

Appendix

1. Definitions

The following definitions are identified:

- *EUROVOLC*: the European Network of Observatories and Research Infrastructures for Volcanology (EUROVOLC) is a H2020-EU.1.4.1.2. - Integrating and opening existing national and regional research infrastructures of European interest project to facilitate communication and integration within the European volcano community, bringing together the wide range of disciplines necessary for effective volcanic research (e.g. seismology, physical volcanology, geodesy, geochemistry, petrology, rock and fluid mechanics, earth observation, meteorology, social sciences, and informatics), European Volcano Supersite e-infrastructures implemented in the FUTUREVOLC and MED-SUV projects and a test bed for validation of new models and integrated techniques.
- *EPOS*: the European Plate Observing System is a long-term plan to integrate national and transnational research infrastructures for solid Earth science in Europe. By improving and facilitating the access, use, and re-use of multidisciplinary solid Earth science data, data products, services, as well as physical access to facilities, EPOS is developing a federated and sustainable research platform to provide coordinated access to harmonized and quality-controlled data from diverse Earth science disciplines, together with tools for their use in analysis and modeling. EPOS fosters worldwide interoperability in Earth sciences and provides services to a broad community of users (Cocco et al., 2022).

2. Description of used metadata

This section provides a general overview of all classes used in the proposed structure. The *Metadata* section reports the field's name and is also helpful for comprehending metadata provisioning. A complete description of the field is proposed in the Usage Note section. It has a hierarchical structure, which represents and follows the logical pathway from the studied area: the location where measurement and/or sampling have been carried out (*site*), the geochemical manifestation (*feature*), the different types of collected samples (*material*), the classes of measured parameters (*category parameters*), the parameters analyzed for each material (*parameters*), the analytical procedure related to each parameter.

In the following section, we describe each class of metadata.

Site class

The sample collection and/or measurement site is detailed with a name associated with a Country. More detailed information concerns the volcano where the samples come from, identified by a Global Volcanism Program ID, latitude and longitude, or the volcanic area, defined by the coordinates of a bounding box.

Indeed, the sample collection and/or measurement site can be further detailed by describing the natural or man-made features under study. Various features are possible: a fumarole, a mofete, a lava flow, a drilled well, a spring, the position of in-plume measurements, etc. When the feature is described, the site class represents a more generic attribute (the volcano, for instance). The class feature should contain as much information as possible about the sampling site, including pictures, sketches, and geometric details.

Site	
Metadata	Usage note (description)
name	Name of the site (e.g. Name of the volcano)
country	Indicate the Country where the site is located
site lat	Spatial latitude of the site
site long	Spatial longitude of the site
volcanic area	Name of the volcanic area where the sample come from
area_longW	Left longitude of the boundary box. Top latitude of the boundary box
area_lonE	Right longitude of the boundary box
area_latS	Bottom latitude of the boundary box
area_latN	Top latitude of the boundary box

Feature class

This class contains all functional characteristics to best describe the samples or the sampling points.

Feature	
Metadata	Usage note (description)
feature_name	Name of the geochemical feature studied during a field survey or node of a permanent sampling network
sample_label	Label used to identify the sample
sample IGSN	IGSN is a persistent identifier for the sample
sample type	Description of the physical characteristics of the sample visible in hand or with low magnification microscopy. The description must use terms of a fixed Vocabulary***
sample eruption	Date of sample's eruption (YYYY/MM/DD)
sampling date	Date of sampling (YYYY/MM/DD)
sampling start	Time of sampling start (YYYY/MM/DD hh:mm:ss)
sampling end	Time of sampling end (YYYY/MM/DD hh:mm:ss)
vent location	A free text, helpful to identify the eruptive vent/fissure producing the sample and/or a locality where the sample has been collected
activity type	Description of the activity of the eruption (eg: effusive, spattering, Strombolian explosions, paroxysm, ash emission, other)
sample texture	Description of the texture of the sample
sample lat	Latitude of the sample/sampling point
sample long	Longitude of the sample/sampling point
sample elevation	Elevation of the sample/sampling point (m a.s.l.)
sampling method	The sampling method used for data collection

sample weight	Weight of the sample (g)
sample_quenching	Information about the sample quenching process
sample collector	Name of the person who collects the samples
sample photo link	Sample's image
geological age	Age of the sample according to scientific literature data
geological unit	Geological unit to which the sample belongs, according to scientific literature data
eruption unit	Name of the eruption
eruption start	Start date of eruption (YYYY/MM/DD)
eruption end	End date of eruption (YYYY/MM/DD)
survey or network info URL	Information about the field campaign, the permanent network, the project URL, or information page link
monitoring or research info	Information about the monitoring network or research details
note	A free text for any helpful information to describe the sample

Person class

This class can be associated with various classes. It lists the information related to the responsible of the sampling campaign, to the sample collector, to the person responsible for the laboratories, and the analysts.

