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SOFTWARE ARTICLE

Spinel web: an interactive web application for visualizing the chemical composition of spinel group minerals

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Abstract

The spinel group minerals provide useful information regarding the geological environment in which the host rocks were formed, constituting excellent petrogenetic indicators, and guides in the search for mineral deposits of economic interest. In this article, we present the Spinel Web, a web application to visualize the chemical composition of spinel group minerals. Spinel Web integrates most of the diagrams commonly used for analyzing the chemical characteristics of the spinel group minerals. It incorporates parallel coordinates and a 3D representation of the spinel prisms. It also provides coordinated views and appropriate interactions for users to interact with their datasets. Spinel Web also supports semi-automatic categorization of the geological environment of formation through a standard Web browser.

Keywords Geology · Tectonic settings · Spinel group minerals · Visualization · Web application · 3D visualization

Introduction

In Geological Sciences, one of the main goals is to reconstruct the geological environments where rocks were formed and the events that subsequently affected them. This allows geologists to understand the geological evolution of the Earth and, therefore, identify regions where natural resources are located, identify areas that present geological risks to human life or to the implementation of engineering works, etc.

In order to characterize a particular geologic region in terms of its tectonic setting, we focus on the study of a particular suite of rocks, mafic and ultramafic rocks carrying spinel group minerals. Each *spinel sample* is characterized by 11 analyzed major chemical elements (those whose content is greater than 0.01% by weight expressed as oxide), and by 22 metadata, called end-members, calculated as combinations of the major chemical elements. However, only 8 of these end-members are routinely used by geologists for representation in specific graphics (see Table 1).

It is common to represent the spinels composition in a prismatic space called spinel prism, a compositional space that represents the solid solution between six end-members. The spinel prism supports two representations: the Magnetite Prism and the Ulvöspinel Prism. The spinel prism can be divided into different fields that represent the different tectonic environments where this group of minerals may be formed. The chemical data corresponding to spinels from a certain tectonic environment are grouped into a specific and unique reference pattern and grouped into a particular region of the prism. To evaluate these data, both 3D prismatic diagrams and the projected information on the faces of the prism are used.

In order to establish the tectonic environment where a spinel with a particular composition could have been formed, geologists typically use the contours defined by Barnes and Roeder (2001a) as empirical tectonic discriminators. Barnes and Roeder compiled a database comprising more than 26000 analyses of spinels from mafic and ultramafic rocks. This enables the delineation

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Table 1 The eight end-members commonly used by geologists for the different analyses, their associated formula, and the corresponding plain-text label for Spinel Web

Minerals	Formula	Label
Spinel	$MgAl_2O_4$	$MgAl2O4$
Hercynite	$Fe^{2+}Al_2O_4$	$FeAl2O4$
Magnesioferrite	$MgFe_2^{3+}O_4$	$MgFe2O4$
Magnetite	$Fe^{2+}Fe_2^{3+}O_4$	$Fe3O4$ or $FeFe2O4$
Magnesiochromite	$MgCr_2O_4$	$MgCr2O4$
Chromite	$Fe^{2+}Cr_2O_4$	$FeCr2O4$
Qandilite	$(Mg, Fe^{3+})_2(Ti, Fe^{3+}, Al)O_4$	$Mg2TiO4$
Ulvöspinel	$Fe_2^{2+}TiO_4$	$Fe2TiO4$

and construction of characteristic compositional fields for spinels of various tectonic environments using data density contour plots (DDCPs).

In this article, we introduce the Spinel Web, an interactive visual analysis web application tool for spinel group minerals. Spinel Web supports semi-automatic categorization of the tectonic environments for the spinel group minerals based on the Barnes and Roeder's contours (Barnes and Roeder 2001a). This application provides a rich set of functionalities required by the geologist, comprising 2D binary plots, ternary plots, and a 3D representation of the spinel prisms. All views are interactive, linked, and integrated into a coordinated multiple views setup. The coordinated multiple views technique is a proven concept in visual analysis (Roberts 2007). The main idea behind this technique is to simultaneously show a dataset with different visualization techniques, depicting multiple views of the data and supporting the *brushing and linking* concept. Brushing and linking allows the user to interactively select (brush) subsets of the data in a view, and all the corresponding data items in all linked views will be consistently highlighted (linking). The use of multiple coordinated views provides analytic power because it allows the exploration of data from a variety of different perspectives. Spinel Web is an online web application, so no installation process is required for its use. It can be accessed from any browser such as Google Chrome, Internet Explorer, etc.

This work is the result of a long term collaboration of an interdisciplinary group of visualization and geology experts. The main goal of the present communication is to make this web application available to the scientific community.

