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

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Abstract: Powered by technologies such as machine learning and deep learning, meaningful patterns are increasingly discovered in earth science big data. In the field of mineralogy, Mindat ("mindat.org") 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 10 2022. Through a project called OpenMindat, an application programming interface (API) to enable open data query and access from Mindat was set up 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 15 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. In real-world applications, these functions only require minor coding for users to get desired datasets, and various other packages in the R environment can be used to analyze and visualize the data. The OpenMindat v1.0.0 package is open on GitHub under the MIT license, together with detailed tutorials and examples. The field of mineralogy and many other geoscience disciplines are facing the opportunities enabled by open data. 20 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 can help accelerate those data-intensive studies and lead to more scientific discoveries.

1 Introduction

As machine learning and deep learning techniques thrive on their ability to discover complex patterns, data-driven geoscience 25 studies yield increasingly more exciting results (Hazen et al., 2011; Bergen et al., 2019; 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 quantitative methods to make informed predictions across varying contexts (Chen et al., 2023). Open access to large and diverse datasets is imperative for data-driven geosciences and calls for attention and actions (Hossain et al., 2016). 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) (Ralph et al., 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 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 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), and the records are actively expanding and updating.

Mindat is widely used by many individuals and 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. The Mindat team provides a website portal (https://www.mindat.org/advanced_search.php) for users to retrieve data by specifying parameters interactively. Although its website has always been open for searching and browsing datasets, a machine interface for Mindat data 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) was set up recently to implement a fully open access, machine-readable, and interoperable architecture for Mindat. Following the FAIR principles (i.e., findable, accessible, interoperable, and reusable) (Wilkinson et al., 2016), a roadmap of OpenMindat was laid out, including the technical approaches to upgrade and reuse existing data resources, tools, and infrastructure. 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 (Zhang, 2024). While the API (https://api.mindat.org) provides a structured and stable channel to the Mindat open data (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 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 such as R Studioand Jupyter, where many other packages can be used together for data analysis.

65   This paper presents our design and implementation of the 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.

2 Architecture of the OpenMindat R Package

The primary objective of the OpenMindat R package is to provide an implementation mechanism to translate users' data
70   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. **Table 1** lists the primary data subjects stored in Mindat and the number of their records.

Table 1: Primary data and the number of records stored in the Mindat database

Data subjects	Brief description	Number
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
occurrences	The links between the mineral data and the locality where they occur.	>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
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

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The API server manages Web requests for datasets. Currently, it provides a separate access endpoint for each data subject. While in the future, as the number of subjects and records in the crowdsourced Mindat database increases, the API server may open or update its data access endpoints. Some new features of our package will be updated according to the endpoints provided by the server. Accordingly, we designed an architecture (**Figure 1**) to connect the user's data needs with the Mindat API server
80   (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, most users' data requirements fall into the following categories: (1) Queries about geomaterials (i.e., mineral, rock, commodity, and other natural geological materials). Users need to filter the geomaterials based on their physical properties