Person	
Metadata	Usage note (description)
person_type	This field specifies the role of the person
family_name	Family name
given_name	Given name
nationality	Report the nation to which he belongs
institution	The institution to which they belong
email	Email address
tel	Telephone number

Physical archive class

The *physical archive* class contains information about where the physical samples are located (e.g., Lithotheque). If this information is available, to know where and how the samples are stored.

<i>Physical archive</i>	
Metadata	Usage note (description)
lithot_corridor	This field specifies the position in the corridor used for the physical archive
lithot_cabinet	This field specifies the position in the cabinet used for the physical archive
lithot_shelf	This field specifies the position on the shelf used for the physical archive

lithot_type	Describe the lithological type
lithot_info	Describes generic info for the sample

The following classes describe sampling materials, which represent the physical object obtained by processing the same physical sample that will be subjected to laboratory chemical analysis. Different types of materials are analyzed with different techniques to achieve different objectives.

Bulk rock class

The *bulk rock* class contains information about the whole rock sample that is properly prepared (generally pulverized or melted) to be analyzed with appropriate instruments.

<i>Bulk rock</i>	
Metadata	Usage note (description)
comment	Chemical composition of volcanic rock
bulk rock label	Label of the bulk rock

Volcanic glass class

This *volcanic glass* class contains information about the natural silicate glass that forms when the magma cools too rapidly to permit crystallization.

<i>Volcanic Glass</i>	
Metadata	Usage note (description)
comment	Chemical composition of volcanic glass
section label glass	Label of the thin section or rock slide where the measure of glass is carried out
volcanic glass label	Label of the spot/area which is measured
volcanic glass type	Specify if the measure of glass is carried out in groundmass or melt inclusion
volcanic glass host mineral	Name of the mineral hosting the glassy melt inclusion
volcanic glass info	A free text for any helpful information to describe the glass analysis
volcanic glass photo	Image of the volcanic glass
volcanic glass shape	A text for any helpful information to describe the f glass
volcanic glass color	Information about the color of the glass
minerals in volcanic glass	Minerals eventually occurring in volcanic glass

Mineral class

Mineral class contains information about a solid, crystalline phases of the rock.

<i>Mineral</i>

Metadata	Usage note (description)
comment	Chemical composition of a mineral phase
section label mineral	Label of the thin section or rock slide where the measure of mineral is carried out
mineral label	Label of the mineral
mineral type	Name of the mineral (e.g. plagioclase, olivine pyroxene, other)
mineral spot label	Label of the spot which is measured
mineral size	Measure (in micron) of the main axis of the mineral
mineral zone	Zone of the mineral where the measure has been carried out (e.g. core, rim, intermediate, other)
mineral info	A free text for any helpful information to describe the mineral and/or analysis
mineral photo	Image of the mineral
mineral glomerophyre	Glomerophytic texture information

Steam condensate class

Steam condensate class represents the features relating to the sample obtained from the condensation of fumarolic steam along the fumarole sampling line.

<i>Steam condensate</i>	
Metadata	Usage note (description)
sampling procedure	Procedure for sample collection
description	Description of the collected material
sampling date	Date of sampling (YYYY/MM/DD)
sampling start	Time of sampling start (YYYY/MM/DD hh:mm:ss)
sampling end	Time of sampling end (YYYY/MM/DD hh:mm:ss)
comment	
steam condensate label	Name of the material "steam condensate"

Dry gas sample class

The *Dry gas sample* class represents the features relating to the gas sample obtained after condensation of the steam along the fumarole sampling line, or gas sample from low-temperature gas vents or soil air.

<i>Dry gas sample</i>	
Metadata	Usage note (description)
sampling procedure	Procedure for sample collection
description	Description of the collected material
sampling date	Date of sampling (YYYY/MM/DD)
sampling start	Time of sampling start (YYYY/MM/DD hh:mm:ss)
sampling end	Time of sampling end (YYYY/MM/DD hh:mm:ss)
comment	
dry gas sample label	Name of the material "Dry gas sample."

Giggenbach bottle class

The Giggenbach bottle is a glass bottle with one or two stopcocks, half-filled with a NaOH solution, able to trap the water vapor (steam), CO₂, S-bearing gas species, HCl, HF (the method was proposed by Giggenbach, 1975). The incondensable gas species, such as He, Ar, Ne, N₂, and O₂, accumulate in the bottle headspace (Giggenbach W. F., 1975).

