OpenMindat v1.0.0 R package: A machine interface to Mindat open data to facilitate data-intensive geoscience discoveries

Xiang Que[1], Jiyin Zhang[1], Weilin Chen[1], Jolyon Ralph[2], Xiaogang Ma[1]

[1]Department of Computer Science, University of Idaho, Moscow, ID 83844, USA
[2]Hudson Institute of Mineralogy, Keswick, VA 22947, USA

Correspondence to: Xiaogang Ma (max@uidaho.edu)

Abstract: Powered by ~~data-driven knowledge discovery~~ technologies such as machine learning and deep learning, ~~increasingly exciting~~meaningful patterns are increasingly discovered in ~~complex~~ earth science big data. ~~One~~In the field of ~~the world's most enormous treasure troves of mineral databases~~mineralogy, Mindat ("mindat.org~~"), contains vast amounts of knowledge that are yet to be mined~~") is one of the largest databases. Although its front-end website is open and free, a machine interface for bulk data query and download had never been set up before 2022. Through a project called OpenMindat, an application programming interface (API) to enable open data query and access from Mindat had been set up~~. This paper presents an open-source R package (OpenMindat v1.0.0) to bridge the data highway, connecting users' overwhelming data needs, facilitating data-intensive query and access, unlocking novel insights, and enabling groundbreaking geoscience discoveries. The package was designed to be user-friendly and extensible. It exploits the capabilities of the Mindat API, including the data subjects of~~ in 2023. To further lower the barrier of Mindat open data to geoscientists with limited coding skills, we developed an R package (OpenMindat v1.0.0) on top of the API. The Mindat API includes multiple data subjects such as geomaterials (e.g., rocks, minerals, synonyms, variety, mixture, and commodity), localities, and the IMA (International Mineralogical Association)-approved mineral list. The OpenMindat v1.0.0 package wraps the capabilities of the Mindat API and is designed to be user-friendly and extensible. In addition to providing functions for querying those data subjects on the API, the package supports exporting data to various formats~~ such as CSV, JSON-LD, and TTL. In~~. In real-world applications, these functions only require minor coding ~~and provide invaluable convenience~~ for users ~~with limited~~to get desired datasets, and various other packages in the R environment ~~experience. The~~can be used to analyze and visualize the data. The OpenMindat v1.0.0 package is open on GitHub under the MIT license~~ and~~, together with detailed ~~tutorial documentation~~tutorials and examples. The field of mineralogy and many other geoscience disciplines are facing the opportunities enabled by open data. Various research topics such as mineral network analysis, mineral association rule mining, mineral ecology, mineral evolution, and critical minerals have already benefited from Mindat's open data~~.~~ efforts in recent years. We hope this R package ~~will~~can help accelerate~~ the process of~~ those data-intensive studies and lead to more scientific discoveries.

1 Introduction

As machine learning and deep learning techniques thrive on their ability to ~~discern intricate~~discover complex patterns~~ and correlations~~, data-driven ~~discoveries in geosciences~~geoscience studies yield increasingly more exciting results (~~Reichstein~~Hazen et al., 2011; Bergen et al., 2019; ~~Bergen~~Reichstein et al., 2019; Que et al., 2024). However, due to the complexity and multifaceted nature of Earth's processes, high-quality data are required to enable the capacity of ~~machine learning and deep learning~~quantitative methods to make informed predictions ~~and classifications~~ across varying contexts (Chen et al., 2023). ~~Therefore, open~~Open access to large and diverse datasets is imperative for data-driven geosciences and calls for attention and actions (Hossain et al., 2016~~), as this can unlock novel insights, enabling groundbreaking discoveries that elucidate the complexities underlying Earth's dynamic processes.~~

). Regarding the field of mineralogy, minerals provide many essential clues for exploring the complex geological history of the Earth and other planetary bodies (Hazen et al., 2019; Prabhu et al., 2021). A rapidly growing volume of mineralogical and geochemical data resources are available for research, such as the IMA (International Mineralogical Association) list of mineral species (rruff.info/ima) (Prabhu et al., 2023), Mindat (mindat.org) (~~Hazen~~Ralph et al., ~~2011~~2022; Ma et al., 2024), RRUFF (rruff.info) (Yang et al., 2011), EarthChem (earthchem.org) (Walker et al., 2005; Lehnert et al., 2007), the Evolutionary System of Mineralogy Database (ESMD; odr.io/esmd) (Chiama et al., 2023), the Mineral Properties Database (odr.io/MPD) (Morrison et al., 2023), and the Astromaterials Data System (Astromat.org) (Chamberlain et al., 2021). Thanks to these big and expanding open datasets, new scientific topics such as mineral evolution (Hazen et al., 2008; Hazen et al., 2014), mineral ecology (Hazen et al., 2015), and mineral informatics (Prabhu et al., 2023) are emerging and developing ~~dramatically~~quickly. Among those data sources, the Mindat, a crowd-sourced and expert-curated database that started running in 2000, is now one of the world's most widely used online ~~database of mineralogical information~~databases about minerals and their distributions. By August 2023, Mindat has recorded 5,960 minerals, 395,558 localities, 1,503,650 occurrences, and 1,291,077 photos, with a total data volume exceeding 25.8 TB (Ralph et al., ~~2022).~~2022), and the records are actively expanding and updating.

~~Although~~ Mindat ~~plays an increasingly significant role in scientific value~~is widely used by many individuals and ~~societal impacts, it still faces the challenges of infrastructure maintenance and development to meet the overwhelming data needs (Ma et al., 2024).~~communities. In 2021 alone, the Mindat website received 44,333,302 views from 10,148,136 unique visitors, and as of August 2023, the number of registered users reached 72,488. ~~However,~~The Mindat ~~relies entirely on donations and sponsorships to maintain and develop the infrastructure to meet growing~~team provides a website portal (https://www.mindat.org/advanced_search.php) for users to retrieve data by specifying constraints interactively. Although its website has always been open for searching and browsing datasets, a machine interface for Mindat data ~~volumes and needs. The undergoing project~~ querying and downloading had never been fully established before 2023. Moreover, multiple constraints on the website require multiple interactions to be performed, and some pages cannot load all the filtered data records at once (due to the size of the data that meet the constraints) or cannot display them efficiently (e.g., in sorted order). In the past years, many researchers have reached out to the Mindat technical team requesting bulk datasets on certain topics, and those requests could only be addressed on a tedious case-by-case situation. To address the challenge, the OpenMindat project (Ma et al., 2024) aimswas set up recently to implement a fully open access, machine-readable, and interoperable architecture for Mindat, making it an active data node in the geoscience cyberinfrastructure ecosystem.

. Following the FAIR principles (i.e., findable, accessible, interoperable, and reusable) (Wilkinson et al., 2016), a roadmap of the OpenMindat project was laid out, including the technical approaches to upgrade and reuse existing data resources, tools, and infrastructure (Ma et al., 2024).. In the Spring of 2023, the preliminary RESTful API (Application Programming Interface) (Richardson and Ruby, 2008) of Mindat was established, for which any registered users can access with an authorized API token. Although data can now be queried and accessed from (Zhang, 2024). While the API (https://api.mindat.orghttps://api.mindat.org) (Zhang et al., 2024), a more friendly R or Python software package oriented to users' provides a structured and stable channel to the Mindat open data needs, is still desired, as (Zhang et al., 2024), users need to know the data subjects available in the API, the parameters of each data subject, as well as moderate coding skills to construct the commands for data retrieval. To further lower the barrier of Mindat open data, we are constructing R and Python software packages on top of the API. Such packages have several advantages. First, they wrap the capability of the API in a variety of functions, for which users only need minimal coding to retrieve datasets of interest. Second, the data querying is fast, and the results can be returned in specified formats. Third, the packages can be easily integrated in workflow platforms of R and Python such as R Markdown and Jupyter are now viral amongst geoscientists. Such an R or Python package of the Mindat API will make the data query and access much more accessible., where many other packages can be used together for data analysis.

This paper presents our design and implementation of anthe R software package, OpenMindat v1.0.0, to meet users' needs for quick and easy access to Mindat's open data. The package is open source for anyone to reuse, and we welcome feedback on improvement and extension. The remainder of this paper is organized as follows: Section 2 presents the technical architecture of the OpenMindat R package. Section 3 introduces the classes and functions in it. Section 4 presents a list of examples using this package, including records about geomaterials, localities, IMA minerals, and their outputs in different formats. Section 5 discusses the capabilities and limitations of the current R package and plans for future extension. Finally, Section 6 summarizes the contributions of this study.

2 Technical Architecture of the OpenMindat R Package

The primary objective of the OpenMindat R package is to provide an implementation mechanism to translate users' data requirements into Mindat API requests. Mindat datasets, especially those made machine-readable through the Mindat RESTful

API, are structured records stored in a relational MySQL database. ~~The primary data subjects include mineral species (>5800), alternative mineral names (>45000), localities (>390000), occurrence records (>1.2 million), photographs (>1.1 million), Mindat ID (>10.3 million), locality age (>5500), literature references (>13.5million), and meteorities (1509 records including 449 petroleum categories). The API server manages HTTP requests for datasets. Currently, it provides a separate access endpoint for each data subject, and it distinguishes HTTP single-record requests and list requests as request query strings. Therefore, the key to building the R package is converting user data requirements into data request strings that the Mindat API can handle.~~**Table 1** lists the primary data subjects stored in Mindat and their volume.

Table 1: Primary data and its volume stored in the Mindat database

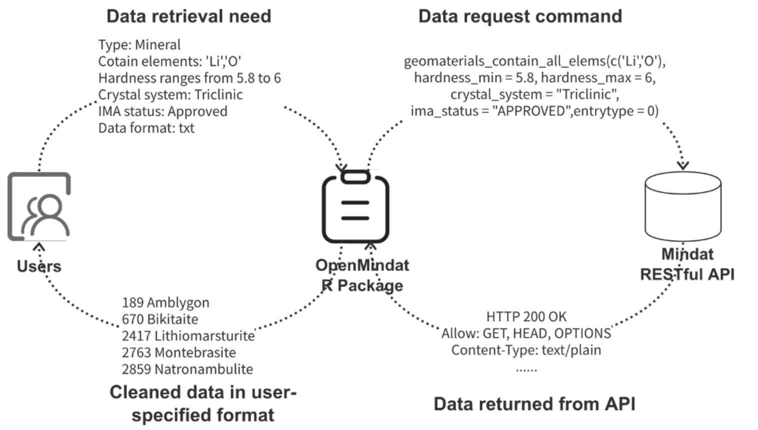
Data subjects	**Brief description**	**Volume**
mineral species	The official list of approved mineral species, including their names, localities, and occurrences.	>5800
alternative mineral names	Alternative names that aren't official IMA-approved mineral species, including varieties, mixtures, synonyms, etc.	>45000
localities	General information about a locality, which may include latitude and longitude or any other relevant information about the locality.	>390000
occurrence records	The link between our mineral data and our locality pages.	>1.2 million
photographs	Mineral photo	>1.1 million
Mindat ID	Identifier for a mineral or related material (rock, mixture) in the Mindat.org database	>10.3 million
locality age	The age of a mineral occurrence and its locality.	>5500
literature references	References formatted within Mindat database	>13.5million
meteoritics	A meteorite is a stony or metallic body that has fallen to the Earth's surface (or any other planetary body on which it is found) from outer space.	>1500

