENTIFIER	Name of the project under which the analyses were originally run.	Sample	String	Required	
SAMPLE_PROJECT_DESCRIPTION	Short description of the project under which the analyses were originally run.	Sample	String	Required	
SAMPLE_DATE_START	Date when the sampling process started, expressed as YYYY-MM-DD HH:MM.	Sample	YYYY-MM-DD HH:MM	Required	(Holden et al., 2011; ISO, 2019a)
SAMPLE_DATE_END	Date when the sampling process ended, expressed as YYYY-MM-DD HH:MM.	Sample	YYYY-MM-DD HH:MM	Optional	ISO (2019a)
SAMPLE_DURATION	The duration of the sampling process, as hours.	Sample	Numeric	Optional	
SAMPLE_TIMEZONE	The time zone of the sampling time.	Sample	String	Optional	
SAMPLE_ID	Unique name of the sample.	Sample	String	Required	
SAMPLE_PID	Unique, permanent URI linked to the data.	Sample	String	Recommended	Klump et al. (2021)
SAMPLE_TYPE	Type of physical material collected from the collection site.	Sample	String	Required	
SAMPLE_SOURCE_TYPE	Describes the material that contained the sample. Further refines Sample Type.	Sample	String	Recommended	
SAMPLE_SOURCE_FORM	The form of the sample at sampling time.	Sample	String	Optional	
SAMPLE_SUBTYPE	Type of subsample analysed in the laboratory.	Sample	String	Recommended	
SAMPLE_SUBSAMPLE_ID	Unique name of the subsample.	Sample	String	Optional	
SAMPLE_AMOUNT	Amount of sample analysed.	Sample	Numeric	Optional	
SAMPLE_UOM	Unit of sample amount.	Sample	String	Optional	
SITE_NAME	Name assigned to the collection site.	Site	String	Recommended	
SITE_DESCRIPTION	Description of the site at which the sample was collected.	Site	String	Recommended	
SITE_NUMBER	Unique ID assigned to the collection site.	Site	String	Optional	
SITE_TYPE	Type of collection site.	Site	String	Optional	
SITE_LATITUDE	Latitude of the sample collection site, in the GDA94 datum.	Site	Numeric	Required	ICSM (2014)
SITE_LONGITUDE	Longitude of the sample collection site, in the GDA94 datum.	Site	Numeric	Required	ICSM (2014)
LAT_LON_PRECISION	The precision of the reported latitude and longitude, determined from GPS or estimated.	Site	Numeric	Optional	ICSM (2014)
SITE_ELEVATION_AHD_M	Elevation or altitude in metres relative to the Australian Height Datum.	Site	Numeric	Required	Australian Height Datum 1971 (AHD71)
SITE_UPPER_DEPTH_M	Upper limit of depth at which field sample was collected, in metres from surface.	Site	Numeric	Optional	BOM (2019)
SITE_LOWER_DEPTH_M	Lower limit of depth at which field sample was collected, in metres from surface.	Site	Numeric	Optional	BOM (2019)
SITE_DEPTH_REFERENCE_UNIT	Unit used to quantify upper and lower depth of a sample.	Site	String	Optional	BOM (2019)
SAMPLE_TEMPERATURE	Temperature of the sample in the field.	Sample	Numeric	Optional	
SAMPLE_SITE_AIR_TEMPERATURE_DEGC	Air temperature at time sample was taken, expressed as degrees Celsius.	Sample	Numeric	Optional	
SAMPLE_STRATIGRAPHIC_UNIT	Describes the body of rock forming a discrete and definable geologic unit defined by lithology independent of relationships to other units. Denotes a 'kind' of rock body characterized by lithology, e.g. basaltic rocks.	Sample	String	Optional	(2017; Raymond and Brown, 1949; Simons et al., 2006)
SAMPLE_COLLECTED_BY	Name of organisation who collected the sample.	Agent	String	Optional	
SAMPLE_CONFIDENTIAL_DATE	Date when data is publicly available.	Sample	YYYY-MM-DD HH:MM	Optional	(ISO, 2019a)
ANALYTE	The feature of interest in the stable isotope analytical procedure, expressed as the most specific component entity, e.g. Element, material, substance or chemical constituent.	Measurement	String	Required	
ISOTOPE	The isotope analysed, expressed as d(number)(element).	Measurement	String	Required	Coplen and Shrestha (2016)
VALUE	The measured result of stable isotope analysis.	Measurement	Numeric	Required	(Coplen, 2011; Skrzypek, 2013)
UNIT	The unit of the result.	Measurement	String	Required	(Coplen, 2011; Coplen et al., 1992; ISO, 2019b; Skrzypek et al., 2022)
SCALE	Scale to which isotope measurements were normalized.	Measurement	String	Required	Skrzypek et al. (2022)
UNCERTAINTY	Analytical uncertainty associated with procedure.	Measurement	Numeric	Recommended	Skrzypek et al. (2022)
UNCERTAINTY_KIND	Analytical uncertainty type. If not provided or unknown, default "Not provided".	Measurement	String	Required	

(continued on next page)

Table 1 (*continued*)

Attribute	Description	Class	Format	Reporting	Reference
SAMPLE_ELEMENT_CONCENTRATION	Concentration of the element measured, related to the isotope analysed.	Sample	Numeric	Optional	
SAMPLE_ELEMENT_CONCENTRATION_UNIT	Unit of concentration.	Sample	String	Optional	
REFERENCE_MATERIAL_USED	Reference material used to normalise stable isotope measurement results.	Traceability	String	Recommended	(Brand et al., 2014; Coplen et al., 2002b)
VALUE_REFERENCE_MATERIAL	Measurement result (Value) of reference material.	Traceability	Numeric	Recommended	(Coplen, 2011; Skrzypek et al., 2022)
UNCERTAINTY_REFERENCE_MATERIAL	Uncertainty of the measured reference material.	Traceability	String	Recommended	Skrzypek et al. (2022)
UNIT_UNCERTAINTY_REFERENCE_MATERIAL	Unit used to calculate uncertainty.	Traceability	String	Recommended	
DATA_OWNER	The organisation to contact for any inquiries, issues, or updates related to the dataset.	Agent	String	Recommended	
ANALYSIS_DATE	Date of analysis.	Agent	YYYY-MM-DD HH: MM	Optional	ISO (2019a)
ANALYSIS_COMMENTS	Any comments or remarks about an analysis.	Agent	String	Optional	
LABORATORY	Laboratory at which the analysis was performed, provided as organisation name.	Agent	String	Optional	
METHOD_SAMPLE_PRETREATMENT	Details on any pretreatment prior to stable isotope analysis.	Method	String	Optional	
METROLOGICAL_TRACEABILITY	Details about the normalisation and data post-measurement.	Traceability	String	Optional	Skrzypek et al. (2022)
TRACEABILITY_ANALYTICAL_PROCEDURE	The analytical technique: i.e. bulk isotope analysis using EA-IRMS (Elemental analyser coupled isotope ratio mass spectrometry) or compound specific isotope analysis which will requiring separation prior to analysis i.e. GC- or LC-IRMS. Sample preparation: i.e. x mg of sample weighed into tin or silver capsules, sample combusted at x temperature, any reduction of combusted gas and removal of water, carrier gas (grade and brand), flow rate, any GC column (brand) used. Instrument and control: i.e. brand and model of peripheral connected to mass spectrometer, software package, version.	Traceability	String	Optional	Skrzypek et al. (2022)
TRACEABILITY_UNCERTAINTY	The delta value must be reported with standard uncertainty/expanded with coverage factor and coverage probability. The measurement uncertainty for the reported values was evaluated from both known sources and uncertainty from the Reference Material used for normalisation.	Traceability	String	Optional	Skrzypek et al. (2022)
DATA_PROCESSING	The measurement model equation or describing the basic principles used to normalise stable isotope measurement results. Any and all corrections applied to instrumental readings.	Traceability	String	Optional	Skrzypek et al. (2022)
UNCERTAINTY_EVALUATION	Standard uncertainty or expanded uncertainty with coverage factor and coverage probability. Conformity of results to the method performance characteristics.	Traceability	String	Optional	Skrzypek et al. (2022)
METHOD_SAMPLE_COLLECTION	Details of method used to collect the sample.	Method	String	Optional	
METHOD_SAMPLE_CONTAINER	Description of the sample container.	Method	String	Optional	
METHOD_SUBSAMPLE_CONTAINER	Description of the subsample container.	Method	String	Optional	
SAMPLE_STORAGE_CONDITIONS	Details on the manner in which the sample was stored and handled until it was tested.	Method	String	Optional	
MODELLED	“yes”, if the result stems from a mathematical model and not from a measurement. “no” otherwise (default).	Measurement	String	Optional	

Table 2
The main object properties defined in the stable isotope ontology.

Object property	Description	Domain	Range
hasMethod	Link to the method associated with Sample or Measurement	Sample or Measurement	Method
hasMeasurement	Link to the Measurement associated with the Sample	Sample	Measurement
associatedWith	Link to the Agent associated with Sample or Measurement	Sample or Measurement	Agent
hasTraceability	Link to Traceability involved in the Measurement	Measurement	Traceability

included.