Related work

It is a common practice to plot spinel chemical compositions on prismatic spaces (spinel prism), which provides a reasonable and easily interpretable 3D chart (Haggerty 1991). Besides, scientists mostly use binary and ternary plots to evaluate correlations between chemical elements expressed as oxides/cations and typically work with different software tools to generate dedicated diagrams (Carr 2002; Bernhardt 2007; Janoušek et al. 2006; Williams et al. 1990) related to the petrogenesis and the provenance of the spinel group minerals. These tools have been developed for better data analysis and representation, but they are usually not interactive.

In 2012, Ganuza et al. (2012) presented a geological visualization application called SpinelViz. The application consists of an interactive 3D viewer, which enables the user to depict and explore different datasets in the spinel prism at the same time. SpinelViz provides the capability to manipulate, view, plot, and project data in 2D and 3D, which helps the user to gain a better insight into the data distribution, but it only runs on Windows 7. In 2014, Spinel Explorer (Ganuza et al. 2014) was presented. Spinel Explorer is an interactive visual analysis framework that integrates the most commonly used plots for spinel sample data exploration with other conventional plots and exploits the coordinated multiple views principle. Later, interactive semi-automatic 2D categorization based on the Barnes and Roeder's contours was integrated into the Spinel Explorer, and the Spinel Explorer++ was presented (Ganuza et al. 2017, 2015).

In this communication, we introduce an interactive visual analysis web application for exploring the chemical composition of the spinel group minerals based on Spinel Explorer++ (Ganuza et al. 2017, 2015). It runs on any browser so it is very easy to access, not requiring any installation by the user. Besides that, it also includes a 3D categorization showed in the prism.

The software - design and implementation

The user interface of the application was designed as a combination of two sections: the logging section (see Fig. 1) and the data upload and multiple views section (see Fig. 2).

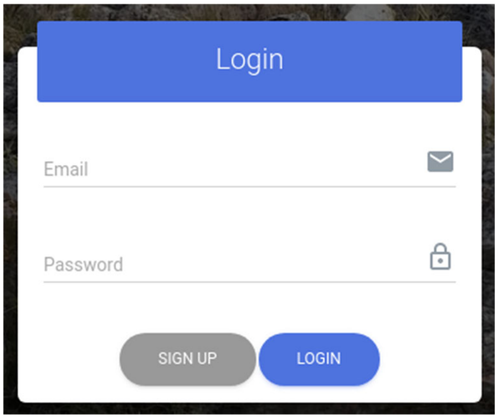

Fig. 1 Screenshot from a login session

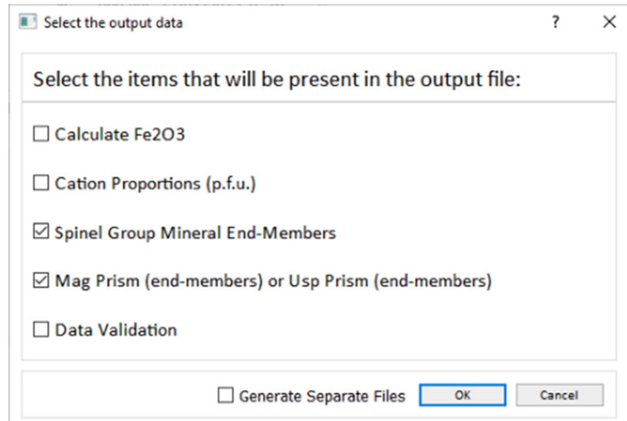

Fig. 3 Configuration for EMG (Ferracutti et al. 2015). When processing their data with EMG, the users are required to select, at least, the options “Spinel Group Mineral End-Members” and “Mag Prism (end-members) or Ulv Prism (end-members)” and deselect the option “Generate Separate Files”, to enable full functionality of the Spinel Web

Data input format

To use Spinel Web, the data must be compiled in the CSV format (*.csv) and must be processed with the EMG program (Ferracutti et al. 2015) or a similar one that allows the calculation of the end-members of the spinel group. To enable the full functionality of Spinel Web, in the configuration of the EMG, the user must select, at least, the options “Spinel Group Mineral End-Members” and “Mag Prism (end-members) or Ulv Prism (end-members)”, and deselect the option “Generate Separate Files” (see Fig. 3). The user can also include the cation proportions or the Fe_2O_3 calculations to the dataset, or any other properties that he/she may want to analyze. An example of the structure of a valid dataset for the Spinel Web is attached as Supplementary Material.

Visualizing data

With the coordinated multiple views, it is possible to simultaneously show the dataset with different visualization techniques. The overall premise of this exploratory technique is

Fig. 2 Screenshot of an analysis session in which geologists interact with different views of the data: spinel prism, ternary plots, scatterplots, and prism projections

that users better understand their data if they can interact with their data viewing it through different representations (Roberts 2007). The purpose of generating multiple views of the same data is to look at and interact with them from different points of view, thus facilitating analysis. The Spinel Web supports scatterplots, ternary plots, and spinel prisms, which are well-known representations in the geology domain. It also includes views of the projection of the spinel prism and parallel coordinates. Figure 4 is a screenshot from an analysis session where most of the available views are shown. In this particular case, a dataset of spinel group minerals (Sp-EMX dataset) associated with Earth Mantle xenoliths (Sp-EMX) from Patagonia, Argentina, has been loaded.