The API server manages Web requests for datasets. Currently, it provides a separate access endpoint for each data subject. Accordingly, we designed ~~a technical~~an architecture (**Figure 1**) ~~oriented to users' data requirements. From the users' side, they do not need to care about the details of the request strings that will finally be sent to the API; they should operate on the functions in the R package and a token~~ to connect ~~to~~the user's data needs with the Mindat API server~~.~~. (For a more detailed technical diagram of the architecture, please refer to the online documentation on our GitHub repository. Links are given in the Code and Data Availability section). From our survey and interactions with geoscientists in the past years, ~~the~~most users' data requirements fall into ~~those~~the following categories: (1) Queries about geomaterials (i.e., mineral, rock, commodity, and other natural geological materials). Users need to ~~query~~filter the geomaterials ~~by~~based on their physical properties~~, such as~~ (e.g., density, hardness, color, refractive index, and crystal structure~~. Besides, users would also like to query datasets by~~); or on their chemical properties (e.g., element inclusion and exclusion states~~). Finally, Users need to filter geomaterial according to the~~); or their entry ~~type, such as~~types (e.g., synonym, variety, rock, mixture, mineral, and series~~.~~). (2) Queries about localities. Mindat's localities record textual addresses, coordinates, area boundaries, and other relevant attributes. It ~~is~~

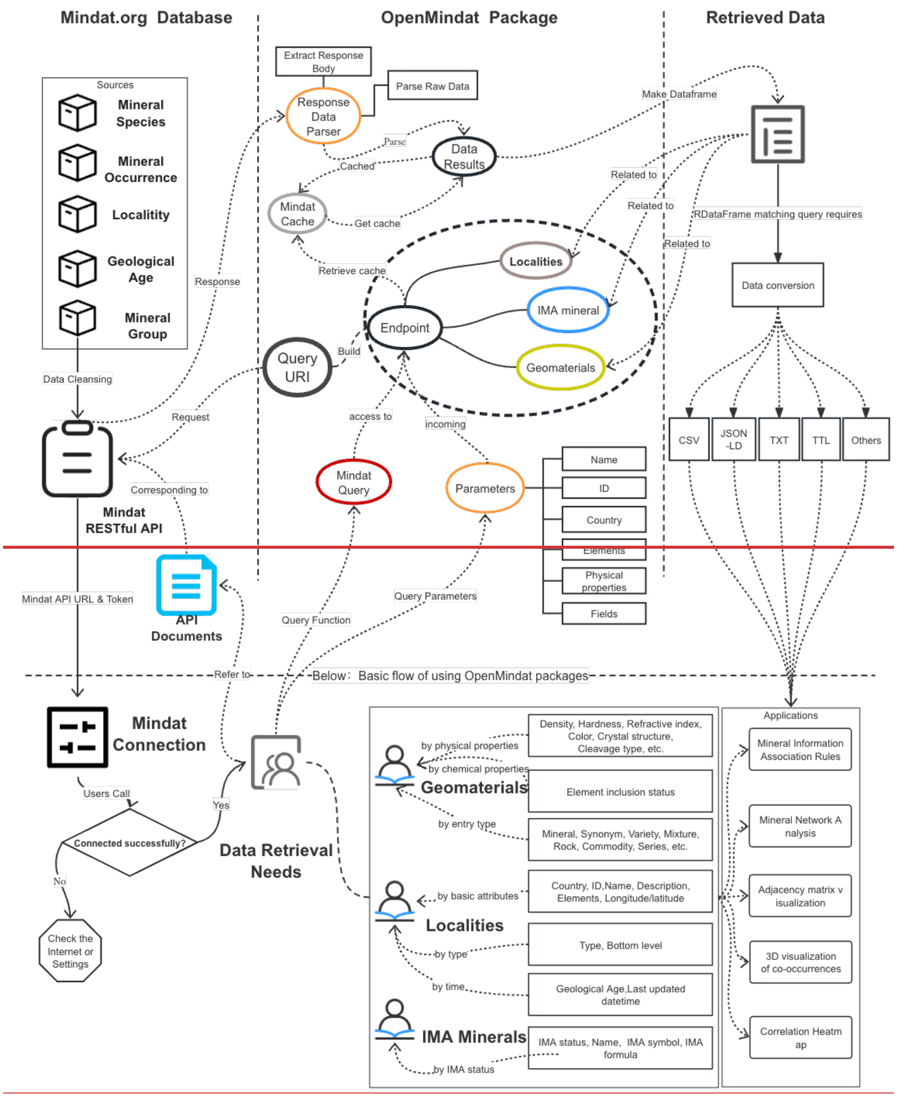
organized infollows a specific hierarchical structure. In most cases, users and naming rule (https://www.mindat.org/a/localityhierarchies). A simple explanation is that the number of levels of an address indicates the level of detail of the address. The larger the value, the more detailed the address. 0 is the top level, usually representing a country, a region, or a plate. Users may need to query the localities bybased on their number of levels, attributes, such as (e.g., name, country, ID, description, and longitude/latitude. In addition, because of the hierarchical structure of localities, many users need to query localities by type, such as queries about whether a locality is at a bottom level or whether there are), coordinate records. Moreover, studies ofinformation, or geological ages (Studies of the mineral evolution (Hazen and Ferry, 2010; Hystad et al., 2019) and the co-evolution of geosphere and biosphere (Hazen et al., 2014; Hazen and Morrison, 2020) ignited the need to retrieve localities with geological ages.). (3) Queries about IMA-approved minerals. The International Mineralogical Association (IMA) is an international group that promotes the science of mineralogy and standardizes the nomenclature of mineral species. Since theThe IMA mineral list is updated frequently, queryingand it is common to query mineral information by the specific IAMIMA status, such as A (approved), G (grandfathered), Rd (redefined), and Q (questionable), has also become one of the common etc. (4) Data format needs. Some applications or analyses, including mineral association rule analysis (Morrison et al., 2023) and mineral network analysis (Liu et al., 2018; Morrison et al., 2020), require filtered data in a specified format, such as CSV.

In the implementation, the core module of the OpenMindat R package will first receive query functions and parameters, and then parse and distribute them to the corresponding endpoints. The API endpoint module will check its local cache, i.e., Mindat Cache, to see if it is already cached. If so, the data results module will return cached data and make a data frame to meet the data need. Otherwise, according to the query functions and parameters, the endpoint will assign query tasks to the specific sub-endpoints, such as localities, geomaterials, or IMA minerals. The sub-endpoint will combine the query parameters and content to build a query URI that the Mindat API server can handle. When the query URI request is handled, the server will return the response data, and then the OpenMindat R package will extract the body of the response and parse the received raw data. The package can help users transform the retrieved data into various required formats, including CSV, TXT, and TTL, and support many

applications, such as mineral association rule analysis (Morrison et al., 2023),



mineral network analysis (Liu et al., 2018; Morrison et al., 2020), and more.



Mindat.org Database
OpenMindat Package
Retrieved Data
Sources
Mineral Species
Mineral Occurrence
Localitity
Geological Age
Mineral Group
Data Cleansing
Mindat RESTful API
Response
Request
Corresponding to
API Documents
Mindat API URL & Token
Extract Response Body
Parse Raw Data
Response Data Parser
Parse
Cached
Data Results
Mindat Cache
Get cache
Retrieve cache
Make Dataframe
Localities
IMA mineral
Geomaterials
Endpoint
Query URI
Build
access to
incoming
Mindat Query
Parameters
Name
ID
Country
Elements
Physical properties
Fields
Related to
Related to
Related to
RDataFrame matching query requires
Data conversion
CSV
JSON -LD
TXT
TTL
Others
Query Function
Query Parameters
Refer to
Below: Basic flow of using OpenMindat packages
Mindat Connection
Users Call
Connected successfully?
Yes
No
Check the Internet or Settings
Data Retrieval Needs
Geomaterials
by physical properties
by chemical properties
by entry type
Density, Hardness, Refractive index, Color, Crystal structure, Cleavage type, etc.
Element inclusion status
Mineral, Synonym, Variety, Mixture, Rock, Commodity, Series, etc.
Localities
by basic attributes
by type
by time
Country, ID,Name, Description, Elements, Longitude/latitude
Type, Bottom level
Geological Age,Last updated datetime
IMA Minerals
by IMA status
IMA status, Name, IMA symbol, IMA formula
Applications
Mineral Information Association Rules
Mineral Network A nalysis
Adjacency matrix v isualization
3D visualization of co-occurrences
Correlation Heatm ap

Figure 1: Technical architectureArchitecture of the OpenMindat R package

3 Capabilities and Usage

Following the designed technical architecture and user need analysis, we developed nine classes: Connection, Mindat Cache, Endpoint, Response Data Parser, Mindat Query, Geomaterials, Localities, IMA Minerals, and Data Maker. We implemented about 100 functions to ensure that the package could work accurately and efficiently.in the R package (to view all the functions, execute “help (package = OpenMindat)” or see the reference manual listed in Table 110), and they are grouped into several classes. Table 2 lists the ninemain classes and briefly describes some of their tasks.

Table 1: Capabilities of the OpenMindat R package (nine functions related to data subjects and formats (A complete list of classes and some of their functions))

Class	Functions	Brief description
Connection	mindat_connection	Initialize the API Call. Setup the base URL, token of Mindat API, response page size per request, and the response format of API.
Mindat Cache	mindat_cache	Create a cache environment.
	mindat_cache_set	Set or allocate a cache by a given name.
	mindat_cache_get	Get cache value by name. If exist return the cached value, otherwise return NULL.
Endpoint	mindat_set_up_endpoints	Set up the base Mindat sub-endpoints (e.g., localities sub-endpoint, geomaterials sub-endpoint, etc.) according to the Mindat API server.
	mindat_uri_builder	Build a query URI based on the query dataset and parameters.
	mindat_setup	Set up a Mindat base URI, endpoints, and cache configuration information.
Response Data Parser	mindat_parse_raw_data	Parse the responded raw data (default is in JSON format) and then convert it to an R dataframe. If the raw data obtained is paged, the function will continue to request the next page of data until all data pages are obtained.
	mindat_extract_response_body	Check the response status for success. If so, text data is returned, otherwise an error is reported.
	mindat_make_data_frame	Convert the responded JSON data to an R dataframe.
	mindat_get_data_from_uri	Retrieve data from a query URI.
	mindat_build_querystring	Construct a query string based on query conditions.

	mindat_query	Basic function to query dataset from a specified endpoint. Entrance to all conditional queries.
	params_to_string	Parses arguments into strings so that the function can handle external conditions entered by the user.
Mindat Query	mindat_geomaterial(mindat_geomaterial_list)	Retrieve a (list of) geomaterial that matched the input conditions.
	mindat_localitiy(mindat_localities_list)	Retrieve a (list of) locality that matched the input conditions.
	mindat_mineral_ima(mindat_mineral_ima_list)	Retrieve a (list of) IMA mineral that matched the input conditions.
	saveMindatDataAs	Save the data frame to file in a specified format.
Data Maker	ConvertDF2JsonLD	Convert the retrieved data frame into a JSON-LD format string.
	ConvertDF2TTL	Convert the retrieved data frame into a TTL format string.
	geomaterials_contain_any_elems	Retrieve geomaterials that contain any of the specified elements.
	geomaterials_contain_all_elems	Retrieve geomaterials that contain all the specified elements.
	geomaterials_without_elems	Retrieve geomaterials that do not contain any of the specified elements.
	geomaterials_contain_only_elems	Retrieve geomaterials that only contain the specified elements.
	geomaterials_contain_all_and_without_elems	Retrieve geomaterials that contain the specified included and excluded elements.
Geomaterials	geomaterials_cleavagetype	Retrieve geomaterials that matched the specified types.
	geomaterials_colour	Retrieve geomaterials that matched the specified colours.
	geomaterials_crystal_system	Retrieve geomaterials that matched the specified crystal system.
	geomaterials_bi_greater_than, geomaterials_bi_less_than	Retrieve geomaterials that had higher (lower) birefringence than the input value.
	geomaterials_dens_range	Retrieve geomaterials that matched the density within a given range.
	geomaterials_diapheny	Retrieve geomaterials that matched the given diapheny.
	localities_list_country	Retrieve the localities list that are found in a specified country.
Localities	localities_list_elems_inc, localities_list_elems_exc	Retrieve the localities that contain (or not contain) the given elements.
	localities_list_description	Retrieve the localities that contain the given description.
	minerals_ima_list	Retrieve the whole IMA mineral list.
IMA Minerals	minerals_ima_list_ima	Retrieve IMA mineral lists with given authorization statuses.
	minerals_ima_retrieve	Retrieve IMA mineral with given ID.