A further 12 attributes are recommended which provide additional context for samples and associated results and include IUPAC recommended reporting requirements. These include a persistent identifier (PID) for the sample, such as an International Generic Sample Number (IGSN) (Klump et al., 2021), site names and a site description, uncertainties and reference material information.

The additional 33 optional attributes further enhance functionality or usability of the data collection and users should be encouraged to use as many as are relevant. Some attributes are only relevant to specific sample types and are included to provide important contextual information.

Table 3
Reporting requirement levels for the stable isotope ontology.

Required	Recommended	Optional
ANALYTE	DATA_OWNER	ANALYSIS_COMMENTS
ISOTOPE	REFERENCE_MATERIAL_USED	ANALYSIS_DATE
PUBLICATION	SAMPLE_PID	DATA_PROCESSING
SAMPLE_DATE_START	SAMPLE_SOURCE_TYPE	LABORATORY
SAMPLE_ID	SAMPLE_SUBTYPE	LAT_LON_PRECISION
SAMPLE_PROJECT_DESCRIPTION	SITE_DESCRIPTION	METHOD_SAMPLE_COLLECTION
SAMPLE_PROJECT_IDENTIFIER	SITE_LAT_LONG_REFERENCE_SYSTEM	METHOD_SAMPLE_CONTAINER
SAMPLE_TYPE	SITE_NAME	METHOD_SAMPLE_PRETREATMENT
SCALE	UNCERTAINTY	METHOD_SUBSAMPLE_CONTAINER
SITE_LATITUDE	UNCERTAINTY_REFERENCE_MATERIAL	METROLOGICAL_TRACEABILITY
SITE_LONGITUDE	UNIT_UNCERTAINTY_REFERENCE_MATERIAL	MODELLED
UNCERTAINTY_KIND	VALUE_REFERENCE_MATERIAL	SAMPLE_AMOUNT
UNIT		SAMPLE_COLLECTED_BY
VALUE		SAMPLE_CONFIDENTIAL_DATE
SITE_ELEVATION_AHD_M		SAMPLE_DATE_END
		SAMPLE_DURATION
		SAMPLE_ELEMENT_CONCENTRATION
		SAMPLE_ELEMENT_CONCENTRATION_UNIT
		SAMPLE_SITE_AIR_TEMPERATURE_DEGC
		SAMPLE_SOURCE_FORM
		SAMPLE_STORAGE_CONDITIONS
		SAMPLE_STRATIGRAPHIC_UNIT
		SAMPLE_SUBSAMPLE_ID
		SAMPLE_TEMPERATURE
		SAMPLE_TIMEZONE
		SAMPLE_UOM
		SITE_DEPTH_REFERENCE_UNIT
		SITE_LOWER_DEPTH_M
		SITE_NUMBER
		SITE_TYPE
		SITE_UPPER_DEPTH_M
		TRACEABILITY_ANALYTICAL_PROCEDURE
		TRACEABILITY_UNCERTAINTY
		UNCERTAINTY_EVALUATION

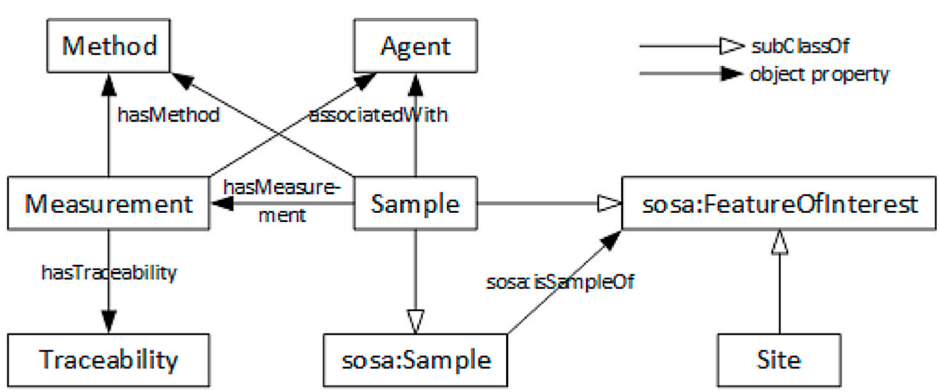

Fig. 2. Main classes and relations of the ontology, which reuses the SOSA (Sensor, Observation, Sample, and Actuator) ontology contained within the Semantic Sensor Network Ontology.

3.5. 3.5 Remarks on vocabulary

The primary purpose of the stable isotope ontology is to contextualise stable isotope data and is designed to be adaptable to specific domains and applications. Therefore, each attribute can be described using custom, domain-specific vocabularies, so that different systems can be used without need to synchronise vocabularies. Each of the attributes has an expected data type – either a numeric value, string or date format. This is to ensure that appropriate values are used throughout the ontology. Field lengths are not character limited, to reflect the various requirements of different data management systems.

The ontology accommodates datasets which contain a single sample type, multiple sample types, multiple samples from a single site, using multiple attributes fields to refine sample material information (e.g. sample material can be described by SAMPLE_TYPE, SAMPLE_SOURCE_TYPE, SAMPLE_SOURCE_FORM, SAMPLE_SUBTYPE).

The cornerstone of the ontology are the MEASUREMENT attributes (ANALYTE, ISOTOPE, VALUE, UNIT, SCALE, UNCERTAINTY, UNCERTAINTY_KIND, MODELLED) (Table 5), for which there are recommended vocabularies. The ISOTOPE attribute should be described according to the IUPAC recommendations (Coplen, 2011; Bond and Hobson, 2012), with further clarification provided by the UNIT and SCALE attributes. The ANALYTE and UNCERTAINTY_KIND attributes are recommended to be described using the Chemical Species and Uncertainty concepts (respectively) from AuScope Geochemistry Network (AGN) Geochemistry and Earth Science Vocabulary (Nixon et al., 2025). The METHOD attributes are suggested to be described according to the recommendations of ecohydrological investigations (Millar et al., 2022).

Table 4
Mapping of main attributes of the stable isotope ontology to the Geoscience Australia data systems (Hawkins et al., 2022; Geoscience Australia, 2021).

Attribute	Class	Format	Reporting	Sr layer - Geochronology and Isotopes web service	Pb regolith layer - Geochronology and Isotopes web service	All Hydrochemistry - Hydrochemistry web service
PUBLICATION	Agent	String	Required	SR_REF	PB_REFERENCE	PROJECT_PUBLICATIONS
SAMPLE_PROJECT_IDENTIFIER	Sample	String	Required	PROJECT	PROJECT	PROJECT
SAMPLE_PROJECT_DESCRIPTION	Sample	String	Required	null	null	null
SAMPLE_DATE_END	Sample	YYYY-MM-DD HH:MM	Optional	null	null	null
SAMPLE_DATE_START	Sample	YYYY-MM-DD HH:MM	Required	SAMPLE_ACQUISITION_DATE	SAMPLE_ACQUISITION_DATE	SAMPLING_DATE
SAMPLE_DURATION	Sample	Numeric	Optional	null	null	null
SAMPLE_TIMEZONE	Sample	String	Optional	null	null	null
SAMPLE_ID	Sample	String	Required	SAMPLE_ID	SAMPLE_ID	SAMPLE_ID
SAMPLE_PID	Sample	String	Recommended	SAMPLE_PID	SAMPLE_PID	SAMPLE_PID
SAMPLE_TYPE	Sample	String	Required	SAMPLE_TYPE	SAMPLE_TYPE	SAMPLE_TYPE
SAMPLE_SOURCE_FORM	Sample	String	Optional	null	null	null
SAMPLE_SOURCE_TYPE	Sample	String	Recommended	MATERIAL_TYPE	MATERIAL_TYPE	MATERIAL_CLASS
SAMPLE_SUBTYPE	Sample	String	Recommended	null	null	null
SAMPLE_SUBSAMPLE_ID	Sample	String	Optional	null	null	null
SAMPLE_AMOUNT	Sample	Numeric	Optional	null	null	null
SAMPLE_UOM	Sample	String	Optional	null	null	null
SITE_NAME	Site	String	Recommended	SAMPLING_FEATURE_NAME	SAMPLING_FEATURE_NAME	SAMPLING_FEATURE_NAME
SITE_DESCRIPTION	Site	String	Recommended	null	null	null
SITE_NUMBER	Site	String	Optional	ENO	ENO	SAMPLING_FEATURE_PID
SITE_TYPE	Site	String	Optional	SAMPLING_FEATURE_TYPE	SAMPLING_FEATURE_TYPE	SAMPLING_FEATURE_TYPE
SITE_LATITUDE	Site	Numeric	Required	LAT_GDA94	GDA94_LAT	LAT_GDA94
SITE_LONGITUDE	Site	Numeric	Required	LONG_GDA94	GDA94_LONG	LONG_GDA94
LAT_LON_PRECISION	Site	Numeric	Optional	ACCURACY_M	ACCURACY_M	null
SITE_ELEVATION_AHD_M	Site	Numeric	Required	ELEV_M_AHD	ELEV_M_AHD	ELEVATION_M_AHD
SITE_UPPER_DEPTH_M	Site	Numeric	Optional	BOREHOLE_TOP_DEPTH_M	BOREHOLE_TOP_DEPTH_M	SAMPLING_INTERVAL_END_M
SITE_LOWER_DEPTH_M	Site	Numeric	Optional	BOREHOLE_BASE_DEPTH_M	BOREHOLE_BASE_DEPTH_M	SAMPLING_INTERVAL_BEGIN_M
SITE_DEPTH_REFERENCE_UNIT	Site	String	Optional	null	null	null
SAMPLE_TEMPERATURE	Sample	Numeric	Optional	null	null	FIELD_TEMPERATURE_DEGC
SAMPLE_SITE_AIR_TEMPERATURE_DEGC	Sample	Numeric	Optional	null	null	null
SAMPLE_STRATIGRAPHIC_UNIT	Sample	String	Optional	STRAT_UNIT_PID, STRAT_UNIT_NAME		null
SAMPLE_COLLECTED_BY	Agent	String	Optional	SAMPLE_ORIGINATOR	SAMPLE_ORIGINATOR	null
SAMPLE_CONFIDENTIAL_DATE	Sample	YYYY-MM-DD HH:MM	Optional	null	null	null
ANALYTE	Measurement	String	Required	MINERAL1		various incl., LEAD_206_LEAD_204_RATIO, ARGON_38_ARGON_36_RATIO
ISOTOPE	Measurement	String	Required	ISOTOPIC_NAME		various incl., LEAD_206_LEAD_204_RATIO, ARGON_38_ARGON_36_RATIO
VALUE	Measurement	Numeric	Required	multiple	multiple	multiple
UNIT	Measurement	String	Required	SR87_SR86_MEASURED (ratio)	ratio	in header for each analyte
SCALE	Measurement	String	Required	null	null	null
UNCERTAINTY	Measurement	Numeric	Recommended	SR87_SR86_UNCERTAINTY	6 columns, ending in _UNC	null
UNCERTAINTY_KIND	Measurement	String	Required	null	null	null
SAMPLE_ELEMENT_CONCENTRATION	Sample	Numeric	Optional	null	null	null
SAMPLE_ELEMENT_CONCENTRATION_UNIT	Sample	String	Optional	in header	in header	null
REFERENCE_MATERIAL_USED	Traceability	String	Recommended	STANDARD_NAME	STANDARD_NAME	null
VALUE_REFERENCE_MATERIAL	Traceability	Numeric	Recommended	null	null	null
UNCERTAINTY_REFERENCE_MATERIAL	Traceability	String	Recommended	null	null	null
UNIT_UNCERTAINTY_REFERENCE_MATERIAL	Traceability	String	Recommended	null	null	null
DATA_OWNER	Agent	String	Recommended	Geoscience Australia	Geoscience Australia	Geoscience Australia