(e.g., density, hardness, color, refractive index, and crystal structure); or on their chemical properties (e.g., element inclusion and exclusion states); or their entry 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 follows a specific hierarchical structure and naming rule (https://www.mindat.org/a/localityhierarchies). A simple explanation is that the number of locality levels indicates the level of detail in the locality hierarchy.. Larger value indicates more details t. 0 is the top level, usually representing a country, a region, or a tectonic plate. Users may need to query the localities based on their number of levels, attributes (e.g., name, country, ID, description, and longitude/latitude), coordinate information, or geological ages. For example,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. IMA promotes the science of mineralogy and standardizes the nomenclature of mineral species. The IMA mineral list is updated frequently, and it is common to query mineral information by specific IMA status, such as A (approved), G (grandfathered), Rd (redefined), and Q (questionable), 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 outputting filtered data in specified formats, such as CSV, TXT, TTL, JSON-LD, etc., for different use cases.
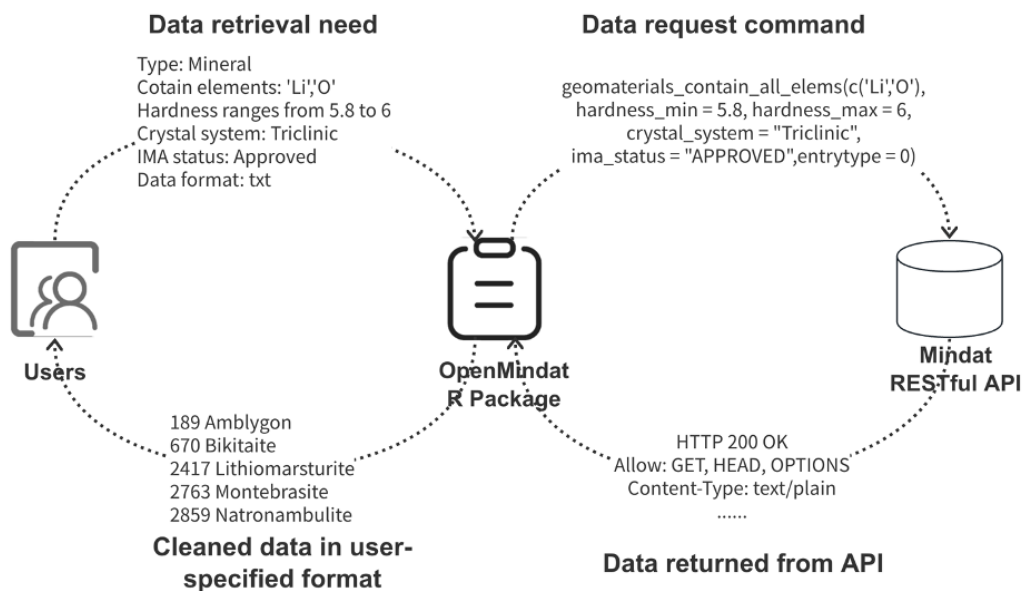
Figure 1: Architecture of the OpenMindat R package

Following the designed architecture and user need analysis, we developed about 100 functions in the R package (to view all the functions, execute "help (package = OpenMindat)" or see the reference manual listed in Table 10), and they are grouped

into several classes. Table 2 lists the main classes and functions related to data subjects and formats (A complete list of classes and functions is available via our online documentation on GitHub): (1) Geomaterials class, which is one of the main data subjects supported by Mindat API, includes sub-subjects of minerals, synonyms, varieties, mixtures, series, group lists, polytypes, rocks, and commodities. The current geomaterial record contains 146 attributes, including descriptions of physical properties, chemical information, optical properties, crystal structure information, and more. (2) Localities class. It consists of 37 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. (3) IMA Minerals class. This class is mainly for retrieving and managing IMA-approved mineral species names, 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.

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

Class	Functions	Brief description
Geomaterials	geomaterials_contain_any_elems	Retrieve geomaterials that contain any of the specified elements.
	geomaterials_cleavagetype	Retrieve geomaterials that matched the specified cleavage type.
	geomaterials_colour	Retrieve geomaterial matched the specified colours.
	geomaterials_crystal_system	Retrieve geomaterial matched the specified crystal system.
	geomaterials_bi_greater_than	Retrieve geomaterials that have higher birefringence than an 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	localities_list_country	Retrieve the localities list that are found in a specified country.
	localities_list_elems_inc	Retrieve the localities that contain the given elements.
	localities_list_description	Retrieve the localities that contain the given description.
IMA Minerals	minerals_ima_list	Retrieve the whole IMA mineral list.
	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.

These classes and functions can be applied flexibly to meet users' specific data needs. The Geomaterials class provides functions that help 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. For some physical properties with numerical values or threshold ranges (e.g., Mohs scale (Broz et al., 2006), density, etc.), it supports filtering records by

relationships such as "greater than", "less than", and "within a given range". For the other non-numerical physical properties, it provides functions for retrieving data records by specifying strings, enumeration variables, and special symbols. It also

125   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 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

130   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. Some examples will be presented in the next section.

3 Examples and Results

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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.