~~From the software developers' point of view, these classes and functions follow a workflow sequence: (1) The Connection~~ is available via our online documentation on GitHub): (1) Geomaterials class~~ helps establish the access configuration between the user and the Mindat API. Since the current API server only accepts data access with authorization, it is necessary to register as a Mindat user and obtain a token to ensure a connection to the server. Users can apply for a token per the instructions via the link: https://www.mindat.org/a/how_to_get_my_mindat_api_key. Once the function "mindat_connection" is successfully executed, other functions of the R package can run normally, and the connection configuration will be cached. (2) The Mindat Cache class manages cached data, e.g., creation, release, acquisition, and more. Mindat data cache can reduce the number of interactions between users and the API server and improve efficiency. (3) The Endpoint class is mainly responsible for configuring and assigning sub-endpoints and constructing request URIs based on the query conditions. The sub-endpoints are configured based on the Mindat API to handle different query datasets. For example, the geomaterials sub-endpoint is set up to handle queries about records of geomaterials. The request URI to be sent to the Mindat API server for geomaterials can thus be built according to the query conditions. (4) The Response Data Parser class processes the response data from Mindat API. It can help check the response status, extract and parse the body of the response data, and convert it into a data frame of R. (5) The Mindat Query is a comprehensive data retrieval class that requires the use of multiple classes mentioned above. It first builds a query URI using an Endpoint instance, then sends a request to the API server via the URI, and finally parses the response data using a Response Data Parser. (6) The Data Maker class is used for data conversion and output. It can convert R data frames to required formats such as CSV, TXT, TTL, etc. (7) The Geomaterials class~~, which is one of the main ~~dataset objects~~data subjects supported by ~~the~~ Mindat API, and it includes sub-subjects of minerals, synonyms, varieties, mixtures, series, group lists, polytypes, rocks, and commodities. The current geomaterial record contains 146 ~~fields~~attributes, including descriptions of physical properties, chemical information, optical properties, crystal structure information, and more. (~~8) The~~2) Localities class~~ is another vital dataset object the Mindat API supports.~~. It records 37 ~~fields~~attributes, including longitude, latitude, coordinate system, link, area, etc., which describe the information of textual address, coordinate point position, locality type boundary polygon, and occurrences. (~~9) The~~3) IMA Minerals class. This class is mainly for retrieving and managing IMA-approved mineral species names, ~~molecular~~chemical formulas, authorization status, and other attributes. (4) Data Maker class. It is for data format conversions and outputs. It can convert R data frames to required formats such as CSV, TXT, TTL, and JSON-LD.

~~For the end users, those classes and functions can be applied flexibly to meet various data needs. For example, they support retrieval of geomaterial records via single or combined query conditions, including filtering records by certain specified chemical elements, hardness within a specified range, color characteristics, refractive index within a specified range, cut type (e.g., imperfect/fair), crystal structure (e.g., amorphous), tenacity (e.g., brittle), and optical type (e.g., biaxial). They also support retrieving localities records, e.g., a specific type (e.g., bottom level) of localities within a specified country (e.g., Sweden). More examples of this will be presented in the next section.~~

4 Examples and Results

To make the OpenMindat R package work adequately, some dependent packages, including "httr" and "jsonlite," should be installed in the running environment. In addition, as mentioned above, an access token is required to establish a connection to the Mindat API server. As shown in the following code, the “mindat_connection” function should be called to complete configuration initialization, and then all other functions can be called according to the user's data retrieval needs.

```
R> library(httr)
R> library(jsonlite)
R> library (OpenMindat)
R> #Replace the following string “aa9c25fa95d8063908cb2bf186c9e79f” with your own Mindat token.
R> mindat_connection(“aa9c25fa95d8063908cb2bf186c9e79f”)
```

The following examples demonstrate how to retrieve data through this OpenMindat R package, including the functions of the three main dataset entity classes: Geomaterials, Localities, and IMA Minerals.

4.1 Geomaterials

To illustrate the capabilities of retrieving geomaterial records, we chose some representative use cases. In terms of chemical elements of geomaterials, the package functions support data retrieval for relations including “contains any,” “contains all,” “contains only,” “does not contain,” “contains all but not,” and “contains any but not.” Some demo codes are as follows:

```
R> geomaterials_contain_any_elems (c('Fe','S'))
R> geomaterials_contain_all_elems (c('Fe','S'))
R> geomaterials_contain_only_elems (c('Fe','S'))
R> geomaterials_not_contain_elems (c('Fe','S', 'O'), fields ="id,name,mindat_formula,elements")
R> geomaterials_contain_all_but_not_elems (c('Fe','S'), c('O'))
R>geomaterials_contain_any_but_not_elems(c('Fe','S'), c('O'))
```

Results show that 10146 geomaterial records (148 fields) containing iron (Fe) or sulfur (S) elements were retrieved using the function “geomaterials_contain_any_elems”. The retrieved number of geomaterial records containing both Fe and S elements sharply dropped down to 1363 using the “geomaterials_contain_all_elems” function. Moreover, only 83 records of geomaterials that containing only Fe and S elements (no other elements) were retrieved by using the “geomaterials_contain_only_elems” function. Besides, 31919 records of geomaterials that did not contain elements Fe, S, and O (Oxygen) (the fields were filtered by id, name, mindat_formula, and elements) were retrieved by using the

~~“geomaterials_not_contain_elems” function. Lastly, 808 records of geomaterials containing Fe and S, but not O elements can be retrieved using the “geomaterials_contain_all_but_not_elems” function. **Table 2** shows the head 3 of geomaterial records in those examples.~~

~~**Table 2: Results of geomaterial records retrieved by chemical elements**~~

Table 2: A partial list of classes and functions in the OpenMindat R package

~~*Function name*~~ *Class*	~~*Head 3 records of some selected fields*~~ *Functions*	*Brief description*		
		~~*name*~~	~~*mindat_formula*~~	~~*elements*~~
Geomaterials	geomaterials_contain_any_elems	~~Ach√©valite~~ Retrieve geomaterials that contain any of the specified elements.	~~FeSe~~	~~Fe Se~~
		~~Actinolite~~	~~◻Ca₂(Mg_{4.5-2.5}Fe_{0.5-2.5})Si₈O₂₂(OH)₂~~	~~Ca Fe Mg Si O H~~
		~~Aegirine~~	~~NaFe³⁺Si₂O₆~~	~~Fe Na Si O~~
	geomaterials_~~*contain_all_elems*~~cleavagetype	~~Aluminocopiapite~~ Retrieve geomaterials that matched the specified cleavage type.	~~Al_{2/3}Fe³⁺₄(SO₄)₆(OH)₂·20H₂O~~	~~Al Fe O S H~~
	~~Alloclasite~~ geomaterials_colour	~~Co_{1-x}Fe_xAsS~~ Retrieve geomaterial matched the specified colours.	~~As Co Fe S~~	
	~~Amarantite~~ geomaterials_crystal_system	~~Fe³⁺₂(SO₄)₂O·7H₂O~~ Retrieve geomaterial matched the specified crystal system.	~~Fe O S H~~	
	geomaterials_~~*contain_only_elems*~~bi_greater_than	~~Gold-bearing Pyrite~~ Retrieve geomaterials that have higher birefringence than an input value.	~~FeS₂~~	~~Fe S~~
		~~Greigite~~	~~Fe²⁺Fe³⁺₂S₄~~	~~Fe S~~
		~~Mackinawite~~	~~FeS~~	~~Fe S~~
	geomaterials_~~*not_contain_elems*~~dens_range	~~Abelsonite~~ Retrieve geomaterials that matched the density within a given range.	~~Ni(C₃₁H₃₂N₄)~~	~~Ni N C H~~
		~~Aluminium~~	~~Al~~	~~Al~~
		~~Algodonite~~	~~(Cu_{1-x}As_x)~~	~~As Cu~~

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	geomaterials_*contain_all_but_not_elems*diapheny	AlloclasiteRetrieve geomaterials that matched the given diapheny.	Co_{1-x}Fe_xAsS	-As-Co-Fe-S-
Localities	Bismuth-bearing Tetrahedritelocalities_list_country	Cu₆(Cu₄(Fe/Zn)₂)(Sb,Bi)₄S₁₂SRetrieve the localities list that are found in a specified country.		-Bi-Cu-Fe-Sb-Zn-S-
	Argentopentlandite	Ag(Fe,Ni)₈S₈		-Ag-Fe-Ni-S-
	localities_list_elems_inc	***geomaterials_contain_any_but_not_elems***Retrieve the localities that contain the given elements.	Achávalite FeSe	-Fe-Se-
	Alloclasitelocalities_list_description	Co_{1-x}Fe_xAsSRetrieve the localities that contain the given description.		-As-Co-Fe-S-
IMA Minerals	Bismuth-bearing Tetrahedriteminerals_ima_list	Cu₆(Cu₄(Fe/Zn)₂)(Sb,Bi)₄S₁₂SRetrieve the whole IMA mineral list.		-Bi-Cu-Fe-Sb-Zn-S-
	minerals_ima_list_ima	Retrieve IMA mineral lists with given authorization status.		
	minerals_ima_retrieve	Retrieve IMA mineral with given ID.		
Data Maker	saveMindatDataAs	Save the data frame to file in a specified format.		
	ConvertDF2JsonLD	Convert the retrieved data frame into a JSON-LD format string.		
	ConvertDF2TTL	Convert the retrieved data frame into a TTL format string.		