(*continued on next page*)

Table 4 (*continued*)

Attribute	Class	Format	Reporting	Sr layer - Geochronology and Isotopes web service	Pb regolith layer - Geochronology and Isotopes web service	All Hydrochemistry - Hydrochemistry web service
ANALYSIS_DATE	Agent	YYYY-MM-DD HH:MM	Optional	ANALYSIS_DATE	ANALYSIS_DATE	null
ANALYSIS_COMMENTS	Agent	String	Optional		PB_ANALYSIS_REMARK	null
LABORATORY	Agent	String	Optional	LABORATORY_NAME	LABORATORY_NAME	null
METHOD_SAMPLE_PRETREATMENT	Method	String	Optional	null	null	null
METROLOGICAL_TRACEABILITY	Traceability	String	Optional	null	null	null
TRACEABILITY_ANALYTICAL_PROCEDURE	Traceability	String	Optional	COLLECTION_TYPE	COLLECTION_TYPE	null
TRACEABILITY_UNCERTAINTY	Traceability	String	Optional	null	null	null
DATA_PROCESSING	Traceability	String	Optional	null		null
UNCERTAINTY_EVALUATION	Traceability	String	Optional	null	RATIO_CONFIDENCE_LEVEL	null
METHOD_SAMPLE_COLLECTION	Method	String	Optional	null	null	null
METHOD_SAMPLE_CONTAINER	Method	String	Optional	null	null	null
METHOD_SUBSAMPLE_CONTAINER	Method	String	Optional	null	null	null
SAMPLE_STORAGE_CONDITIONS	Method	String	Optional	null	null	null
MODELLED	Measurement	String	Optional	null	null	null
				null	null	null

4. Discussion

4.1. Facilitating interoperability

Creating ontologies is a time-intensive and resource-intensive process, so publication of this ontology intends to reduce the burden for others. The stable isotope ontology aims to provide the basic metadata foundations to which complexity can be added to in the future. As the available isotopic data was originally collected for a variety of purposes, consideration was given to the flexibility of the ontology to include additional, domain-specific properties. This ontology can harmonise different datasets and ultimately transform them into a common format, without interrupting existing data models or introducing burdensome overhead to established workflows.

While this ontology was developed with a limited list of stable isotopes, the ontology is designed to be extensible to other stable isotopes (Coplen et al., 2002b), as well as compound-specific stable isotope data and radioisotope data. There are no anticipated limitations to expanding beyond the initial stable isotopes used or adding additional domain-specific attributes. The Sedimentary Geochemistry and Paleoenvironments (SGP) database, which assembles multi-proxy sedimentary geochemical data from fine-grained siliciclastic rocks, includes an extended list of isotope attributes (e.g. $\delta^{34}S$, $\delta^{53}Cr$, $\delta^{56}Fe$, $\delta^{7}Li$, $\delta^{26}Mg$, $\delta^{98}Mo$, $\delta^{51}V$, $\delta^{66}Zn$) (Farrell et al., 2021). Using the attribute "delta_s34" as an example, we can map the measurement attributes of ISOTOPE, UNIT, VALUE, and SCALE (Fig. 3).

The AusTraits Plant Dictionary vocabulary defines the concept of stable isotope composition as the mineral and ion content trait within the biochemical traits of plant functional ecology and plant morphology (Falster et al., 2021; Wenk et al., 2024). This concept can be described by the stable isotope ontology, using the MEASUREMENT attributes (Fig. 4).

The stable isotope ontology is designed as a straightforward data stewardship tool to improve the findability, accessibility, interoperability and reuse of stable isotope data produced across disciplines and ultimately published in publicly accessible data repositories, in peer-reviewed literature and/or grey literature. As an example, the $\delta^{13}C$ data from a large-scale vegetation survey (Munroe et al., 2021) collected as part of the Australian Terrestrial Ecosystem Research Network (TERN) can be accommodated by the ontology and retain the information from the peer-reviewed study (Munroe et al., 2024) (Table 6).

Utilising a modular architecture, it can be extended to other fields across a broad range of vocabularies and fields in the Earth Sciences. For example, "WaterSAMPLE" is a subclass of "Sample" class with 14 additional attributes (Table 7) which can be used to align with hydrology and water resources ontologies (Brodaric et al., 2019; Cheatham et al., 2020). These 14 domain-specific concepts provide additional contextual information, including salinity, flow rates, humidity and pH. Used in this way, the stable isotope ontology can function as a foundational ontology, so that related concepts from other domains can be applied, inheriting the attributes to acknowledge the interdisciplinary nature of stable isotope data. Therefore, users can utilise data from elsewhere to increase applicability and include additional relevant attributes that are not currently included in the ontology.

4.2. Challenges and limitations

While the ontology is designed to increase the interoperability of stable isotope data, there are additional challenges and complexities it does not resolve.

The use of persistent identifiers across the research ecosystem is uneven. While identifiers for datasets and publications (i.e. digital object identifiers, DOI) and researchers (ORCID) are widely used, identifiers for research organisations (Research Organisation Registry, ROR), research projects (Research Activity identifiers, RAiD), and instrumentation are not yet commonplace. To encourage and promote the broader use of

Table 5
Examples to describe the non-numeric Measurement attributes.