140   **Table 3: Geomaterial data retrieval use cases**

Function category	*Function name & Input*	*Output & Description*	*Demo codes & Results*
chemical elements' inclusion and exclusion relationships	geomaterials_contain_any_but_not_elem(c('Fe','S'), c('O'))	Records of geomaterials that containing Fe and S, but not O.	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retriev_Geomaterials_by_elements.ipynb
	geomaterials_not_contain_elems(c('Fe','S','O'),fields="id,name,mindat_formula,elements")	Records of geomaterials without Fe, S, and O, only contain the following fields: id, name, mindat_formula, and elements.	
physical properties with numerical values or threshold ranges	geomaterials_hardness_gt (9)	Records of geomaterials with a Mohs hardness greater than 9.	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_physical_prop_1.ipynb
	geomaterials_dens_range(3,3.2)	Records of geomaterials with a density ranging from 3 to 3.2.	
non-numerical physical properties	geomaterials_colour(c("bright blue"))	Records of geomaterials that have bright blue color.	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_physical_prop_2.ipynb
	geomaterials_cleavagetype(c("Poor/Indistinct"))	Records of geomaterials with a cleavage type of "Poor/Indistinct".	
wildcard names, non-null fields, etc.	geomaterials_name("_u_r_z")	Records of geomaterials whose names has 6-character where 2, 4, and 6 characters were specified.	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Geomaterials_by_wildcard_names.ipynb
	geomaterials_name("qu*")	Records of geomaterials whose names had the first two characters 'q' and 'u'.	
	geomaterials_field_exists("meteoritical_code",TRUE)	Records of geomaterials whose "meteoritical_code" field had non null values.	
	geomaterials_varietyof(3337)	Records of geomaterials that were varieties of Quartz (3337 is the Mindat ID of Quartz).	