Code

These above classes and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Retriev_Geomaterials_by_elements.ipynb

In addition to chemical elements, the package also supports geomaterial dataset retrieval by usingfunctions can be applied flexibly to meet users' specific data needs. The Geomaterials class provides functions that help us easily filter records by the following relationships: "contains any", "contains all", "contains only", "does not contain", "contains all but not", and "contains any but not". It also provides functions to filter records by specifying the physical properties, including density, hardness, birefringence, optical 2v, crystal system, fracture type, color, streak, diaphaneity, lustre type, optical sign, optical type, poly type, cleavage type, tenacity, and more. Some demo codes are as follows:

R> For some *geomaterials_hardness_gt (9)*

R> geomaterials_hardness_lt (1)

R> geomaterials_hardness_range(3,3.5)

R> geomaterials_dens_range(3,3.2)

R> geomaterials_optical2v_range (9,10)

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Table 3 shows the head 3 of retrieved geomaterial records that the numerical physical properties meet the given conditions. For example, the hardness of geomaterials in the Mindat database, ranging from 0 to 10, usually refers to the with numerical values or threshold ranges (e.g., Mohs scale (Broz et al., 2006). The "geomaterials_hardness_gt" and "geomaterials_hardness_lt" functions retrieve geomaterial records with hardness higher and lower than a given value, respectively. The "geomaterials_hardness_range" function retrieves the), density, etc.), it supports filtering records whose density is by relationships such as "greater than", "less than", and "within a specific interval. In addition to hardness, records of similargiven range". For the other non-numerical physical properties (e.g., density or optical 2v) can also be retrieved , it provides functions for retrieving data records by calling the corresponding functions such as "geomaterials_dens_range"specifying strings, enumeration variables, and "geomaterials_optical2v_range".

Table 3: Results of geomaterial records retrievedspecial symbols. It also provides functions to retrieve geomaterial records based on wildcard names, non-null fields, Mindat IDs, mineral varieties, and more. The Localities class also provides functions for retrieving records by **using physical**specifying the chemical elements' inclusion and exclusion relationships. It can support filtering locality records by level, country name, Mindat ID, description, etc. The "age_id" attribute of the Mindat locality, if not null, shows a unique identifier that can be associated with a locality age record. This record contains geological time information about the locality. The IMA Minerals class provides functions to retrieve IMA minerals records. It helps retrieve the complete list of IMA-authorized mineral names, including their chemical formulas, description information, etc. Users can also retrieve data by specifying their approved status or ID. The Data Maker class provides functions to help export the retrieved records into the required format. All the provided functions support the expansion of the input parameter, which enables data retrieval based on combined properties **in numeric forms**. Some examples will be presented in the next section.

3 Examples and Results

3.1 Geomaterial data retrieval

To illustrate the capabilities of retrieving geomaterial records, **Table 3** lists some basic use cases and their descriptions. In the list each use case only involves the simple usage of one function from the R package.

Table 3: Geomaterial data retrieval use cases

Function category	***Function -name & Input*** ***name***	***Head 3 records of some selected fieldsOutput & Description*** ***min_value***	***Demo codes & Results*** ***max_value***
geomaterials_hardness_gtchemical elements' inclusion	Bahianitegeomaterials_contain_any_but_not_elem(c('Fe','S'), c('O'))	9Records of geomaterials that containing Fe and S, but not O.	9https://github.com/quexiang/OpenMindat/blob/main/notebook/Retriev_Geomaterials_by_elements.ipynb

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and exclusion relationships			
	Bromellite	9	9
	Chromium	9	9
geomaterials_hardness_lt	Acetamidegeomaterials_not_contain_elems(c('Fe','S','O'),fields="id,name,mindat_formula,elements")	1Records of geomaterials without Fe, S, and O, only contain the following fields: id, name, mindat_formula, and elements.	1.5
	Aliettite	1	2
	Aluminite	1	2
geomaterials_hardness_rangephysical properties with numerical values or threshold ranges	Abelsonitegeomaterials_hardness_gt (9)	2Records of geomaterials with a Mohs hardness greater than 9.	3https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_physical_prop_1.ipynb
	Abernathyite	2.5	3
	Acuminite	3.5	3.5
geomaterials_dens_range	Actinolitegeomaterials_dens_range(3,3.2)	3.03Records of geomaterials with a density ranging from 3 to 3.2.	3.24
non-numerical physical properties	Akrochorditegeomaterials_colour(c("bright blue"))	3.194Records of geomaterials that have bright blue color.	3.35https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_physical_prop_2.ipynb
	Amblygonitegeomaterials_cleavagetype(c("Poor/Indistinct"))	3.04Records of geomaterials with a cleavage type of "Poor/Indistinct".	3.11
geomaterials_optical2v_rangewildcard names, non-null fields, etc.	Autunitegeomaterials_name("_u_r_z")	10Records of geomaterials whose names has 6-character where 2, 4, and 6 characters were specified.	53https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_wildcar_names.ipynb
	Bario-orthojoaquinitegeomaterials_name("qu*")	10Records of geomaterials whose names had the first two characters ‘q’ and ‘u’.	15
	Beidellitegeomaterials_field_exists("meteoritical_code",TRUE)	9Records of geomaterials whose “meteoritical_code” field had non null values.	16
	geomaterials_varietyof(3337)	Records of geomaterials that were varieties of Quartz (3337 is the Mindat ID of Quartz).	

Code and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_physical_prop_1.ipynb

The geomaterial records can also be retrieved using special symbols and strings representing different physical features. The following codes show some examples:

R> geomaterials_crystal_system(c("Icosahedral"))

R> geomaterials_fracturetype(c("Step-Like"))

R>

In some other situations even just one function can achieve a relatively heavy task. The code below demonstrates three such tasks: One is to retrieve a hierarchical taxonomy of petrological names and their definitions (e.g., get the rock hierarchy information), and the other is to list mineral species containing nickel or cobalt, with sulphur but without oxygen, which was discussed in Ma et al. (2023) as a typical use case.

```
geomaterials_colour(c("bright blue"))
R> geomaterials_streak("orange")
R> geomaterials_diapheny("Transparent")
R> geomaterials_lustretype(c("Adamantine"))
R> geomaterials_opticalsign("-")
R> geomaterials_polytypeof(0)
R> geomaterials_cleavagetype(c("Poor/Indistinct"))
```

Table 4 shows part of the results retrieved by symbols or strings with actual physical meaning. The last column is the field that matches the input string or symbols (except for the field of "commentcrystal"), and the remaining columns are some related fields. Results only list the head 3 records that meet the conditions (all those with less than 3 records are also listed), showing that these implemented functions can run accurately and efficiently.

Table 4: Results of geomaterial records retrieved by using physical properties in symbol and string forms

Function Name	***Head 3 records of some selected fields***				
	name	***elements***	***csystem***	***commentcrystal***	
geomaterials_crystal_system	Icosahsedrite	-Al-Cu-Fe-	Icosahedral	The structure is not reducible to a single three-dimensional unit cell, so neither cell parameters nor Z can be given. The X-ray powder pattern was indexed on the basis of six integer indices, as conventionally used with quasicrystals, where the lattice parameter (in six-dimensional notation) is measured to be a6D = 12.64 √Ö, with probable space group Fm-3-5.	
	Decagonite	-Al-Fe-Ni-	Icosahedral	P105/mmc.	
	Unnamed (Mn-Si-Cr-Al-Ni Quasicrystal)	-Al-Cr-Mn-Ni-Si-	Icosahedral		
geomaterials_fracturetype	***name***	***elements***	***csystem***	***cleavagetype***	***fracturetype***
	Bytownite	-Al-Ca-Na-Si-O-	Triclinic	Perfect	Step-Like
	Clinoatacamite	-Cl-Cu-O-H-	Monoclinic	Perfect	Step-Like

	Daomanite	As Cu Pt S	Orthorhombic	Distinct/Good	Irregular/Uneven,Step-Like
geomaterials_colour	***name***	***elements***	***csystem***	***colour***	
	Astrocyanite-(Ce)	Ce Cu La Nd O C H U	Hexagonal	Bright blue	
	Chlorothionite	Cl Cu O K S	Orthorhombic	Bright blue.	
	Lautenthalite	Cu Pb O S H	Monoclinic	Green, bright blue	
geomaterials_streak	***name***	***elements***	***csystem***	***colour***	***streak***
	Alacránite	As S	Monoclinic	Orange to pale gray with rose-yellow internal reflections	Yellow-orange
	Berzeliite	As Ca Mg Na O	Isometric	Yellow, Orange, colorless, brownish-orange; colorless to orange in transmitted light.	Nearly white to yellow-orange
	Cassedanneite	Cr Pb O H V	Monoclinic	Orange-red	Yellow-orange
geomaterials_diapheny	***name***	***elements***	***csystem***	***colour***	***diapheny***
	Abenakiite-(Ce)	Ce Na Si O P C S	Trigonal	Pale brown	Transparent
	Abernathyite	As O K H U	Tetragonal	yellow	Transparent
	Abhurite	Cl Sn O H	Trigonal	Colourless	Transparent
geomaterials_lustretype	***name***	***elements***	***csystem***	***lustre***	***lustretype***
	Aerugite	As Ni O	Trigonal		Sub-Adamantine,Sub-Vitreous,Resinous
	Annabergite	As Ni O H	Monoclinic	Weakly adamantine, vitreous, earthy when powdery.	Sub-Adamantine,Sub-Vitreous,Pearly,Earthy
	Ardennite-(As)	Al As Mg Mn Si O H	Orthorhombic		Sub-Adamantine
geomaterials_opticalsign	***name***	***elements***	***colour***	***csystem***	***opticalsign***
	Abenakiite-(Ce)	Ce Na Si O P C S	Pale brown	Trigonal	-
	Abernathyite	As O K H U	yellow	Tetragonal	-
	Acetamide	N O C H	Colourless, grey	Trigonal	-

geomaterials_polytypeof	***name***	***elements***	***csystem***	***opticalbireflectance***	***polytypeof***
	Barikaite	Ag As Pb Sb S	Monoclinic	distinct bireflectance in grey tones,	0
	Pašavaite	Pb Pd Te	Orthorhombic	strong bireflectance	0
	Batisivite	Ba Si Ti O V	Triclinic	weakly bireflected	0

geomaterials_cleavagetype	***name***	***elements***	***csystem***	***cleavage***	***cleavagetype***
	Abelsonite	Ni N C H	Triclinic	Probable on <mi>{11_1}</mi>.	Poor/Indistinct
	Abenakiite-(Ce)	Ce Na Si O P C S	Trigonal	{0001}	Poor/Indistinct
	Aikinite	Bi Cu Pb S	Orthorhombic	on {010}	Poor/Indistinct

Code and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_physical_prop_2.ipynb

Besides the above-mentioned, geomaterial records can be retrieved using wildcard names, specifying non-null fields of interest (whether the specified fields are empty), Mindat ID, mineral varieties, and more. These functions can sometimes greatly facilitate data retrieval needs. Some demo codes are as follows:

```
R> geomaterials_search_name("Quartz")
R> geomaterials_name("qu_rtz")
R> geomaterials_name("_u_r_z")
R> geomaterials_name("qu*")
R> geomaterials_field_exists("meteoritical_code",TRUE)
R> mindat_geomaterial(id=3337)
R> geomaterials_varietyof(3337)
R> geomaterials_entrytype(c('1'))
R> mindat_geomaterial_list(ids = c('3','3337'))
```

Table 5 shows the geomaterial records retrieved by wildcard name, non-null fields, Mindat ID, and entry type. A brief *(''), entrytype=7, fields = c ("name","* *description* of the function and the meaning of the arguments are also included. *short", "rock_parent","rock_parent2"))*

Table 5: Results*R>unique(rbind(geomaterials_contain_all_but_not_elems(c("Ni","S"),c('O')),geomaterials_contain_all_but_not_elems(c("Ni","S"), c('O'))))*