ANALYTE	ISOTOPE	UNIT	SCALE	UNCERTAINTY_KIND	MODELLED
SO4	3H	ratio	VSMOW	1 sigma	Yes
NO3	87Sr/86Sr	ppm	Air - N2	2 sigma	No
H2O	d18O	permille	PDB	95 % confidence	
CH4	d15 N	TU	TDIC	1 standard error	
CO2	d13C		VPDB	2 standard error	
DOC	d17O			1 sigma internal	
DIC	d14C			2 sigma internal	
NH4	d2H			95 % confidence internal	
Bulk	d34S			1 sigma external	
				2 sigma external	
				95 % confidence external	
				1 sigma propagated (int + ext)	
				2 sigma propagated (int + ext)	
				95 % confidence propagated (int + ext)	
				1 sigma propagated sqrt[(int)ˆ2+(ext)ˆ2]	
				2 sigma propagated sqrt[(int)ˆ2+(ext)ˆ2]	
				95 % conf. propagated sqrt[(int)ˆ2+(ext)ˆ2]	
				Weighted standard deviation	
				other	
				Unknown	
				No Uncertainty Given	

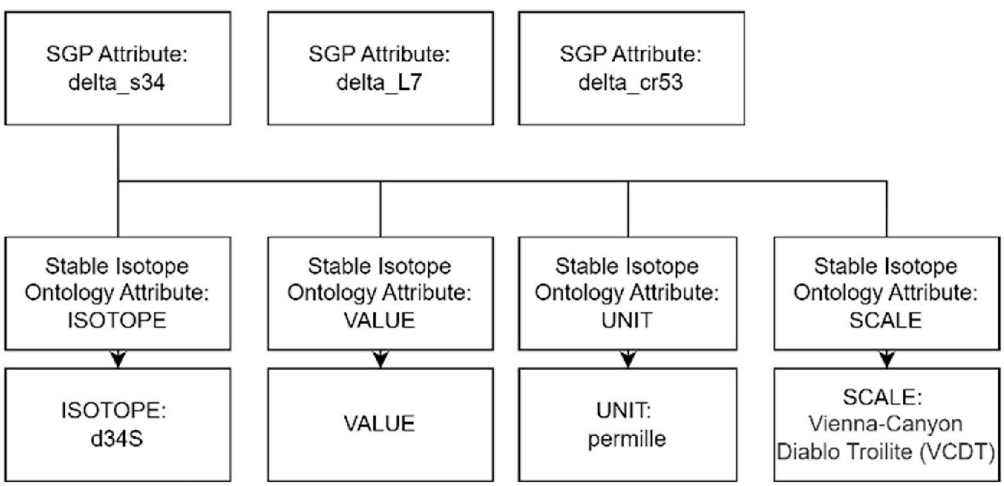

Fig. 3. Relationship between the SGP database attribute $\delta^{34}S$ to the stable isotope ontology attributes (adapted from Farrell et al., 2021).

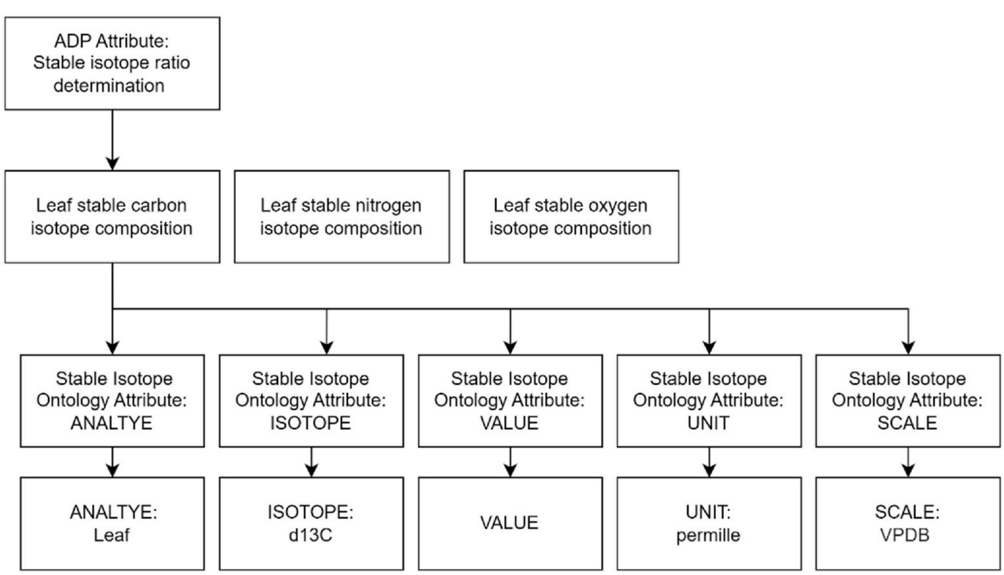

Fig. 4. Comparison of AusTraits Plant Dictionary Vocabulary to the stable isotope ontology (adapted from Falster et al., 2021).

Table 6
Ontology properties used to describe stable isotope data from a large-scale vegetation survey (Munroe et al., 2021, 2024).

Attribute	Description	Requirement	Study Specific Description
SAMPLE_ID	Unique name of the sample.	Required	Unique name of the sample, uses TERN primary genetic barcode of plant specimen.
SITE_LATITUDE	Latitude of the sample collection site, in the GDA94 datum.	Required	Latitude of the sample collection site.
SITE_LONGITUDE	Longitude of the sample collection site, in the GDA94 datum.	Required	Longitude of the sample collection site, in the GDA94 datum.
SAMPLE_DATE_START	Date when the sampling process started, expressed as YYYY-MM-DD HH:MM.	Required	Date the plant specimen was collected.
SITE_NAME	Name assigned to the collection site.	Recommended	Site number assigned to the plot from which the TERN plant sample was collected. This code can be used to search for more information on the plot via TERN's “ausplotsR” R package.
SITE_NUMBER	Unique ID assigned to the collection site.	Recommended	Unique ID assigned to the collection site. This code can be used to search for more information on the plot via TERN's “ausplotsR” R package.
ISOTOPE	The isotope analysed, expressed as d (number) (element).	Required	The isotope analysed, expressed as d (number) (element).
ANALYTE	The sample of interest in the stable isotope analytical procedure. Expressed as the most specific component entity, eg. Element, material, substance or chemical constituent.	Required	The material of interest in the stable isotope analytical procedure.
SCALE	Scale to which isotope measurements were normalized.	Required	Scale to which isotope measurements were normalized.
VALUE	The measured result of stable isotope analysis	Required	The measured result of stable isotope analysis.
UNIT	The unit of the result.	Required	The unit of the result.
UNCERTAINTY	Analytical uncertainty associated with procedure.	Recommended	Analytical uncertainty associated with procedure.
UNCERTAINTY_KIND	Analytical uncertainty type. If not provided or unknown, default “Not provided".	Required	Analytical uncertainty type.
SAMPLE_TYPE	Type of physical material collected from the collection site.	Required	Type of physical material collected from the collection site.
SAMPLE_SOURCE_TYPE	Describes the material that contained the sample. Further refines Sample Type.	Recommended	This column lists the species name of the plant specimen.

persistent sample identifiers (e.g. ISGN), while acknowledging the inconsistent approaches, the SAMPLE_PID is a recommended attribute and PUBLICATION and DOI are required attributes.

The distributed custodianship and heterogeneity of data may require reconciling multiple samples taken from the one site (i.e. groundwater bores) at different points in time and by different organisations. In the case of groundwater bores, there are often multiple identifiers used by regulatory authorities and national data repositories. Resolving multiple and/or conflicting sample or site identifiers is beyond the scope of this ontology. However, by complementing existing standards (Brodaric et al., 2018) the stable isotope ontology can highlight instances of overlapping or ambiguous records through the data provenance (Traceability attributes) and ownership attributes (Agent attributes).

The stable isotope ontology delineates measured data and data produced from data-based models and interpolations using the binary attribute MODELLED. This does not suggest that measured and modelled data can be easily compared. Comparison of measured data and modelled data should be undertaken with the full understanding of the underlying models or interpolations.

The attribute REFERENCE_MATERIAL_USED creates a text string, which may result in clumsy formats or introduce repetition of site level metadata. However, as the reporting of reference materials and normalisation procedures is not yet consistently included in stable isotope datasets, imperfect reporting is better than none.

Additionally, the stable isotope ontology does not provide any provisions for user access or confidentiality clauses. Instead, the responsibility of data access falls to the respective data custodian or organisation. This does not prevent private or embargoed data from adhering to the ontology, rather it acknowledges that these data are outside of the public domain and thus cannot be tracked.

4.3. Users and implementation

The objective is to enable existing datasets and repositories to become cohesive, interoperable and discoverable across the entire measurement pipeline. The stable isotope ontology can be adapted by data generators in analytical laboratories, to include sample collection and data analytics, as well as users across domains including other isotope scientists, and anyone else wishing to access stable isotope data.

Table 7
Summary of additional properties that provide domain-specific contextual information for Sample Class: WaterSample.

Attribute	Description	Class	Format
SITE_AIR_PRESSURE	Air pressure at time sample was taken.	Water sample	Numeric
SITE_DO	The concentration of the amount of oxygen present in water sample, expressed as milligrams of dissolved oxygen per litre of water (mg/L).	Water sample	Numeric
SITE_ELECTRICAL_CONDUCTIVITY	Electrical conductivity of the water sample, expressed as μS/cm (micro-Siemens/ centimetre).	Water sample	Numeric
SITE_FLOW_RATE	Flow rate at the sample water site.	Water sample	Numeric
SITE_HUMIDITY	The humidity of air at the time of sampling.	Water sample	Numeric
SITE_MOISTURE_CONTENT	Moisture content percentage of the sample.	Water sample	Numeric
SITE_ORP	Oxidation-reduction potential (ORP) of the water body.	Water sample	Numeric
SITE_pH	pH of the sample.	Water sample	Numeric
SAMPLE_PRECIPITATION	Average or composite measurement over the duration of a composite sample, Amount of precipitation recorded (as mm).	Water sample	Numeric
SITE_SALINITY	Measurement of the salinity of the water sample, expressed as parts per million (ppm).	Water sample	Numeric
SITE_TURBIDITY	Measurement of the turbidity of the water sample, expressed as Nephelometric Turbidity Units (NTU).	Water sample	Numeric
SITE_WATER_LEVEL	Measurement of the water level of the water body sampled.	Water sample	Numeric
SITE_WATER_TEMPERATURE_DEGC	Average or composite measurement over the duration of a composite sample. Temperature of a water sample, expressed as degrees Celsius.	Water sample	Numeric
SAMPLE_H2O_VAPOUR_PRESSURE	Measurement of the vapour pressure of water (expressed as %). Either average or composite measurement over the duration of a composite sample.	Water sample	Numeric

This will assist in: i) reducing the need for human data manipulation for or by the end user, which can be prone to errors; ii) providing a machine-readable format for new and emerging technology use-cases, and iii) helping stable isotope data to align with FAIR (Cox et al., 2021; Wilkinson et al., 2016) and responsible data principles (Stitzlein et al., 2021).