In some other situations even just one function can achieve a relatively heavy task. The code below demonstrates two 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.

```
R> mindat_geomaterial_list(ids = c (''), entrytype=7, fields = c ("name","description_short", "rock_parent","rock_parent2"))
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 properties, a single function can also support complex data request needs. For example, if we need to retrieve records of the IMA-approved minerals, containing lithium (Li) and oxygen (O) elements, with Mohs hardness between 5.8 and 6, and have a triclinic crystal structure. We can use the following 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 4: Results of geomaterial records retrieved by combined properties

Name	elements	hmin	hmax	csystem	ima_status	entrytype
Records (only some relevant fields are shown)						
Amblygonite	"Al", "Li", "O", "P", "F"	5.5	6	Triclinic	"APPROVED", "GRANDFATHERED"	0
Bikitaite	"Al", "Li", "Si", "O", "H"	6.0	6	Triclinic	"APPROVED", "GRANDFATHERED"	0
Lithiomarsturite	"Ca", "Li", "Mn", "Si", "O", "H"	6.0	6	Triclinic	"APPROVED"	0
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

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 (Arsenic)) or geomaterials containing certain literal descriptions (e.g., volcano) (**Figure 2**).

Table 5: Locality data retrieval use cases

Function category	Function name & Input	Output & Description	Demo codes & Results
Name, ID, and Description	localities_list_country ("China")	Records of localities of China	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Localities_by_desc.ipynb
	localities_retrieve_id(id = 22)	Records of localities in Algeria (The 22 is the locality ID of Algeria).	
	localities_list_description("volcano")	Records of localities with its descriptions containing the word "volcano".	
chemical elements' inclusion and exclusion relationships	localities_list_elems_inc(c("Dy"))	Records of localities that contain the Dysprosium (Dy) element.	https://github.com/quexiang/OpenMindat/blob/main/notebook/Retrieve_Localities_by_elems.ipynb
	localities_list_elems_inc_exc(c("Dy"), c("Li"))	Records of localities containing Dysprosium (Dy) but no lithium (Li).	
Locality age	locality_age_list()	All records of locality age.	
	locality_age(id = 60)	Records of locality age with its locality ID is 60.	

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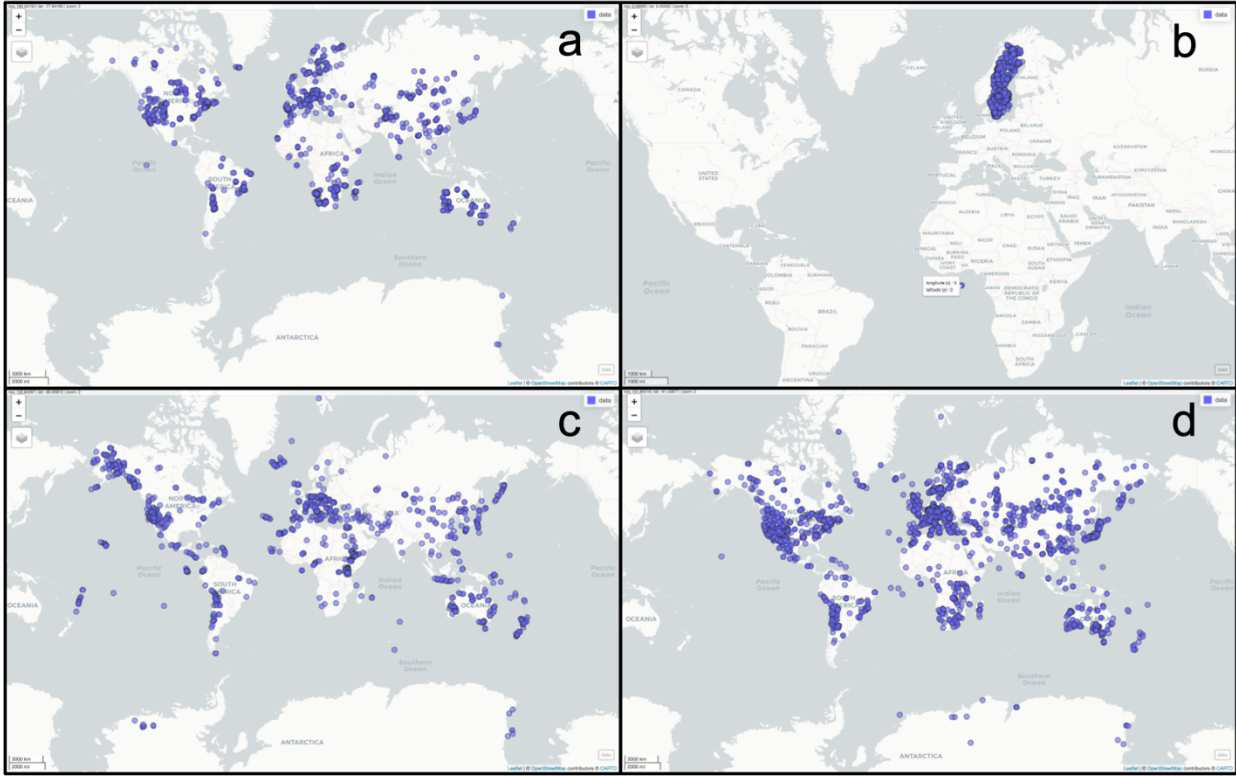
Figure 2: Mapping locality records retrieved by the OpenMindat R package: (a) As-containing minerals, (b) localities in Sweden, (c) locality descriptions containing 'volcano', and (d) type localities of IMA-approved minerals. Base map © OpenStreetMap contributors 2024. Distributed under the Open Data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

175 **3.3 IMA mineral list retrieval**

This package can support retrieval of records 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")
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 minerals list, IMA status, and 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 data exploration or analysis needs, and many of them require just a few lines 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 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.
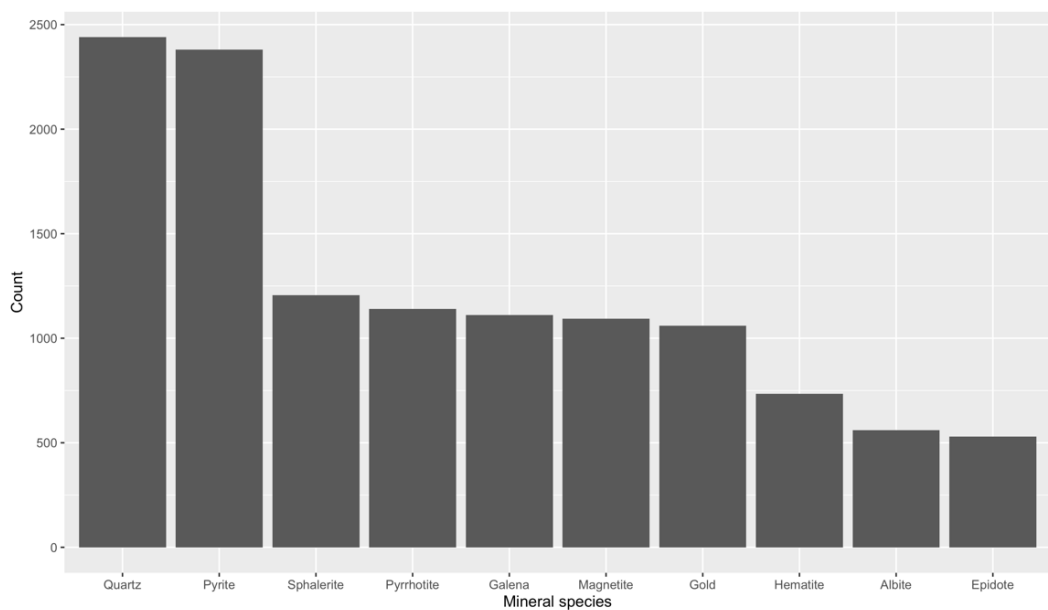
Figure 3: Top 10 IMA-approved mineral species found in Canada.

3.4 Output the retrieved data into different formats

Users can output their retrieved data in a specified format, such as CSV, JSON, TXT, JSON-LD, and TTL. The function "saveMindatDataAs" will identify the suffix of the input file name and convert the retrieved R data frame into a corresponding format. For the data conversion to the JSON-LD and TTL formats, two Excel template files (i.e., OpenMindat_Schema_JSON-LD.xlsx and OpenMindat_Schema_TTL.xlsx) are required. 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). There are two sheets in the template file; the first one is for the context settings 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. **Table 8** shows the second sheet, where "fields" record the field names that need output corresponding to the Mindat API. 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 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/

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Table 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

220 With the above configuration, we can obtain the exported file shown in **Table 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 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 ",
```