With appropriate combination of geomaterial records retrieved by wildcard names, non-null fields, and entry type

Function name & its brief description	Head 3 records of some selected fields		
geomaterials_search_name		***id***	***name***
Input: "Quartz", a full name of geomaterials **Output**: The records that match or contain the input full name		1877	\Herkimer-style\" Quartz"
		6124	α-Quartz
		10773	Alpha-Quartz
geomaterials_name		***id***	***name***
Input: "qu_rtz". **Output**: records of geomaterials whose names match the input 6-character wildcard names, where the third character were arbitrary.		3337	Quartz
		6747	Quertz
Input: "_u_r_z". **Output**: records of geomaterials whose names match the input 6-character wildcard names, where the first, third, and fifth characters were arbitrary.		3337	Quartz
		6747	Quertz
Input: "qu*". **Output**: records of geomaterials whose names had the first two characters matched the input two characters (i.e., q and u).		3335	Quadridavyne
		3336	Quadruphite
		3337	Quartz
geomaterials_field_exists	***id***	***name***	***meteoritical_code***
Input: "meteoritical_code", a field of geomaterials. TRUE, Boolean value. **Output**: records of geomaterials that had non-null values of the field "meteoritical_code".	11263	Lodranite meteorite	Lodranite
	49515	Chondrite meteorite	Chondrite-uncl
	49517	Chondrite-fusion crust meteorite	Chondrite-fusion crust
mindat_geomaterial		***id***	***name***
Input: id=3337 or 3337, specify a mindat id.**Output**: records of geomaterials that had the same mindat id as the input id.		3337	Quartz
		3337	Quartz
geomaterials_varietyof	***id***	***name***	***varietyof***
Input:3337, which is the mindat id of Quartz. **Output**: records of geomaterials that were varieties of Quartz.	198	Amethyst	3337
	398	Star Quartz	3337
	436	Aventurine	3337
geomaterials_entrytype	***id***	***name***	***entrytype***
Input: 2, an integer.**Output**: records of geomaterials that match the input entry type, which can be one value of below:0: mineral;	8	Absite	2
	12	Acarbodavyne	2
	22	Adamsite	2

1: synonym; 2: variety;3: mixture; 4: series; 5: grouplist; 6: polytype;7: rock; 8: commodity				
mindat_geomaterial_list	***id***	***longid***	***name***	
Input: ids = c ('3','3337'), a list of mindat IDs. **Output**: records of geomaterials with the same Mindat ID as the input ID list.	3	1:1:3:3	Abernathyite	
	3337	1:1:3337:0	Quartz	

Code and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_wildcar_names.ipynb

Lastly, the packageproperties, a single function can also retrieve geomaterial datasets based on combined conditionssupport complex data request needs. For example, if we would likeneed to retrieve an records of the IMA-approved minerals record, containing elements lithium (Li) and oxygen (O,) elements, with Mohs hardness between 5.8 and 6, and in thehave a triclinic crystal structure,. We can use the following function can be used:code. **Table 4** shows the returned geomaterial records.

R> geomaterials_contain_all_elems(c('Li','O'), hardness_min = 5.8, hardness_max = 6, crystal_system = "Triclinic", ima_status = "APPROVED",", ", entrytype = 0)

Table 6 shows the retrieved records matching those conditions. Users can choose a related function as the main query function (e.g., the "geomaterials_contain_all_elems" function). Then additional conditions can be added to the main query function according to the actual data needs and conditions. The field names in the additional conditions can be seen in the online Mindat API document (https://api.mindat.org/schema/redoc).

Table 6: Results of geomaterial records retrieved by combined conditions

Table 4: Results of geomaterial records retrieved by combined properties

Function Name & input description / ***Name***	***Head 3 records of Records (only some selected relevant fields are shown)*** ***id***	***name***	***elements***	***hmin***	***hmax***	***csystem***	***ima_status***	***entrytype***
geomaterials_contain_all_elems	189	Amblygonite	"Al", "Li", "O", "P", "F"	5.5	6	Triclinic	"APPROVED", "GRANDFATHERED"	0
Input: c('Li','O'), contain Li and O elements.	670	Bikitaite	"Al", "Li", "Si", "O", "H"	6.0	6	Triclinic	"APPROVED", "GRANDFATHERED"	0
hardness_min = 5.8 and hardness_max = 6, crystal_system = "Triclinic", crystal structure is Triclinic. ima_status =	2417	Lithiomarsturite	"Ca", "Li", "Mn", "Si", "O", "H"	6.0	6	Triclinic	"APPROVED"	0

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"APPROVED", IMA approved. entrytype = 0, entrytype is mineral. **Output**:Geomaterials records that matched the combined conditions.						
Montebrasite	"Al", "Li","O", "H"	5.5	6	Triclinic	"APPROVED", "GRANDFATHERED"	0
Natronambulite	"Na", "Li", "Mn", "Ca", "O","H"	5.5	6	Triclinic	"APPROVED"	0

Code and results shared on GitHub:
https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_combined_conds.ipynb

4.2 Localities

The current package supports Mindat locality dataset retrieval by using country name, Mindat ID, element inclusion relationship, and other conditions. Some example codes are given below：

R> localities_list_country ("China")
R> localities_retrieve_id(id = 22)
R> localities_list_description("volcano")

As shown in **Table 7**, users can easily retrieve the locality records by a given country through the function “localities_list_country”. The current API will return Mindat locality records containing 37 fields, among which commonly used fields including id, country, txt (text), latitude, longitude, element, age, level, etc. Mindat locality follows a specific hierarchical structure and naming rules; users can refer to this link: https://www.mindat.org/a/localityhierarchies. The “latitude” and “longitude” fields record the coordinates of a locality, and the “txt” field records a text string of locations that follows the hierarchy described above. The number of locality levels reflects the level of detail of the address. The larger the value, the more specific the address information is. Thus, 0 is the top level and usually represents a country, a region, or a tectonic plate. The field “description_short” briefly introduces the locality. Users can retrieve records of terms contained in the “description_short” field using the “localities_list_description” function. The field “element” records the elements of the locality, that is, the list of elements in all the mineral species found at this locality. Users can quickly obtain records of “contains”, “does not contain”, and “contains but does not contain” chemical element relationships through the “localities_list_elems_inc”, “localities_list_elems_exc”, and “localities_list_elems_inc_exc” functions respectively. The "age" field of Mindat Locality records the "age_id" of a locality age. In addition, although the current locality record does not include a mineral list, we are aware of the needs of many users. We are planning to implement it in a future extension.

3.2 Locality data retrieval

Users can apply the package to retrieve locality data as needed. **Table 5** lists some use cases. Once the locality dataset is retrieved, many other third-party packages and functions in the R environment can be leveraged in data visualization and analysis. For example, we can use a map window to view the spatial distribution of minerals containing certain elements (e.g., As) or geomaterials containing certain literal descriptions (e.g., volcano) (**Figure 2**).

Table 75: Locality records retrieved by different inputting conditionsdata retrieval use cases

Function category		***Function name & descriptionInput***	***Head 3 records of some selected fieldsOutput & Description***			*Demo codes & Results*			
Name, ID, and Description		localities_list_country **Input**: “ ("China”, a country name. **Output**: The localities records occur or are within the specified country. A total of 10026 records returned.")	idRecords of localities of China			countryhttps://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Localities_by_desc.ipynb	***element***	***latitude***	***longitude***	***level***	***Txt***
693	China	Ag S Fe Se Ca Mg Si O H As Zn Al K Na Ti C Ce Nd Y F Bi Cu Pb Cl Hg Mn Th Te La Sb Co Ba Li P Sr Ru Ni Au Be Pd Ge Nb Sn U Pt Tl Zr B Mo Ta Rh V Br N Cr Ir In Os W Cs Cd Hf I Sc Ga Rb	0	0	0	China			
694	China	Ca Fe Mg Si O Al Ti K F H C Cl P Cr Cu Na Ni S Zn	33.83333	115.83333	5	Boxian meteorite, Xiaoyanzhuang, Qiaocheng District, Bozhou, Anhui, China			

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695	China	Ag S Ca Fe Mg Si O H Mn Al Na Bi Pb Te Sb C As Ni Cl Cu Ba Ti K F B Be Sn Co Sr Zn Cr Hg U Au Cd Mo P W Li Ta Zr	3 3 3 0	3 3 3 0	2	Haixi Mongol and Tibetan Autonomous Prefecture, Qinghai, China		
localities_retrieve_id(id = 22)		Records of localities_retrieve_id **Input**: " in Algeria (The 22", Mindat Id. **Output**: is the locality matches the input ID. of Algeria).	*id*	***country***	***element***	***latitude***	***longitude***	***level*** ***Txt***
22	Algeria	As Ba Fe O H	36.5213888889	7.295	4	Djebel Debar, Roknia, Hammam Debagh District, Guelma Province, Algeria		
localities_list_description **Input**: "("volcano", an enter terms that must be contained in the descriptive text (i.e., field of description_short). **Output**: records of localities that matched the input string. A total of 1729 records return. ")		*id*Records of localities with its descriptions containing the word "volcano".	***country***	***element***	***latitude***	***longitude***	***level***	***Description_short***
chemical elements'	38localities_list_elems_inc(c("Dy"))	Antar	Al Ca Fe Mg Na Si O K S H	-77.	167.	4	Ross Island is an island formed by four volcanoes in the Ross Sea near	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Localities_by_elems.ipynb

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inclusion and exclusion relationships		etiea	Cl-C-Ti-F-P-Au-Mn-	52608838	0800781		the continent of Antarctica, off the coast of Victoria Land in McMurdo Sound. Ross Island lies within the boundaries of Ross Dependency, an area of Antarctica claimed by New Zealand.Records of localities that contain the Dysprosium (Dy) element.
	113localities_list_elems_inc_exc(c("Dy"), c("Li"))	Australia	-Fe-Na-Si-O-Ti-Al-H-Ca-Mg-Cl-Zr-K-	-31.315	149.185	4	The shield volcano that made the Warrumbungle ranges was active about 13-17 million years ago. The volcano had a roughly circular outcrop 50 km in diameter, but is now heavily eroded and dissected, with prominent sub-volcanic dykes (Duggan 1989).Records of localities containing Dysprosium (Dy) but no lithium (Li).
Locality age	locality_age_list()						All records of locality age.
	120locality_age(id = 60)	Australia	-Ca-Fe-Mg-Si-O-H-Al-Na-K-Be-Cl-Cu-P-U-C-Ba-S-Ti-F-Bi-V-Sn-Li-B-Nb-Y-Zn-Pb-Au-Ag-Mo-Mn-	-22.986666667	134.920868333	3	Harts Range is about 190 kilometres by dirt road (Stuart and Plenty Hwys) north-east of Alice Springs. Areas most accessible and interesting tend to be along the northern limits of the ranges. The eastern and southern sections can be accessed by a trac...Records of locality age with its locality ID is 60.