There is demand for technical and field-specific ontologies to facilitate greater collaboration and data sharing. While some users in the data generation pipeline have access to OGC (Open Geospatial Consortium) compliant web services, many are reliant on simple spreadsheets. Using a flat structure, the stable isotope ontology becomes a tool so that users can use their existing “tools in the shed” without creating an additional technical barrier. The aim is to facilitate uptake by anyone who uses stable isotope data regardless of whether they have access to data modelling or relational database software, or spreadsheets and text documents.

Using a simplified data structure, the stable isotope ontology facilitates integration of stable isotope data from different organisations with different corporate goals, data infrastructure, operating models and specialist skills. This stable isotope ontology improves data traceability and data management practices for users. As a stand-alone file structure, the ontology can be used across organisations or data infrastructures, providing flexibility to adapt and develop as needed. Creating a community-driven ontology we aim to reduce the likelihood of a black-box situation, where data can be entered but not updated. Implementation by the national science organisations, which can act as generalist data repositories, will provide ongoing maintenance and foster adoption, by setting the precedence for the stable isotope ontology in regular use.

4.4. Future governance

The stable isotope ontology is intended to evolve as needed, based on feedback from the stable isotope community. As such, updates to this ontology will continue through a consultative steering committee (IsotopesAU Steering Committee), consisting of the original contributing organisations and an expanded SOUG. This Steering Committee will continue to develop and maintain this ontology, based on user needs and feedback. Future updates and versions will be published through the CSIRO Data Access Portal at https://doi.org/10.25919/aa8d-yw93. The stable isotope ontology will be made available through Research Vocabularies Australia (RVA) to increase wider use and engagement.

A federated data platform, www.isotopes.au (Welti et al., 2024), applies this ontology, creating a single-point access to the harmonised stable isotope datasets used to develop this ontology. The intention is to identify appropriate domain repositories and create user-submitted pathways to increase the data federated into this platform. Users can access data through the platform and create unified data outputs structured according to this ontology. The platform is free to use and open to all. The platform management and governance are formalised through the same consultative steering committee that includes the governance of the stable isotope ontology.

While the governance group is Australian based, it is not limited to Australian-only participation. The members of the steering committee are active in their wider scientific communities (e.g. European Association of Geochemistry, OneGeochemistry, AuScope, International Science Council's Committee on DATA (CODATA), Research Data Alliance, International Atomic Energy Agency) and international conferences (e.g. EGU General Assembly, Goldschmidt, and AGU Fall Meeting, IsoEcol) where they seek feedback and participation in this effort. This is a community-oriented research consortium, and we welcome suggestions on how to best move toward our shared goals. Anyone who is interested to join the effort is welcomed and can find contact details at www.isotopes.au.

5. Conclusions

Across all fields of science data volumes are growing exponentially, and standardised ontologies are a way to manage data for interoperability across agencies and purposes. Stable isotope data is collected for different purposes using domain-specific collection regimes, using comparable analytical methodologies and standards. This diversity makes converting data into a single standard impractical. Instead, the stable isotope ontology provides a structured framework for mapping and harmonising disparate datasets, enabling differences in data formats, schemas, and terminology to be systematically reconciled and integrated into a unified, interoperable model. The stable isotope ontology is important to ensure common understanding and continue to reduce the barriers to entry in a complex field – both as a user and contributor of data.

The stable isotope ontology aims to reduce duplication and create a standard approach that is generic and flexible. Whilst not explicitly requiring the original data structures to be altered, a standard approach allows the reuse of data, enabling disparate data to be compatible across purpose and easily brought into a common system. The aim is to resolve discrepancies in syntax (data format), structure (conceptual schema), and semantics (intended meanings of words) relating to stable isotope data and reduce the barriers to creating interoperable datasets. By providing a mechanism to effectively sort and share data, the stable isotope ontology enables translation of research outputs, regardless of differences within the data itself.

CRediT authorship contribution statement

Nina Welti: Writing – original draft, Validation, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Data curation, Conceptualization. **Steph Hawkins:** Writing – original draft, Visualization, Validation, Supervision, Project administration, Methodology, Investigation, Data curation. **Kathryn Waltenberg:** Writing – original draft, Supervision, Methodology, Investigation, Data curation. **Cath Hughes:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Data curation, Conceptualization. **Jagoda Crawford:** Validation, Software, Methodology, Formal analysis. **Yanfeng Shu:** Methodology. **Regina Campbell:** Methodology. **Alex Leslie:** Methodology. **Athina Puccini:** Validation, Data curation. **Christoph Gerber:** Validation, Methodology, Data curation. **Axel Suckow:** Writing – review & editing, Validation, Software, Resources, Methodology, Formal analysis. **Geoff Fraser:** Writing – original draft, Supervision, Project administration, Investigation, Funding acquisition, Conceptualization. **Lian Flick:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Data curation.

Declaration of competing interest

The authors, listed below, of *A Common Ontology for Stable Isotope Data* declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

This project received financial support (https://doi.org/10.47486/DC103) from the Australian Research Data Commons (ARDC) as part of their Food Security Data Challenges program (https://ardc.edu.au/program/food-security-data-challenges/). The project is a partnership between the Commonwealth Scientific and Industrial Research Organisation (CSIRO), Geoscience Australia (GA), the Australian Nuclear Science and Technology Organisation (ANSTO), the National Measurement Institute and ARDC. The Food Security Data Challenges program is developing innovative digital infrastructure solutions to current data challenges in food security research, with the aim of improving Australia's production, consumption and distribution of safe and high-quality food. The ARDC is enabled by the National Collaborative Research Infrastructure Strategy (NCRIS).

Acknowledgements

The authors would like to acknowledge the members of the Science and User Group who provided feedback throughout the ontology development: Ryan McAllister, Anthony Dosseto, Georgy Falster, Justin Maroccia, Nicole Stubing, Greg Skrzypek. The authors would like to acknowledge Robert Barlow, Ellyse Bunney, Brendan Boesen, Fong Liu, Mark Lewin, Abhijt Paul, Aaron Sedgmen, Steve Szarvas, Tim Stobaus, and Stefan Terzer for providing additional input and insight.

Data availability

Data are available through the CSIRO Data Access Portal at https://doi.org/10.25919/aa8d-yw93.

References

Australia, C.o., 2022. Data Availability and Transparency Act 2022. Canberra.

Australia, C.o., 2023. In: Digital, D.a. (Ed.), Data and Digital Government Strategy and Implementation Plan. Commonwealth of Australia, Canberra.

BOM, 2019. The National Industry Guidelines for Hydrometric Monitoring, Part 2: Site Establishment and Operations. Commonwealth of Australia, Bureau of Meteorology.

Bond, A.L., Hobson, K.A., 2012. Reporting stable-isotope ratios in ecology: recommended terminology, guidelines and best practices. Waterbirds 35 (2), 324–331. https://doi.org/10.1675/063.035.0213.

Boone, S.C., Dalton, H., Prent, A., Kohlmann, F., Theile, M., Gréau, Y., Florin, G., Noble, W., Hodgekiss, S.-A., Ware, B., Phillips, D., Kohn, B., O'Reilly, S., Gleadow, A., McInnes, B., Rawling, T., 2022. AusGeochem: an open platform for geochemical data preservation, Dissemination and Synthesis. Geostand. Geoanal. Res. 46 (2), 245–259. https://doi.org/10.1111/ggr.12419.

Brand, W.A., Coplen, T.B., 2012. Stable isotope deltas: tiny, yet robust signatures in nature. Isot. Environ. Health Stud. 48 (3), 393–409. https://doi.org/10.1080/10256016.2012.666977.

Brand, W.A., Coplen, T.B., Vogl, J., Rosner, M., Prohaska, T., 2014. Assessment of international reference materials for isotope-ratio analysis (IUPAC Technical Report). Pure Appl. Chem. 86 (3), 425–467. https://doi.org/10.1515/pac-2013-1023.

Brodaric, B., Boisvert, E., Chery, L., Dahlhaus, P., Grellet, S., Kmoch, A., Létourneau, F., Lucido, J., Simons, B., Wagner, B., 2018. Enabling global exchange of groundwater data: GroundWaterML2 (GWML2). Hydrogeol. J. 26 (3), 733–741. https://doi.org/10.1007/s10040-018-1747-9.