<i>Giggenbach bottle</i>	
Metadata	Usage note (description)
sampling procedure	Procedure for sample collection
Description	Description of the collected material
sampling date	Date of sampling (YYYY/MM/DD)
sampling start	Time of sampling start (YYYY/MM/DD hh:mm:ss)
sampling end	Time of sampling end (YYYY/MM/DD hh:mm:ss)
Comment	
Giggenbach bottle label	Name of the material "Giggenbach bottle"

The following classes represent the parameters categories, which include the groups of parameters that can be determined in each material. These categories should be considered parameter reservoirs, containing any parameter with specific geochemical attributes.

For bulk rock samples, the parameters in the analyzed categories are Major Elements, Trace Elements, and Isotopes, which contain specific groups of elements and compounds.

Major elements class (for rock samples)

Major elements, which are the most abundant elements in a rock (Si, Ti, Al, Fe, Mn, Mg, Ca, Na, K, P) are expressed as oxide and the concentrations are expressed as weight percent (wt%) .

<i>Major elements</i>	
Metadata	Usage note (description)
SiO ₂	Value of the Silicon Dioxide
TiO ₂	Value of the Titanium Dioxide
Al ₂ O ₃	Value of the Aluminium Oxide
Fe ₂ O ₃	Value of the Ferric Oxide
FeO	Value of the Ferrous Oxide
FeOT	Value of the calculated Total Iron
MnO	Value of the Manganese Oxide
MgO	Value of the Magnesium
CaO	Value of the Calcium Oxide
Na ₂ O	Value of the Sodium Oxide
K ₂ O	Value of the Potassium Oxide
P ₂ O ₅	Value of the Phosphorus Oxide
LOI	Value of the Loss on Ignition
S	Value of the Sulfur
Cl	Value of the Chlorine

CO2	Value of the Carbon Dioxide
H2O	Value of the Water content
Total	Total

Trace elements class (for rock samples)

Trace elements' abundance t is less than 0.1%; the concentrations are expressed in parts per million (ppm).

<i>Trace elements</i>	
Metadata	Usage note (description)
As	Value of Arsenic
Ba	Value of Barium
Be	Value of Beryllium
Bi	Value of Bismuth
Cd	Value of Cadmium
Ce	Value of Cerium
Co	Value of Cobalt
Cr	Value of Chrome
Cs	Value of Cesio
Dy	Value of the Dysprosium
Er	Value of the Erbium
Eu	Value of the Europium
Ga	Value of the Gallium
Gd	Value of the Gadolinium
Ge	Value of the Germanium
Hf	Value of the Hafnium
Ho	Value of the Holmium
In	Value of the Indium
La	Value of the Lanthanum
Lu	Value of the Lutetium
Mo	Value of the Molybdenum
Nb	Value of the Niobium
Nd	Value of the Neodymium
Ni	Value of the Nickel
Pb	Value of the Lead
Pr	Value of the Praseodymium
Rb	Value of the Rubidium
Sc	Value of the Scandium
Sb	Value of the Antimony
Sm	Value of the Samarium
Sn	Value of the Tin
Sr	Value of the Strontium
Ta	Value of the Tantalum
Tb	Value of the Terbium
Th	Value of the Thorium
Tm	Value of the Thulium
U	Value of the Uranium

V	Value of the Vanadium
W	Value of the Tungsten
Y	Value of the Yttrium
Yb	Value of the Ytterbium
Zn	Value of the Zinc
Zr	Value of the Zirconium

Isotopes class (for rock samples)

Isotopes are radiogenic or stable isotopes of selected elements.

<i>Isotopes</i>	
Metadata	Usage note (description)
Sr87 Sr86	Value of the Sr isotopic ratio
Nd143 Nd144	Value of the Nd isotopic ratio
Sr_isotope_error	The quoted error (± 2 s) of the Sr ratio which refers to the last digit.
Nd_isotope_error	The quoted error (± 2 s) of the Nd ratio which refers to the last digit.

Major elements class

Major elements for liquid samples are elements or compounds whose concentration is in the order of mg/L.

<i>Major elements</i>	
Metadata	Usage note (description)
C	Value of the Carbon concentration
SO4	Value of the Sulfate concentration
Cl	Value of the Chlorine concentration
Na	Value of the Sodium concentration
K	Value of the Potassium concentration
Ca	Value of the Calcium concentration
Mg	Value of the Magnesium concentration
Br	Value of the Bromine concentration
F	Value of the Fluorine concentration

Isotopes class (for gas samples)

Isotopes class collects information about the ratios between elements with the same atomic number but different masses (i.e. $^{13}\text{C}/^{12}\text{C}$, $^3\text{He}/^4\text{He}$, $^{40}\text{Ar}/^{36}\text{Ar}$, $^{18}\text{O}/^{16}\text{O}$, D/H, etc.).