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W-Ta-Th-
Zr-

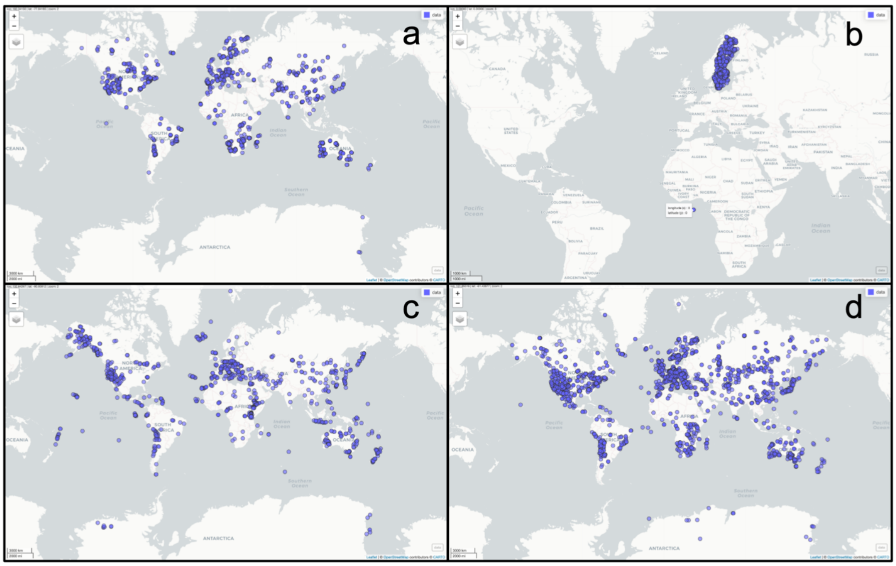

Figure 2: Mapping locality records retrieved by the OpenMindat R package: (a) As-containing minerals, (b) localities in Sweden, (c) locality descriptions containing 'volcano', and (d) type localities of IMA-approved minerals. Base map © OpenStreetMap contributors 2024. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

3.3 IMA mineral list retrieval

This package can support the record retrieval according to their IMA status. **Table 6** lists some basic use cases. We can also use some other functions to validate alternative mineral/rock names. For example, if the name 'amethyst' is input, it would return that the correct mineral species is 'quartz' and 'amethyst' is a varietal name (Ma et al., 2023). We can use the following code to realize that need.

```
R> df_gm_amethyst <- geomaterials_name("Amethyst")
```

Note: code and results: https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Localities_by_desc.ipynb

In addition to the above locality record retrieval functions, the locality age, status, type, and other fields can also be used to filter records from the Mindat API. However, there are some limitations due to the safety protection set on the API server to reduce extremely heavy data outputs. Our R package currently only implements some functions related to the locality age. For example:

R> localities_list_elems_exc(c("H", "O", "Si", "Al", "Fe", "Ca", "Na", "K", "P", "C", "Mn", "F", "Mg", "S"))

395 *R> R> mindat_geomaterial_list(ids = c(df_gm_amethyst $varietyof), entrytype=0, ima_status = "APPROVED")*

Table 6: Use cases of IMA mineral list retrieval

Function category	***Function name & Input***	***Output & Description***	***Demo codes & Results***
IMA status, ID	minerals_ima_list()	Records of all IMA-approved mineral species with detailed properties	https://github.com/quexiang/OpenMindat/blob/main/notebook/IMA_minerals.ipynb
	minerals_ima_list_ima(1)	Records of minerals that IMA-approved status is Approved.	
	minerals_ima_retrieve(2)	Records of Abenakiite-(Ce) (2 is the Mindat ID of Abenakiite-(Ce)).	

The functions in the OpenMindat package can be used together with many other packages and functions in the R environment to achieve
400 data exploration or analysis needs, and many of them require just a few rows of code. For example, we can retrieve and visualize the top 10 IMA-approved mineral species (by occurrence count) found in a country, such as Canada (**Figure 3**). To achieve that, we need to perform the following steps: (1) Execute the OpenMindat function "localities_list_country("Canada",expand = "~all")" to retrieve the list of localities in Canada and the lists of geomaterials recorded in each locality, which is currently stored in the "locentries" field of locality, and can only be accessed by adding the "expand" parameter. (2) Summarize the number of occurrences of each geomaterial ID and sort in descending
405 order. (3) Check each geomaterials ID to see if it is an IMA-approved mineral, and if so, retrieve the corresponding record by using the "minerals_ima_retrieve" function. The code and results of this example are shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Top10_IMA-Approved%20Minerals%20in%20a%20specified%20country(e.g.%20Canada).ipynb.

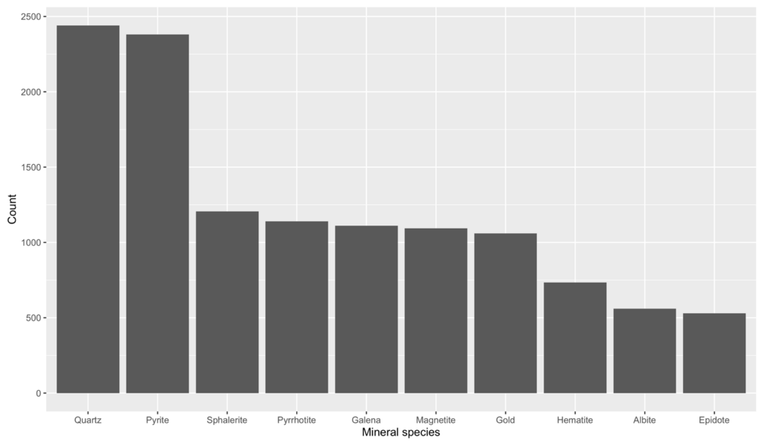

Figure 3: Top 10 IMA-approved mineral species found in Canada.

3.4 Output the retrieved data into *localities_list_elems_inc(c("Dy"))*

R> localities_list_elems_inc_exc(c("Dy"), c("Li"))

R> locality_age_list()

R>locality_age(id = 60)

As shown in **Table 8**, the locality age records can be retrieved by the "locality_age_list" function, and the results showed that the geological time interval of a locality was recorded via the "age_mav" and "age_ma2v" fields. The "age_id" is the unique identifier associated with the locality and locality age, i.e., if a locality has its corresponding locality age, then the "age_id" of locality age will be recorded in the "age" field. The field "agemethod" recorded the method used to obtain the estimated geological time.

Table 8: Results of locality records retrieved by status, age, type, and a few other fields

Function name & its brief description	***Head 3 records of some selected fields***					
localities_list_elems_exc	***country***	***elements***	***latitude***	***longitude***	***level***	***Txt***
Input: c ("H", "O", "Si", "Al", "Fe", "Ca", "Na", "K", "P", "C", "Mn", "F",	Afghanistan	-	0	0	2	Mohammad Agha District, Logar, Afghanistan

"Mg", "S"). **Output**: records of localities that do not contain the input elements. A total of 223622 records returned.	Australia	-Au-	-30.23207267	151.8779073	4	Aberfoyle River deep lead, Aberfoyle River, Clarke Co., New South Wales, Australia
	Australia	-Ag-Cl-	-36.5889328	143.244155	4	Silver Mines (Silver Reef), St Arnaud, Northern Grampians Shire, Victoria, Australia
localities_list_elems_inc **Input**: c("Dy"), elements that the localities contain. **Output**: records of localities that include the input elements. 9 records returned.	Germany	-As-O-K-H-U-Ag-S-Ca-Fe-Mg-Si-Zn-Al-Na-Cu-Nd-Y-Ce-Dy-La-Bi-Pb-Cl-Sb-Co-N-Ti-C-Ni-Be-Sr-Ba-Ge-F-Mn-Au-P-Zr-Se-Br-V-Sn-Nb-Cr-Hg-Li-W-B-Th-Cd-Tl-I-Mo-	0	0	1	Baden-Württemberg, Germany
	Germany	-Ag-S-As-Fe-Al-O-F-H-U-Ca-P-Ba-Na-Si-Bi-Cu-C-Y-Pb-Se-K-Li-Mg-Au-Co-Nd-N-Ni-Mn-Zn-W-Dy-	47.83888889	8.048888889	0	Krunkelbach Valley Uranium deposit, Menzenschwand, St Blasien, Waldshut, Freiburg Region, Baden-Württemberg, Germany
	Germany	-As-O-K-H-U-Ag-S-Zn-Cu-Nd-Y-Ce-Dy-Bi-Pb-Co-Fe-Al-Si-Ti-Ca-C-Ni-F-Mn-Ba-Mg-Cl-Hg-Na-P-Sb-Mo-N-	48.33810891	8.343429565	5	Wittichen, Schenkenzell, Rottweil, Freiburg Region, Baden-Württemberg, Germany
localities_list_elems_inc_exc **Input**: c("Dy"), elements that the localities contain. c("Li"), elements that the localities does not contain. **Output**: records of localities that match the input condition.3 records returned.	Germany	-As-O-K-H-U-Ag-S-Zn-Cu-Nd-Y-Ce-Dy-Bi-Pb-Co-Fe-Al-Si-Ti-Ca-C-Ni-F-Mn-Ba-Mg-Cl-Hg-Na-P-Sb-Mo-N-	48.33810891	8.343429565	5	Wittichen, Schenkenzell, Rottweil, Freiburg Region, Baden-Württemberg, Germany
	Germany	-As-O-K-H-U-Ag-S-Ca-Fe-Mg-Si-Zn-Cu-Nd-Y-Ce-Dy-Bi-Pb-Co-Al-Ti-C-Ni-F-Mn-Ba-Cl-Hg-Na-P-Sb-Mo-	0	0	4	Schenkenzell, Rottweil, Freiburg Region, Baden-Württemberg, Germany
	Germany	-As-O-K-H-U-Ag-S-Ca-Fe-Mg-Si-Zn-Cu-Nd-Y-Ce-Dy-Bi-Pb-Co-Al-Ti-C-Ni-F-Mn-Ba-Cl-Be-Hg-Na-P-Sb-B-Mo-	0	0	3	Rottweil, Freiburg Region, Baden-Württemberg, Germany

locality_age_list	***age_id***	***age_mav***	***age_ma2v***	***agemethod***
	3	170.3	157.3	K/Ar
	17	4574.7	4574.7	Pb-Pb isochrons

	36	590	590	Pre-1977 K-Ar, Ar-Ar and Rb-Sr ages recalculated using the decay constants of Steiger and Jager (1977)
locality_age	60	717.4	660	Re-Os

Code and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Localities_by_elems.ipynb

4.3 IMA minerals

The R package makes retrieving an IMA-approved mineral list relatively easy. The code below shows how to retrieve IMA minerals in a whole list, by their status, or by ID. Table 9 lists a few fields in the results. The field "type locality" denotes where the original material came from for the formal definition of the mineral species.

```
R> minerals_ima_list()
R> minerals_ima_list_ima(1)
R> minerals_ima_retrieve(2)
```

Table 9: Results of IMA minerals records retrieved by different constraint conditions

Function name	*Head 3 records of some selected fields*				
minerals_ima_list	***name***	***Type_localities***	***ima_formula***		***ima_status***
	Abelsonite	39262	NiC₃₁H₃₂N₄		APPROVED
	Abenakiite-(Ce)	599	Na₂₆Ce₆(Si₆O₁₈)(PO₄)₆(CO₃)₆(SO₂)O		APPROVED
	Abernathyite	4145	K(UO₂)(AsO₄) · 3H₂O		c("APPROVED","GRANDFATHERED")
minerals_ima_list_ima(1)	***name***	***Type_localities***	***mindat_formula_note***	***ima_status***	***ima_formula***
	Paramolybdomenite	333762	PbSeO₃	c("APPROVED", "PENDING_PUBLICATION")	
	Mckelveyite-(Nd)	435543	NaCaBa₃Nd(CO₃)₆·3H₂O	c("APPROVED", "PENDING_PUBLICATION")	NaCaBa₃Nd(CO₃)₆ · nH₂O