All views are linked and the system supports interactive selection. If the user selects a subset of the data in one view, the selected data is highlighted in the other views as well. In all views, each sample is represented with a graphic mark and has an associated color and size. By default, each sample is represented as a blue or gray point, but the user can change the color and shape of the graphic object.

To reduce the cognitive load and to make analysis much more efficient, Spinel Web offers a predefined view arrangement for spinels categorization. When the spinel prism is depicted, the corresponding projections are shown below or next to it.

Scatterplot

Scatterplots are commonly used in the studies of the spinel group minerals to show the relationship between the cations in the tetrahedral site (X) against those which are expected to be in the octahedral site of the crystalline framework (Y) of spinels. They also show the chemical variations in the dataset and allows the representation of the lateral and basal faces of the spinel prism with magnetite or ulvöspinel, if the correct oxides are selected to construct the diagram.

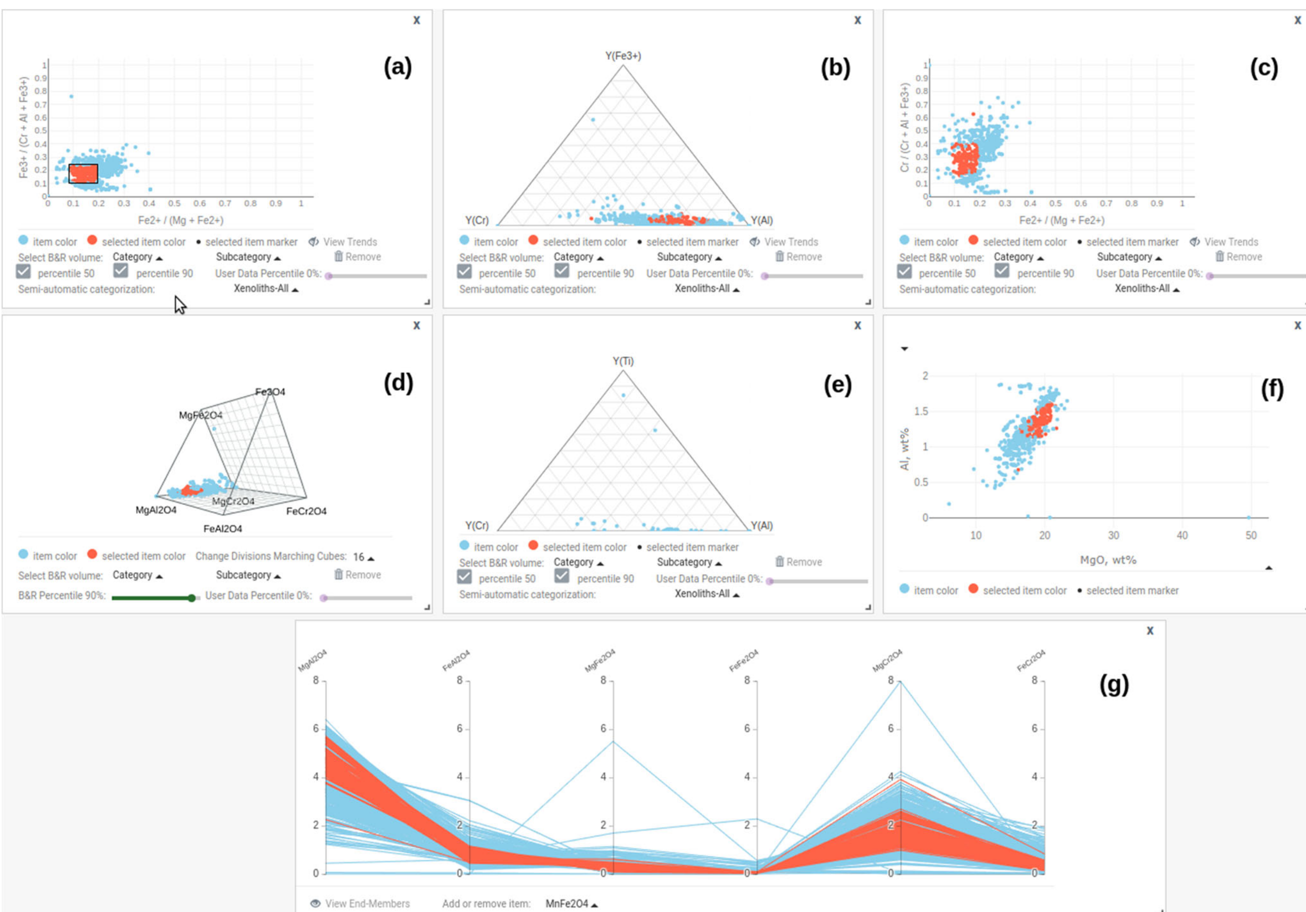

Fig. 4 Correlated views in Spinel Web. The Sp-EMX dataset has been loaded and depicted using different views at the same time. 2D projections of the datasets loaded into the prismatic space are drawn in 2D spaces (the faces of the prism). **a** Lateral front projection of the magnetite prism, **b** Triangular front projection, **c** Base front projection. **d** The magnetite prism view. **e** A ternary plot depicting the relation between Al, Ti, and Cr. **f** A scatterplot showing the relation between MgO and Al. **g** The parallel coordinates view. A rectangular brush active in (**a**) and highlighted in red color in all the other coordinated views

Therefore, they can be used to easily detect correlations between two attributes (elements/oxides/cations).

Spinel Web provides a simple way to generate scatterplots and it supports rectangular selection. The rectangular selection allows the user to draw a rectangle inside the view and automatically select the points included therein. As a result, all the corresponding items in all linked views will be consistently highlighted. Figure 4f shows a scatterplot depicting the relation between MgO and a cation, in this case, Al, which corresponds to Sp-EMX.

Ternary plot

Ternary diagrams are employed to represent groups of three chemical elements that sum to a constant. These are very useful in geological studies to show the relative compositions of soils and rocks and for the interpretation of the chemical analyses of spinel group minerals.

Figure 4e illustrates a ternary diagram, in this particular case showing the relationship between Al, Ti, and Cr cations. The user is responsible for choosing the attributes significant for the analysis. Also, as in scatterplots, Spinel Web supports a rectangular selection for ternary plots.

Spinel prism

The spinel prism is a compositional space that represents the solid solution between six end-members. The vertices correspond to each end-member of the compositional space. The magnetite prism is used to plot the chemical compositions of the solid solution between hercynite, spinel, magnesioferrite, magnetite, magnesiochromite, and chromite end-members, while the ulvöspinel prism is used to plot the chemical compositions for the solid solution represented by hercynite, spinel, ulvöspinel, qandilite, magnesiochromite, and chromite end-members.