Brodaric, B., Hahmann, T., Gruninger, M., 2019. Water features and their parts. Appl. Ontol. 14 (1), 1–42. https://doi.org/10.3233/ao-190205.

de Caritat, P., Cooper, M., 2011. National Geochemical Survey of Australia: the Geochemical Atlas of Australia. Geoscience Australia. https://doi.org/10.11636/Record.2011.020. Record 2011/020.

de Caritat, P., Dosseto, A., Dux, F., 2022. A strontium isoscape of inland southeastern Australia. Earth Syst. Sci. Data 14 (9), 4271–4286.

de Caritat, P., Dosseto, A., Dux, F., 2023. A strontium isoscape of northern Australia. Earth Syst. Sci. Data 15 (4), 1655–1673. https://doi.org/10.5194/essd-15-1655-2023.

de Caritat, P., Dosseto, A., Dux, F., 2025. A strontium isoscape of southwestern Australia and progress toward a national strontium isoscape. Earth Syst. Sci. Data 17 (1), 79–93. https://doi.org/10.5194/essd-17-79-2025.

Cheatham, M., Varanka, D., Arauz, F., Zhou, L., 2020. Alignment of surface water ontologies: a comparison of manual and automated approaches. J. Geogr. Syst. 22 (2), 267–289.

Cheng, C., Messerschmidt, L., Bravo, I., Waldbauer, M., Bhavikatti, R., Schenk, C., Grujic, V., Model, T., Kubinec, R., Barceló, J., 2024. A general primer for data Harmonization. Sci. Data 11 (1), 152. https://doi.org/10.1038/s41597-024-02956-3.

Coplen, T.B., 2011. Guidelines and recommended terms for expression of stable-isotope-ratio and gas-ratio measurement results. Rapid Commun. Mass Spectrom. 25 (17), 2538–2560. https://doi.org/10.1002/rcm.5129.

Coplen, T.B., Shrestha, Y., 2016. Isotope-abundance variations and atomic weights of selected elements: 2016 (IUPAC Technical Report). Pure Appl. Chem. 88 (12), 1203–1224. https://doi.org/10.1515/pac-2016-0302.

Coplen, T.B., Krouse, H.R., Böhlke, J.K., 1992. Reporting of nitrogen-isotope abundances (technical report). Pure Appl. Chem. 64 (6), 907–908. https://doi.org/10.1351/pac199264060907.

Coplen, T.B., Böhlke, J.K., De Bièvre, P., Ding, T., Holden, N.E., Hopple, J.A., Krouse, H.R., Lamberty, A., Peiser, H.S., Révész, K., Rieder, S.E., Rosman, K.J.R., Roth, E., Taylor, P.D.P., Vocke, R.D., Xiao, Y.K., 2002a. Isotope-abundance variations of selected elements -: (IUPAC Technical Report). Pure Appl. Chem. 74 (10), 1987–2017. https://doi.org/10.1351/pac200274101987.

Coplen, T.B., Hopple, J.A., Böhlke, J.K., Peiser, H.S., Rieder, S.E., Krouse, H.R., Rosman, K.J.R., Ding, T., Vocke Jr, R.D., Revesz, K.M., Lamberty, A., Taylor, P., De Bievre, P., 2002b. Compilation of minimum and maximum isotope ratios of selected