~~*minerals_ima_retrieve(2)*~~	~~*id*~~	~~*name*~~	~~*mindat_formula*~~	~~*ima_status*~~	~~*elements*~~	~~*sigelements*~~
	~~Naalasite~~	~~190910~~	~~NaAl(AsO₃OH)₂·H₂O~~	~~c("APPROVED", "PENDING_PUBLICATION")~~		
	~~2~~	~~Abenakiite-(Ce)~~	~~Na₂₆Ce₆(Si₆O₁₈)(PO₄)₆(CO₃)₆(SO₂)O~~	~~APPROVED~~	~~Ce~~	~~Ce~~
	~~2~~	~~Abenakiite-(Ce)~~	~~Na₂₆Ce₆(Si₆O₁₈)(PO₄)₆(CO₃)₆(SO₂)O~~	~~APPROVED~~	~~Na~~	~~Na~~
	~~2~~	~~Abenakiite-(Ce)~~	~~Na₂₆Ce₆(Si₆O₁₈)(PO₄)₆(CO₃)₆(SO₂)O~~	~~APPROVED~~	~~Si~~	~~Si~~

~~Code and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/IMA_minerals.ipynb~~

~~4.4 Output files in~~ different formats

~~The current R package supports users in outputing~~ Users can output their retrieved data in ~~various formats, including~~ a specified format, such as CSV, JSON, TXT, JSON-LD, and TTL. The function "saveMindatDataAs" will identify the suffix of the ~~output~~input file name and ~~then~~ convert the retrieved R data frame into ~~the~~a corresponding format. For the data conversion to the JSON-LD and TTL formats, ~~the~~ two Excel template files (i.e., OpenMindat_Schema_JSON-LD.xlsx and OpenMindat_Schema_TTL.xlsx) ~~were~~are required~~, which can be accessed via https://github.com/quexiang/OpenMindat/tree/main/inst/extdata.~~. Users can configure their settings in the Excel template to customize files that meet their needs for the output. The default versions can be accessed via https://github.com/quexiang/OpenMindat/tree/main/inst/extdata. Here, we take the JSON-LD template as an example to briefly introduce its basic settings (similar template settings in TTL format). ~~own needs for the output. Here, we take the JSON-LD template as an example to briefly introduce its basic settings (similar template settings in TTL format). Two Excel~~There are two sheets ~~are~~ in the template file; the first one is ~~about~~for the context settings~~. **Table 10**~~ and the other one is for the field setting. **Table 7**（i.e., the first sheet) shows the names of all schemas and how their corresponding URLs are configured. ~~The other concerns are field settings, as shown in Table 11~~**Table 8** shows the second sheet, where "fields" record the field names that need output corresponding to the Mindat API. ~~In this sheet, the~~The "ref_fields" records the output field name list of JSON-LD, "context_name" records all schema names corresponding to the field, and "type" records the type of schema to which the field belongs. All the values of the three fields are in the form of a list, separated by commas. Besides, the "ref_field_num" indicates which name is to be output in JSON-LD (e.g., 1 represents the name before the first comma of "ref_fields").

Table ~~10~~7: Context settings of the JSON-LD template

context_name	***context_url***
mindat	https://mindat.org/
schema	https://schema.org/
gsog	https://w3id.org/gso/geology/

Table ~~11~~8: Field settings of the JSON-LD template

fields	***ref_fields***	***context_name***	***type***	***ref_field_num***
id	mindat:id, ,	mindat,schema,gsog	mindat:Geomaterials,schema:Dataset,gsog:Mineral_Material	1
longid	identifier, ,	mindat,schema,gsog	mindat:Geomaterials,schema:Dataset,gsog:Mineral_Material	1
name	mindat:name, ,	mindat,schema,gsog	mindat:Geomaterials,schema:Dataset,gsog:Mineral_Material	1
ima_formula	mindat:ima_formula, ,	mindat,schema,gsog	mindat:Geomaterials,schema:Dataset,gsog:Mineral_Material	1

The full JSON-LD template share on GitHub:
https://github.com/quexiang/OpenMindat/blob/main/inst/extdata/OpenMindat_Schema_JSON-LD.xlsx

~~According to~~With the above configuration, we can obtain the exported file shown in **Table ~~12~~9** by executing the following code~~: ~~.

```
R> library(readxl)
R> saveMindatDataAs(geomaterials_hardness_gt(9.8, fields = "id,longid,name ,ima_formula"),"df_geomaterials.jsonld ")
```

Table ~~12~~9: Output file in JSON-LD format

df_geomaterials.jsonld


```
{
 "@context": {
          "mindat":"https://mindat.org/",
          "schema":"https://schema.org/",
           "gsog":"https://w3id.org/gso/geology/"},
"@graph": [{"@type": ["mindat:Geomaterials " ,  "schema:Dataset " ,  gsog:Mineral_Material "] ,
                    " mindat:id ":" 1282 ",
                    " identifier ":" 1:1:1282:5 ",
                    " mindat:name ":" Diamond ",
                    " mindat:ima_formula ":" C "
           }
```

```
, {"@type": ["mindat:Geomaterials " ,  "schema:Dataset " ,  gsog:Mineral_Material "] ,
        " mindat:id ":" 43792 ",
        " identifier ":" 1:1:43792:7 ",
        " mindat:name ":" Qingsongite ",
        " mindat:ima_formula ":" BN "
 } ,
{"@type": ["mindat:Geomaterials " ,  "schema:Dataset " ,  gsog:Mineral_Material "] ,
        " mindat:id ":" 52913 ",
        " identifier ":" 1:1:52913:0 ",
        " mindat:name ":" Uakitite ",
        " mindat:ima_formula ":" VN "
 }
 ]
}
```

Code and results shared on GitHub: https://github.com/quexiang/OpenMindat/blob/main/notebook/Output_DF2File.ipynbhttps://github.com/quexiang/OpenMindat/blob/main/notebook/Output_DF2File.ipynb

5 Discussion

We have fully implemented the designed architecture of the OpenMindat R package and built examples for almost all the developed functions. The3.5 Package releases, scientific applications, and update

The OpenMindat R package and its source code were shared on GitHub (https://github.com/quexiang/OpenMindathttps://github.com/quexiang/OpenMindat), together with detailed tutorials on how to install and run the package in the R environment (https://quexiang.github.io/OpenMindathttps://quexiang.github.io/OpenMindat). The first version of this R package (version 1.0.0) was also released in the comprehensive R archive network (CRAN) (Hornik, 2012) (https://cran.r-project.org/web/packages/OpenMindat) on February 15, 2024. A list of Jupyter Notebook files (https://github.com/quexiang/OpenMindat/tree/main/notebook), including those shown in the previous section, was also shared to demonstrate the functions and parameters for data query and access from the Mindat API.

What we presented above was from the perspective of the software developers to illustrate the architectural design, the data availability, and the functionality of the OpenMindat R package.https://cran.r-project.org/web/packages/OpenMindat) on February 15, 2024. Scientists can use those functions flexibly to conduct scientifically meaningful data queries and access tasks. A big advantage of using the OpenMindat Rthis package is that it reduces the scientists' efforts on coding, i.e., with relatively minor coding, they can retrieve a specific piece of data from the Mindat API. For example, using the package, the four use cases discussed by Ma et al. (2023) can each be realized with just a few lines of R code.A list of examples and their Jupyter Notebook files (https://github.com/quexiang/OpenMindat/tree/main/notebook), including those shown in the previous section, was also shared to demonstrate the functions and parameters for data query and access from the Mindat API. Readers can also refer to the Data and Code Availability section at the end of the article for a structured list of weblinks to all those resources mentioned above.

4 Discussion

The development of the OpenMindat R package provides geoscientists with a user-friendly, efficient, and reproducible tool for accessing and analyzing mineralogical data from Mindat. By wrapping the capabilities of the Mindat API into structured functions, the package overcomes barriers faced by researchers working with large-scale datasets. One of the primary advantages of the OpenMindat R package is its ability to simplify data access for geoscientists. Previously, obtaining bulk data from Mindat required manual interventions with the webpages or complex API queries that demanded advanced coding skills. The package eliminates these obstacles by providing predefined functions centered on data subjects, such as geomaterials and localities, enabling users to retrieve datasets with minimal effort. This accessibility is particularly beneficial for geoscientists who may not have extensive programming skills but rely on large datasets to drive their research. The package's ability to export data in multiple formats ensures compatibility with various analytical workflows. These formats are widely used across disciplines, allowing researchers to seamlessly integrate Mindat data into existing pipelines for visualization, statistical modeling, and geospatial analysis.

The OpenMindat R package embodies the principles of Findable, Accessible, Interoperable, and Reusable (FAIR) data. By providing an intuitive interface to the Mindat API, the package ensures that mineralogical data are not only accessible but also easily integrated into diverse analytical workflows. This alignment with FAIR principles fosters a culture of openness and collaboration in the geosciences, where shared resources and tools can accelerate innovation. Reproducibility is a cornerstone of scientific research, as the concept of open science is increasingly accepted in the global geoscience community. The OpenMindat R package enhances this by allowing users to embed data retrieval processes directly into their R scripts. By automating the translation of user queries into API requests, the package ensures that data retrieval steps are transparent and replicable. This transparency not only strengthens the reliability of results but also facilitates collaboration among researchers. Shared R scripts or R Markdown documents can precisely reproduce datasets, fostering greater trust in geoscientific analyses. Accordingly, we envision the Mindat open data API and the R package as a catalyst for data-driven discoveries in mineralogy and many other related geoscience disciplines. By providing a structured and efficient interface to the Mindat database, the package empowers researchers to explore complex relationships within mineralogical data. Moreover, the package's integration with R's extensive suite of analytical tools enables advanced applications such as network analysis, clustering, and predictive modeling. Researchers studying critical minerals, for instance, can use the package to analyze the geographic and paragenetic distributions of these resources, supporting strategies for sustainable extraction and utilization.

The Mindat open data API is maintained by the Mindat technical team. They review and permit user registration requests, monitor the status of the server, and defend cyber-attacks or malicious mass downloads. For individual researchers, the default API usage limit is 1,000 requests per hour. Based on our experience in the past two years, that should be enough to meet the needs of most people. Specific users who need more frequent and larger data access can contact the Mindat technical team for permission. The Mindat technical team is planning a hardware upgrade to the server in early 2025, which will further stabilize the API. It is also noteworthy that the computational efficiency of the OpenMindat R package reduces the time and effort required for data retrieval and processing on the server side. By leveraging the API's pagination capabilities, the package ensures smooth handling of large datasets without overloading system memory. The caching mechanism further enhances efficiency by minimizing redundant queries, a critical feature for workflows involving iterative analyses. Scalability is another key strength. As geoscientific studies grow increasingly data-intensive, the ability to handle complex, multi-condition queries becomes necessary. The package's flexibility to combine various conditions, such as element inclusion, locality attributes, and IMA status, enables users to conduct sophisticated analyses tailored to specific research questions.