<i>Isotopes</i>	
Metadata	Usage note (description)
DELTA_D	Value of the delta_D
DELTA_O18(H2O)	Value of the delta_18O(H2O)
DELTA_C13(CO2)	Value of the delta_13C(CO2)

DELTA_O18(CO2)	Value of the delta_18O(CO2)
He3_He4(R/Ra)	Value of the 3He and 4He ratio, referred to air (R/Ra)
Ar40_Ar36	Value of the 40Ar/36Ar ratio
DELTA_N15	Value of the delta N15
Note	A free text for any information useful to describe the isotopes

Gas chemistry class

Gas chemistry contains the chemical composition of the gas phase in a dry gas sample.

<i>Gas chemistry</i>	
Metadata	Usage note (description)
CO2	Value of the Carbon dioxide concentration
CH4	Value of the Methane concentration
He	Value of the Helium concentration
H2	Value of the Hydrogen concentration
O2	Value of the Oxygen concentration
N2	Value of the Nitrogen concentration
CO	Value of the Carbon monoxide concentration
Ar40	Value of the Argon-40 concentration
Ar+O2	Value of the Argon + Oxygen concentrations
H2S	Value of the Hydrogen sulfide concentration
Note	A free text for any information useful to describe the gas chemistry

Fumarole chemistry class

Fumarole chemistry contains chemical composition of the fumarole vapour (steam + other gas species).

<i>Fumarole chemistry</i>	
Metadata	Usage note (description)
H2O	Value of water concentration
CO2	Value of the Carbon dioxide concentration
HCl	Value of the Hydrogen chloride concentration
H2S	Value of the Hydrogen sulfide concentration
Stot	Value of the Sulfur total concentration
SO2	Value of the Sulfur dioxide concentration
CH4	Value of the Methane concentration
Ar	Value of the Argon concentration
Ar+O2	Value of the Argon +Oxygen concentrations
CO	Value of the Carbon monoxide concentration
H2	Value of the Hydrogen concentration
N2	Value of the Nitrogen concentration
He	Value of the Helium concentration
O2	Value of the Oxygen concentration
Note	A free text for any information useful to describe the fumarole chemistry

Soda solution chemistry class

Soda solution chemistry is the chemical composition of the soda solution in the Giggenbach bottles.

<i>Soda solution chemistry</i>	
Metadata	Usage note (description)
C	Value of the Carbon
S	Value of the Sulfur
Cl	Value of the Chlorine
Note	A free text for any information useful to describe the soda solution chemistry

Headspace chemistry class

Headspace chemistry is the chemical composition of the gas phase in the Giggenbach bottles.

<i>Head space chemistry</i>	
Metadata	Usage note (description)
He	Value of the Helium concentration
H2	Value of the Hydrogen concentration
CO	Value of the Carbon monoxide concentration
CH4	Value of the Methane concentration
Ar	Value of the Argon concentration
O2	Value of the Oxygen concentration
N2	Value of the Nitrogen concentration
Note	A free text for any information useful to describe the headspace chemistry

Parameter class

This class contains any parameter (element, compound, isotopic ratio, physico-chemical parameter) that can be measured in the field or in the laboratories. The single parameter can be included or not in a category of parameters. The metadata related to every parameter are

- the name of the parameter, referred to a vocabulary, possibly acknowledged by the scientific community; in this work, we adopted the vocabulary proposed by Earthchem (<http://www.earthchem.org/>);
- the measure units;
- the analytical precision;
- the analytical procedure, including eventual treatments before the analyses and the measurement technique;
- the instrument used for the analyses;
- the detection limit;
- the calibration type and the range of concentration of the standards.

Each parameter is related to the *Category parameters* class and to the *Instrument_info* class.

Some parameters are measured in the field and, therefore, they are directly related to the *Feature* class. Other parameters could be part of a dataset, related to a field campaign, or a given temporal interval.

Parameter	
Metadata	Usage note (description)
parameter name or group	Name of the parameter/group of parameters
unit	Unit of measure
precision	Precision of the measurement provided by the laboratory
analytical method	Method of analysis
detection limit	The lower concentration that can be measured
standard range	The range of concentration of the used standards
calibration type	Type of calibration (linear, exponential...))
reference	Literature data concerning the analytical method used

Instrument info class

This class contains all the information about the instruments used in the field and the laboratories. The manufacturer and model identify the instrument and should be associated with the laboratory where it is installed and the reference person responsible for its use and maintenance.

Instrument info	
Metadata	Usage note (description)
instrument_name	Commercial name of the instrument
instrument_manufacture	Manufacturer of the instrument
instrument_description	Description of the instrument
instrument_laboratory	Laboratory where the Instrument is located