elements in naturally occurring terrestrial materials and reagents. Water-Resources Investigations Report. https://doi.org/10.3133/wri014222.
Cox, S.J.D., Gonzalez-Beltran, A.N., Magagna, B., Marinescu, M.-C., 2021. Ten simple rules for making a vocabulary FAIR. PLoS Comput. Biol. 17 (6), e1009041.
Desem, C.U., de Caritat, P., Woodhead, J.D., Maas, R., Carr, G., 2023. National geochemical survey of Australia: lead isotopes dataset. National topographic map series. Geoscience Australia. https://dx.doi.org/10.26186/5ea8f6fd3de64.
Devaraju, A., Mokrane, M., Cepinskas, L., Huber, R., Herterich, P., de Vries, J., Akerman, V., L'Hours, H., Davidson, J., Diepenbroek, M., 2021. From Conceptualization to implementation: FAIR Assessment of research data objects. Data Sci. J. https://doi.org/10.5334/dsj-2021-004.
Donarski, J., Camin, F., Fauhl-Hassek, C., Posey, R., Sudnik, M., 2019. Sampling guidelines for building and curating food authenticity databases. Trends Food Sci. Technol. 90, 187–193. https://doi.org/10.1016/j.tifs.2019.02.019.
Eftimov, T., Ispirova, G., Potocnik, D., Ogrinc, N., Seljak, B.K., 2019. ISO-FOOD ontology: a formal representation of the knowledge within the domain of isotopes for food science. Food Chem. 277, 382–390. https://doi.org/10.1016/j.foodchem.2018.10.118.
Falster, D., Gallagher, R., Wenk, E.H., Wright, I.J., Indiarto, D., Andrew, S.C., Baxter, C., Lawson, J., Allen, S., Fuchs, A., Monro, A., Kar, F., Adams, M.A., Ahrens, C.W., Alfonzetti, M., Angevin, T., Apgaua, D.M.G., Arndt, S., Atkin, O.K., Atkinson, J., Auld, T., Baker, A., von Balthazar, M., Bean, A., Blackman, C.J., Bloomfield, K., Bowman, D.M.J.S., Bragg, J., Brodribb, T.J., Buckton, G., Burrows, G., Caldwell, E., Camac, J., Carpenter, R., Catford, J.A., Cawthray, G.R., Cernusak, L.A., Chandler, G., Chapman, A.R., Cheal, D., Cheesman, A.W., Chen, S.-C., Choat, B., Clinton, B., Clode, P.L., Coleman, H., Cornwell, W.K., Cosgrove, M., Crisp, M., Cross, E., Crous, K.Y., Cunningham, S., Curran, T., Curtis, E., Daws, M.I., DeGabriel, J.L., Denton, M.D., Dong, N., Du, P., Duan, H., Duncan, D.H., Duncan, R.P., Duretto, M., Dwyer, J.M., Edwards, C., Esperon-Rodriguez, M., Evans, J.R., Everingham, S.E., Farrell, C., Firn, J., Fonseca, C.R., French, B.J., Frood, D., Funk, J.L., Geange, S.R., Ghannoum, O., Gleason, S.M., Gosper, C.R., Gray, E., Groom, P.K., Grootemaat, S., Gross, C., Guerin, G., Guja, L., Hahs, A.K., Harrison, M.T., Hayes, P.E., Henery, M., Hochuli, D., Howell, J., Huang, G., Hughes, L., Huisman, J., Ilic, J., Jagdish, A., Jin, D., Jordan, G., Jurado, E., Kanowski, J., Kasel, S., Kellermann, J., Kenny, B., Kohout, M., Kooyman, R.M., Kotowska, M.M., Lai, H.R., Laliberté, E., Lambers, H., Lamont, B.B., Lanfear, R., van Langevelde, F., Laughlin, D.C., Laugier-Kitchener, B.-A., Laurance, S., Lehmann, C.E.R., Leigh, A., Leishman, M.R., Lenz, T., Lepschi, B., Lewis, J.D., Lim, F., Liu, U., Lord, J., Lusk, C.H., Macinnis-Ng, C., McPherson, H., Magallón, S., Manea, A., López-Martinez, A., Mayfield, M., McCarthy, J.K., Meers, T., van der Merwe, M., Metcalfe, D.J., Milberg, P., Mokany, K., Moles, A.T., Moore, B.D., Moore, N., Morgan, J.W., Morris, W., Muir, A., Munroe, S., Nicholson, Á., Nicolle, D., Nicotra, A.B., Niinemets, Ü., North, T., O'Reilly-Nugent, A., O'Sullivan, O.S., Oberle, B., Onoda, Y., Ooi, M.K.J., Osborne, C.P., Paczkowska, G., Pekin, B., Guilherme Pereira, C., Pickering, C., Pickup, M., Pollock, L.J., Poot, P., Powell, J.R., Power, S.A., Prentice, I.C., Prior, L., Prober, S.M., Read, J., Reynolds, V., Richards, A.E., Richardson, B., Roderick, M.L., Rosell, J.A., Rossetto, M., Rye, B., Rymer, P.D., Sams, M.A., Sanson, G., Sauquet, H., Schmidt, S., Schönenberger, J., Schulze, E.-D., Sendall, K., Sinclair, S., Smith, B., Smith, R., Soper, F., Sparrow, B., Standish, R.J., Staples, T.L., Stephens, R., Szota, C., Taseski, G., Tasker, E., Thomas, F., Tissue, D.T., Tjoelker, M.G., Tng, D.Y.P., de Tombeur, F., Tomlinson, K., Turner, N.C., Veneklaas, E.J., Venn, S., Vesk, P., Vlasveld, C., Vorontsova, M.S., Warren, C.A., Warwick, N., Weerasinghe, L.K., Wells, J., Westoby, M., White, M., Williams, N.S.G., Wills, J., Wilson, P.G., Yates, C., Zanne, A.E., Zemunik, G., Ziemińska, K., 2021. AusTraits, a curated plant trait database for the Australian flora. Sci. Data 8 (1), 254.
Farrell, Ú.C., Samawi, R., Anjanappa, S., Klykov, R., Adeboye, O.O., Agic, H., Ahm, A.-S. C., Boag, T.H., Bowyer, F., Brocks, J.J., Brunoir, T.N., Canfield, D.E., Chen, X., Cheng, M., Clarkson, M.O., Cole, D.B., Cordie, D.R., Crockford, P.W., Cui, H., Dahl, T.W., Mouro, L.D., Dewing, K., Dornbos, S.Q., Drabon, N., Dumoulin, J.A., Emmings, J.F., Endriga, C.R., Fraser, T.A., Gaines, R.R., Gaschnig, R.M., Gibson, T. M., Gilleaudeau, G.J., Gill, B.C., Goldberg, K., Guilbaud, R., Halverson, G.P., Hammarlund, E.U., Hantsoo, K.G., Henderson, M.A., Hodgskiss, M.S.W., Horner, T. J., Husson, J.M., Johnson, B., Kabanov, P., Brenhin Keller, C., Kimmig, J., Kipp, M. A., Knoll, A.H., Kreitsmann, T., Kunzmann, M., Kurzweil, F., LeRoy, M.A., Li, C., Lipp, A.G., Loydell, D.K., Lu, X., Macdonald, F.A., Magnall, J.M., Mänd, K., Mehra, A., Melchin, M.J., Miller, A.J., Mills, N.T., Mwinde, C.N., O'Connell, B., Och, L.M., Ossa Ossa, F., Pagès, A., Paiste, K., Partin, C.A., Peters, S.E., Petrov, P., Playter, T.L., Plaza-Torres, S., Porter, S.M., Poulton, S.W., Pruss, S.B., Richoz, S., Ritzer, S.R., Rooney, A.D., Sahoo, S.K., Schoepfer, S.D., Sclafani, J.A., Shen, Y., Shorttle, O., Slotznick, S.P., Smith, E.F., Spinks, S., Stockey, R.G., Strauss, J.V., Stüeken, E.E., Tecklenburg, S., Thomson, D., Tosca, N.J., Uhlein, G.J., Vizcaíno, M. N., Wang, H., White, T., Wilby, P.R., Woltz, C.R., Wood, R.A., Xiang, L., Yurchenko, I.A., Zhang, T., Planavsky, N.J., Lau, K.V., Johnston, D.T., Sperling, E.A., 2021. The sedimentary geochemistry and Paleoenvironments project. Geobiology 19 (6), 545–556. https://doi.org/10.1111/gbi.12462.
Geoscience Australia, 2021. ISOTOPE Database. Commonwealth of Australia (Geoscience Australia). https://doi.org/10.26186/131588.
Hawkins, S., 2023. In: Australia, G. (Ed.), Relational Databases for Geoscience Data: HYDROCHEM, a Case Study. Geoscience Australia, Canberra. https://doi.org/10.26186/147856.
Hawkins, S., Northey, J., Schroder, I., Lem, A., Sedgmen, A., Peljo, M., 2022. Hydrochemistry Database (HYDROCHEM), Geoscience Australia. https://dx.doi.org/10.26186/147298.
Hawkins, S.G., Waltenberg, K., Sedgmen, A., Sunketa, A., Seedhouse, M., Cherukoori, R., Farmakis, B., Khan, A., Lem, A., Clark, D., 2024. Facilitating dynamic geoscientific data delivery for the GeoInsight pilot. A Methodology for Database, Web Service and Application Development. Geoscience Australia, Canberra. https://doi.org/10.26186/149368.
Hofstra, A.H., Lisitsin, V., Corriveau, L., Paradis, S., Peter, J., Lauzière, K., Lawley, C., Gadd, M., Pilote, J.-L., Honsberger, I., Bastrakov, E., Champion, D., Czarnota, K., Doublier, M., Huston, D., Raymond, O., VanDerWielen, S., Emsbo, P., Granitto, M., Kreiner, D.C., 2021. Deposit classification scheme for the Critical minerals mapping initiative global geochemical database. Open-File Report. Reston, VA.
Holden, N.E., Bonardi, M.L., Bièvre, P.D., Renne, P.R., Villa, I.M., 2011. IUPAC-IUGS common definition and convention on the use of the year as a derived unit of time (IUPAC Recommendations 2011). Pure Appl. Chem. 83 (5), 1159–1162. https://doi.org/10.1351/PAC-REC-09-01-22.
ICSM, 2014. GDA94 2, 4 ed. Commonwealth of Australia (ICSM).
ISO, 2019a. ISO 8601-2:2019, Date and Time — Representations for Information Interchange International Organization for Standardization.
ISO, 2019b. ISO 80000-9 Physical Chemistry and Molecular Physics.
Klöcking, M., Wyborn, L., Lehnert, K.A., Ware, B., Prent, A.M., Profeta, L., Kohlmann, F., Noble, W., Bruno, I., Lambart, S., Ananuer, H., Barber, N.D., Becker, H., Brodbeck, M., Deng, H., Deng, K., Elger, K., de Souza Franco, G., Gao, Y., Ghasera, K. M., Hezel, D.C., Huang, J., Kerswell, B., Koch, H., Lanati, A.W., ter Maat, G., Martínez-Villegas, N., Nana Yobo, L., Redaa, A., Schäfer, W., Swing, M.R., Taylor, R. J.M., Traun, M.K., Whelan, J., Zhou, T., 2023. Community recommendations for geochemical data, services and analytical capabilities in the 21st century. Geochem. Cosmochim. Acta 351, 192–205. https://doi.org/10.1016/j.gca.2023.04.024.
Klump, J., Lehnert, K., Ulbricht, D., Devaraju, A., Elger, K., Fleischer, D., Ramdeen, S., Wyborn, L., 2021. Towards Globally unique Identification of physical samples: governance and technical implementation of the IGSN global sample number. Data Sci. J. 20 (1), 33. https://doi.org/10.5334/dsj-2021-033.
Lithologic unit. https://cgi.vocabs.ga.gov.au/object?uri=http%3A//resource.geosciml.org/classifier/cgi/geologicunittype/lithologic_unit, 2017.
Meija, J., Coplen, T.B., Berglund, M., Brand, W.A., De Bièvre, P., Gröning, M., Holden, N. E., Irrgeher, J., Loss, R.D., Walczyk, T., Prohaska, T., 2016. Isotopic compositions of the elements 2013 (IUPAC technical report). Pure Appl. Chem. 88 (3), 293–306. https://doi.org/10.1515/pac-2015-0503.
Millar, C., Janzen, K., Nehemy, M.F., Koehler, G., Hervé-Fernández, P., Wang, H., Orlowski, N., Barbeta, A., McDonnell, J.J., 2022. On the urgent need for standardization in isotope-based ecohydrological investigations. Hydrol. Process. 36 (10), e14698. https://doi.org/10.1002/hyp.14698.
Miller, D.H., Kavinga, Dempsey, James, Tregeagle, Sean, Sathya Moorthy, Sathish, Sullivan, Brendan, 2012. A System for Extracting and Updating Common Organisational Metadata into a Central Authoritative Source. CSIRO.
Munroe, S.E.M., McInerney, F.A., Andrae, J., Welti, N., Guerin, G.R., Leitch, E., Hall, T., Szarvas, S., Atkins, R., Caddy-Retalic, S., Sparrow, B., 2021. The photosynthetic pathways of plant species surveyed in Australia's national terrestrial monitoring network. Sci. Data 8 (1), 97.
Munroe, S., McInerney, C., Andrae, J., Welti, N., Guerin, G., Emrys, L., Hall, T., Szarvas, S., Atkins, R., Caddy-Retalic, S., Holtum, J., Sparrow, B., 2024. Stable carbon isotope values of plant bulk tissue from 540 species surveyed across Australia between 2011 and 2022. v3. https://doi.org/10.25919/0khp-ya20.
Nixon, A.L., Boone, S.C., Gréau, Y., Kohlmann, F., Theile, M., Noble, W., Prent, A., Foden, J., Barnes, S., Wainwright, A.N., Wade, B., Goemann, K., Gilbert, S., Evans, N. J., Dalton, H., Ware, B., McInnes, B.I.A., 2025. Volcanoes to vugs: demonstrating a FAIR geochemistry framework with a diverse application of major and trace element data through the AuScope EarthBank platform. Chem. Geol. 696, 123092. https://doi.org/10.1016/j.chemgeo.2025.123092.
Overton, M., Larson, S., Carlson, L.J., Kleinschmit, S., 2022. Public data primacy: the changing landscape of public service delivery as big data gets bigger. Global Public Policy and Governance 2 (4), 381–399.
Pauli, J.N., Newsome, S.D., Cook, J.A., Harrod, C., Steffan, S.A., Baker, C.J.O., Ben-David, M., Bloom, D., Bowen, G.J., Cerling, T.E., Cicero, C., Cook, C., Dohm, M., Dharampal, P.S., Graves, G.R., Gropp, R., Hobson, K.A., Jordan, C., MacFadden, B., Birchs, S.P., Poelen, J., Ratnasingham, S., Russell, L., Stricker, C.A., Uhen, M.D., Yarnes, C.T., Hayden, B., 2017. Why we need a centralized repository for isotopic data. Proceedings of the National Academy of Sciences of the United States of America 114 (12), 2997–3001. https://doi.org/10.1073/pnas.1701742114.
Plomp, E., Stantis, C., James, H.F., Cheung, C., Snoeck, C., Kootker, L., Kharobi, A., Borges, C., Moreiras Reynaga, D.K., Pospieszny, Ł., Fulminante, F., Stevens, R., Alaica, A.K., Becker, A., de Rochefort, X., Salesse, K., 2022. The IsoArcH initiative: working towards an open and collaborative isotope data culture in bioarchaeology. Data Brief 45, 108595. https://doi.org/10.1016/j.dib.2022.108595.
Raymond, O.L., Brown, C.E., 1949. Australian Stratigraphic Units Database. Geoscience Australia, Canberra.
Raymond, O., Boisvert, E., Sen, M., Duffy, T., Laxton, J., Cipolloni, C., Vuollo, J., Richard, S., Simons, B., Ritchie, A., 2016. GeoSciML Version 4.0 - a Coming of Age.
Schroder, I.F., de Caritat, P., Wallace, L., Trihey, J.M., Boreham, C., Tobin, J., English, P. E., Sohn, J., Palatty, P., Coghlan, R.A., Flower, C., Maher, P., Main, P.T., Thorose, M., Long, I., Byass, J., Jinadasa, N., 2020. Northern Australia Hydrogeochemical Survey: Final Data Release and Hydrogeochemical Atlas for EFTF. Record Geoscience Australia, Canberra. https://doi.org/10.11636/Record.2020.015.
Sen, M., Duffy, T., 2005. GeoSciML: development of a generic GeoScience markup language. Comput. Geosci. 31 (9), 1095–1103. https://doi.org/10.1016/j.cageo.2004.12.003.
Shipley, O.N., Dabrowski, A.J., Bowen, G.J., Hayden, B., Pauli, J.N., Jordan, C., Anderson, L., Bailey, A., Bataille, C.P., Cicero, C., Close, H.G., Cook, C., Cook, J.A., Desai, A.R., Evaristo, J., Filley, T.R., France, C.A.M., Jackson, A.L., Kim, S.L., Kopf, S., Loisel, J., Manlick, P.J., McFarlin, J.M., McMeans, B.C., O'Connell, T.C., Pilar Birch, S.E., Putman, A.L., Semmens, B.X., Stantis, C., Stricker, C.A., Szejner, P.,