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

3.5 Package releases, scientific applications, and update

The OpenMindat R package and its source code were shared on GitHub (https://github.com/quexiang/OpenMindat), together with detailed tutorials on how to install and run the package in the R environment (https://quexiang.github.io/OpenMindat). The first version of this package (version 1.0.0) was also released in the comprehensive R archive network (CRAN) (Hornik,

230   2012) (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 this 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. A list of examples and their Jupyter Notebook files (https://github.com/quexiang/OpenMindat/tree/main/notebook), including those shown in the previous section, is also shared to demonstrate the functions and parameters for data query and access from

235   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 resources mentioned above.

4 Discussion

The development of the OpenMindat R package provides geoscientists with a user-friendly, efficient, and reproducible data querying tool for accessing and analyzing mineralogical data from Mindat. By wrapping the capabilities of the Mindat API

240   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 interactions with the webpage 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

245   beneficial for geoscientists who may not have extensive programming skills, but require 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.

250 The OpenMindat R package embodies the principles of Findable, Accessible, Interoperable, and Reusable (FAIR) data. It is worth noting that data can be FAIR but not open. The "A" in FAIR stands for "Accessible under well-defined conditions," meaning the data doesn't have to be freely accessible to everyone (Jeffery, 2021). So, it is commendable that Mindat data is open and free; users can access the data by registering with Mindat to get free tokens. 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

255 analytical workflows. This openness and alignment with FAIR principles fosters a culture of 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 demandedin 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

260 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

265 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,

270 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

275 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

280 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., 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. 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 is the foundation to facilitate data-driven discoveries, and the work presented in this paper is a building block for that ecosystem.

Despite its benefits and potential, the OpenMindat R package faces certain limitations and needs further extension. For instance, the current version does not support user-friendly 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 introduces the OpenMindat R package, a tool designed to facilitate efficient data retrieval from Mindat, one of the world's largest databases for mineral species and their distributions. By providing a structured interface to the Mindat open data API, the package simplifies the process of accessing and utilizing mineralogical data, making it more accessible to geoscientists who rely on the R programming environment for data analysis and visualization. The OpenMindat R package addresses a gap by enabling streamlined data retrieval for a variety of use cases. Its functionality includes querying geomaterials based on chemical and physical properties, crystal structures, and 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 to data-intensive research and foster innovation in mineral informatics. Continued development of both the Mindat

API and the R package will further expand their utility, encouraging new research directions and collaborations in the geoscience community.

Code and Data Availability

320 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

330 **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

335   The authors declare no competing interests.

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