Looking into the future, we are confident about the broad variety of scientific applications enabled by the Mindat API and the OpenMindat R package. In mineral evolution studies (Hazen et al., 2008; Hazen et al., 1. Retrieve a full list of all IMA-approved mineral species with detailed properties:

```
R> df_ima_minerals <- minerals_ima_list()
```

2. Retrieve a list of mineral species matching certain chemical criteria, such as 'mineral species containing nickel or cobalt, with sulphur but without oxygen':

```
R> df_Ni_S_without_O<- geomaterials_contain_all_but_not_elems(c("Ni","S"), c('O'))
R> df_Co_S_without_O<- geomaterials_contain_all_but_not_elems(c("Ni","S"), c('O'))
R> df_Ni_or_Co_and_S_without_O<- unique (rbind (df_Ni_S_without_O, df_Co_S_without_O))
```

3. Validate alternative mineral/rock names. For example, if the name 'amethyst' is sent, then it would return that the correct mineral species is 'quartz', and that 'amethyst' is a varietal name:
2014), for example, the package can facilitate analyses of temporal and spatial patterns in mineral diversity, shedding light on the co-evolution of Earth's geosphere and biosphere (Hazen et al., 2014; Hazen and Morrison, 2020). In mineral ecology (Hazen et al., 2015), researchers can use the package to investigate statistical relationships between mineral species and their

geological contexts, contributing to predictive models of mineral formation and distribution. The package also holds promise for cross-disciplinary collaborations. By integrating mineralogical data with environmental, economic, and social datasets, researchers can address pressing global challenges such as critical mineral supply chains and sustainable resource management.

R> df_gm_amethyst <- geomaterials_name("Amethyst")

R> df_ima_mineral_name <- mindat_geomaterial_list(ids = c(df_gm_amethyst $varietyof), entrytype=0, ima_status = "APPROVED")

4. Provide a hierarchical taxonomy of petrological names and their definitions (e.g., get the rock hierarchy information):

R> df_gm_rock_parent <- mindat_geomaterial_list(ids = c(''), entrytype=7, fields = c("name","description_short", "rock_parent","rock_parent2"))

Once the dataset is retrieved, many other packages and functions in the R environment can be leveraged in data visualization and analysis. Visualizing georeferenced records, such as localities in a map window, is straightforward. **Figure 2** shows a few examples.

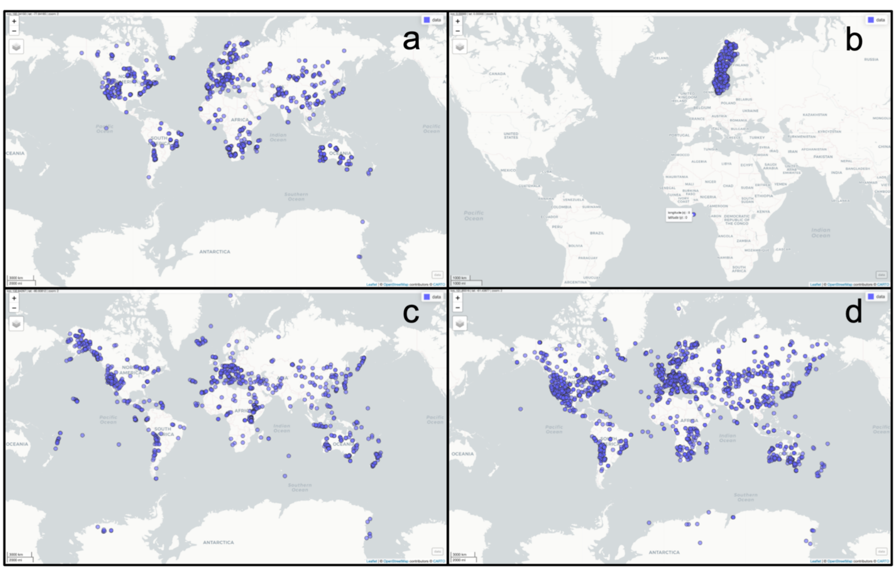

Figure 2: Mapping locality records retrieved by the OpenMindat R package: (a) As-containing minerals, (b) localities in Sweden, (c) locality descriptions containing 'volcano', and (d) type localities of IMA-approved minerals. Base map © OpenStreetMap contributors 2024. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

The Mindat API is constantly upgrading to release more data subjects and fields. Accordingly, we will revise the classes and functions in the OpenMindat R package. We also collect users' feedback on the Mindat API and the package (from the Mindat online forum, Slack channels, and direct emails) and incorporate them into our development plans. For example, when this paper was under preparation in November and December of 2023, the Mindat API did not provide access to the mineral occurrence records (due to heavy data records and concerns about workloads added to the data server). That puts limitations on certain data query conditions. For example, it could not retrieve "minerals that contain cobalt but not oxygen and are found in South Africa or Zambia". The Mindat API technical team (led by Jolyon Ralph) was aware of the users' needs on mineral occurrence records and has been working on an extension to the API to open the data correctly. Once that extension is fully implemented on the API, we will also make extensions to the R package, such as functions to query locality records of certain mineral species or vice versa.

We can envision a broad variety of applications based on the Mindat API and the OpenMindat R package, such as those in mineral evolution (Hazen et al., 2008; Hazen et al., 2014), mineral ecology (Hazen et al., 2015), and the co-evolution of geosphere and biosphere (Hazen et al., 2014; Hazen and Morrison, 2020). According to the discussion on mineral informatics (Prabhu et al., 2023), the work plan of the OpenMindat project (Ma et al., 2024; Que et al., 2024), and the vision of the Deep-time Data-Driven Discovery (4D) Initiative (4D Initiative, 2019), a cyberinfrastructure ecosystem based on many open geoscience data resources (including Mindat) will gradually be built to facilitate data-driven discoveries. This includes the databases, software packages, use cases, and many training activities. Some preliminary work has been implemented. For example, based on the Mindat API and the OpenMindat R package, we recently built an R Shiny app that uses adjacency matrices to explore a variety of correlations in mineral properties, occurrences, and associations (Que et al., 2024). It is foreseeable that, as part of this cyberinfrastructure ecosystem, the machine-readable Mindat data, including this R package and the API, will play an increasingly active role in data-intensive studies.is the foundation to facilitate data-driven discoveries, and the work presented in this paper is a building block for that ecosystem.

6

Despite its benefits and potentials, the OpenMindat R package faces certain limitations and needs further extension. For instance, the current version does not friendly support queries involving mineral occurrences due to restrictions in the Mindat API. This limitation constrains studies that require detailed spatial analysis of mineral distributions. For example, retrieving "minerals that contain cobalt but not oxygen and are found in South Africa or Zambia" is almost impossible or may require complex commands for the current version of package. Additionally, some users may encounter challenges in navigating the package's advanced features, underscoring the need for more detailed tutorials, examples and user support. To address these issues, the development team is actively working on expanding the package's functionality. Planned updates include incorporating mineral occurrence records as the API evolves, enhancing the package's documentation, and developing interactive tutorials to guide users through complex queries. We are also collecting feedback from the geoscientific community to shape these improvements.

5 Conclusions

This paper ~~presents an R package called~~introduces the OpenMindat ~~for simple, fast, and~~R package, a tool designed to facilitate efficient data retrieval from Mindat, one of the world's largest databases for mineral species and their ~~distribution. This R package is of potentially significant use by various scientists because it bridges the data highway, connecting users' data requirements to the Mindat API server. The machine~~distributions. By providing a structured interface to the Mindat open data ~~enabled by~~API, the package ~~will accelerate~~simplifies the process of accessing and utilizing mineralogical data~~-driven geoscience discoveries, as many~~, making it more accessible to geoscientists ~~use~~who rely on the R programming environment ~~intensively in their work.~~

~~This work fills~~for data analysis and visualization. The OpenMindat R package addresses a gap ~~in leveraging technology to expand its underlying cyberinfrastructure ecosystem. The current R package meets most~~by enabling streamlined data retrieval ~~needs of Mindat, including retrieval of~~ for a variety of use cases. Its functionality includes querying geomaterials ~~according to~~based on chemical ~~properties,~~and physical properties, crystal structures, and ~~more. It also supports data retrieval of localities and IMA materials, and the built-in compound retrieval functions~~ other attributes, as well as accessing locality and IMA-approved mineral data. The package's support for multiple output formats ensures compatibility with a wide range of analytical workflows commonly used in geoscience research. Moreover, the availability of open and FAIR mineralogy data through this package aligns with broader efforts to enhance data-driven discoveries in the geosciences. By enabling researchers to integrate Mindat data into their workflows with greater efficiency, we hope the OpenMindat R package can provide solid support ~~a wide range of application requirements. Moreover, it enables bulk~~to data~~-retrieval~~-intensive research and ~~output~~foster innovation in ~~various formats, including CSV, JSON-LD, TXT, and TTL, which are popular amongst geoscientists.~~

~~Open and FAIR mineralogy data, in terms of~~ mineral informatics~~, will bring many advantages that revolutionize how we study and understand the Earth (Hazen, 2014; Hazen et al., 2019). Looking forward to the future, as~~. Continued development of both the Mindat API and the ~~OpenMindat R package gradually improve, we hope the Mindat open data will accelerate research and innovation in many research fields, enabling the development of~~ R package will further expand their utility, encouraging new ~~predictive models, analytical tools, and exploration strategies and leading to many new scientific discoveries~~research directions and collaborations in the geoscience community.

Code and Data Availability

The installation guideline, demos, and documentation of the OpenMindat R package v1.0.0 are accessible at https://cran.r-project.org/web/packages/OpenMindat (Que and Ma, 2024). The code for the OpenMindat R package v1.0.0 can be accessed at the Harvard Dataverse through its DOI: https://doi.org/10.7910/DVN/9NWCDK. The documentation of the Mindat open data API is available at https://api.mindat.org/schema/redoc/. The tutorial on obtaining and using the API token is accessible at: https://www.mindat.org/a/how_to_get_my_mindat_api_key.

The OpenMindat R package v1.0.0 is free and open source. The web links for its installation guidelines, source code, tutorials, examples, and related documentation are listed in Table 10.

Table 10: Online resources for the OpenMindat R package

name	***url***
CRAN OpenMindat R package v1.0.0	https://cran.r-project.org/web/packages/OpenMindat
Source code of the OpenMindat R Package	https://github.com/quexiang/OpenMindat/
Tutorials	https://quexiang.github.io/OpenMindat/
Examples	https://github.com/quexiang/OpenMindat/tree/main/notebook
Reference manual	https://cran.r-project.org/web/packages/OpenMindat/OpenMindat.pdf
How to setup Jupyter Notebook for R?	https://developers.lseg.com/en/article-catalog/article/setup-jupyter-notebook-r
How to get the Mindat API?	https://www.mindat.org/a/how_to_get_my_mindat_api_key
Description of Geomaterial fields	https://github.com/smrgeoinfo/How-to-Use-Mindat-API/blob/main/geomaterialfields.csv
Mindat API online documentation	https://api.mindat.org/schema/redoc/

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Author Contributions

Xiang Que: Conceptualization, Methodology, Software, Writing - Original Draft, Writing - Review & Editing; **Jiyin Zhang**: Methodology, Validation, Writing - Review & Editing; **Weilin Chen**: Validation, Writing - Review & Editing; **Jolyon Ralph**: Data Curation, Writing - Review & Editing; **Xiaogang Ma**: Conceptualization, Methodology, Funding acquisition, Validation, Writing - Review & Editing.

Competing Interests

The authors declare no competing interests.

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