Trammell, T.L.E., Uhen, M.D., Weintraub-Leff, S., Wooller, M.J., Williams, J.W., Yarnes, C.T., Vander Zanden, H.B., Newsome, S.D., 2024. Design, development, and implementation of IsoBank: a centralized repository for isotopic data. PLoS One 19 (9), e0295662.

Simons, B., Boisvert, E., Brodaric, B., Cox, S., Duffy, T.R., Johnson, B.R., Laxton, J.L., Richard, S., 2006. GeoSciML: enabling the exchange of geological map data. ASEG Extended Abstracts 2006 (1), 1–4. https://doi.org/10.1071/ASEG2006ab162.

Simons, B.A., Raymond, O., Jackson, I., Lee, K., 2012. OneGeology-Improving Global Access to Geoscience, 5th Global Workshop on Digital Soil Mapping. AUSTRALIA, Sydney, pp. 265–269.

Simons, B., Wilson, P., Ritchie, A., Cox, S., 2013. ANZSoilML: an Australian - New Zealand Standard for Exchange of Soil Data.

Skrzypek, G., 2013. Normalization procedures and reference material selection in stable HCNOS isotope analyses: an overview. Anal. Bioanal. Chem. 405 (9), 2815–2823. https://doi.org/10.1007/s00216-012-6517-2.

Skrzypek, G., Allison, C.E., Böhlke, J.K., Bontempo, L., Brewer, P., Camin, F., Carter, J.F., Chartrand, M.M.G., Coplen, T.B., Gröning, M., Hélie, J.F., Esquivel-Hernández, G., Kraft, R.A., Magdas, D.A., Mann, J.L., Meija, J., Meijer, H.A.J., Moossen, H., Ogrinc, N., Perini, M., Possolo, A., Rogers, K.M., Schimmelmann, A., Shemesh, A., Soto, D.X., Thomas, F., Wielgosz, R., Winchester, M.R., Yan, Z., Dunn, P.J.H., 2022. Minimum requirements for publishing hydrogen, carbon, nitrogen, oxygen and sulfur stable-isotope delta results (IUPAC Technical Report). Pure Appl. Chem. 94 (11–12), 1249–1255. https://doi.org/10.1515/pac-2021-1108.

Stitzlein, C., Fielke, S., Waldner, F., Sanderson, T., 2021. Reputational risk associated with big data research and development: an interdisciplinary perspective. Sustainability 13 (16), 9280. https://doi.org/10.3390/su13169280.

Suckow, A., Dumke, I., 2001. A database system for geochemical, isotope hydrological, and geochronological laboratories. Radiocarbon 43 (2A), 325–337. https://doi.org/10.1017/S0033822200038182.

Trihey, J., HarrisPascal, C., 2021. Exploring for the Future — Groundwater Hydrochemistry Data Release: East Kimberley Project, Northern Territory. Geoscience Australia, Canberra. https://doi.org/10.11636/Record.2020.043.

Urvois, M., Grellet, S., Lorenz, H., Haener, R., Loiselet, C., Harrison, M., Krivic, M., Pedersen, C.B., Wiese, M.B., Baptie, A., Nayembil, M., Trench, J., Marsh, I., Cipolloni, C., D'Ambrogi, C., Congi, M.P., 2022. Integrating geological data in Europe to foster multidisciplinary research. Ann. Geophys. 65 (3). https://doi.org/10.4401/ag-8817.Dm319.

Walker, G., Taylor, P., Cox, S., Sheahan, P., 2009. Water Data Transfer Format (WDTF): Guiding Principles, Technical Challenges and the Future, Combined IMACS World Congress/Modelling and Simulation Society-of-Australia-and-New-Zealand (MSSANZ)/18th Biennial Conference on Modelling and Simulation. Cairns, AUSTRALIA, pp. 4381–4387.

Washington, N., Lewis, S., 2008. Ontologies: scientific data sharing made easy. Nature Education 1 (3), 5.

Welti, N., Flick, L., Mustakov, A., Campbell, R.S., Axel, Gerber, C.S., Steve, Puccini, A., Hughes, C., Crawford, J., Paul, A., Stobaus, T., Fraser, G., Hawkins, S., Waltenberg, K., 2024, Service Collection. http://hdl.handle.net/102.100.100/701351?index=1.

Wenk, E.H., Sauquet, H., Gallagher, R.V., Brownlee, R., Boettiger, C., Coleman, D., Yang, S., Auld, T., Barrett, R., Brodribb, T., Choat, B., Dun, L., Ellsworth, D., Gosper, C., Guja, L., Jordan, G.J., Le Breton, T., Leigh, A., Lu-Irving, P., Medlyn, B., Nolan, R., Ooi, M., Sommerville, K.D., Vesk, P., White, M., Wright, I.J., Falster, D.S., 2024. The AusTraits plant dictionary. Sci. Data 11 (1), 537.

Wilkinson, M.D., Dumontier, M., Aalbersberg, I.J., Appleton, G., Axton, M., Baak, A., Blomberg, N., Boiten, J.-W., da Silva Santos, L.B., Bourne, P.E., Bouwman, J., Brookes, A.J., Clark, T., Crosas, M., Dillo, I., Dumon, O., Edmunds, S., Evelo, C.T., Finkers, R., Gonzalez-Beltran, A., Gray, A.J.G., Groth, P., Goble, C., Grethe, J.S., Heringa, J., 't Hoen, P.A.C., Hooft, R., Kuhn, T., Kok, R., Kok, J., Lusher, S.J., Martone, M.E., Mons, A., Packer, A.L., Persson, B., Rocca-Serra, P., Roos, M., van Schaik, R., Sansone, S.-A., Schultes, E., Sengstag, T., Slater, T., Strawn, G., Swertz, M. A., Thompson, M., van der Lei, J., van Mulligen, E., Velterop, J., Waagmeester, A., Wittenburg, P., Wolstencroft, K., Zhao, J., Mons, B., 2016. The FAIR Guiding Principles for scientific data management and stewardship. Sci. Data 3 (1), 160018. https://doi.org/10.1038/sdata.2016.18.

Wilson, S.L., Way, G.P., Bittremieux, W., Armache, J.P., Haendel, M.A., Hoffman, M.M., 2021. Sharing biological data: why, when, and how. FEBS Lett. 595 (7), 847–863.