Spinel Web provides support for 3D views for both prisms: the magnetite and the ulvöspinel prisms. Both representations are interactive and can be freely rotated and zoomed in/out for closer observation.

Figure 4d shows the dataset depicted in the magnetite prism view.

Spinel prism projections

One of the most important features of the application is to provide 2D views of the projected faces of the spinel prisms. These projections are calculated automatically after loading a sample dataset and are available throughout the whole analysis session. This allows the exploration of the 3D prismatic space and the 2D projections at the same time. Figure 4a, b and c show the dataset projected into three faces of the magnetite prism.

Parallel coordinates

The parallel-coordinates view shows several dimensions simultaneously (Inselberg 2009). The main idea is to use one vertical axis per dimension and connect the values of a sample using a polyline or a curve. Although the geology community is not familiar with the use of parallel coordinates, this technique has good potential in the geological domain as it supports comparisons of more than three dimensions. With this technique, geologists can explore relationships between the 22 end-members at the same time. Figure 4g illustrates the Sp-EMX dataset depicted in parallel coordinates, which shows the relationship between the six end-members of the magnetite prism at the same time.

Interactive semi-automatic categorization

The Spinel Web introduces a semi-automatic, interactive detection of tectonic settings for an arbitrary dataset based on the contours provided by Barnes and Roeder (2001a). These contours can be depicted in the projections of the 3D spinel prism, and the users can select which contour they want to overly with their data (see Fig. 5).

At that point, Spinel Web can search for the contours that contain most of the end-members of the dataset and automatically rank Barnes and Roeder's contours based on the number of points that they include. The user can provide two thresholds by default corresponding to the 50th and 90th percentiles contours. All contours containing a higher amount of points than the user-provided threshold are listed as potential tectonic-setting categories. These categorization lists are provided for each of the 2D projections separately.

Figure 5 shows the Sp-EMX dataset depicted on three projections of the prism. In Fig. 5, the 50th and the 90th percentile contours are shown in dark green and light green, respectively and in Fig. 5a the categorization list is shown. Information for both, the 50th and the 90th percentile contours, are shown in the list.

Besides, the Spinel Web allows the creation of density-based percentile contours from the user's dataset (Fig. 6) for all prism projections. The user has full control of the contour creation parameters and can freely create percentile contours in the range from 1 % to 100 %. The possibility of displaying contours of different percentiles generated from the set of user samples helps experts to get a deeper insight into their data. Once the contours are created, they can be overlaid and compared with Barnes and Roeder's contours (see Fig. 7).

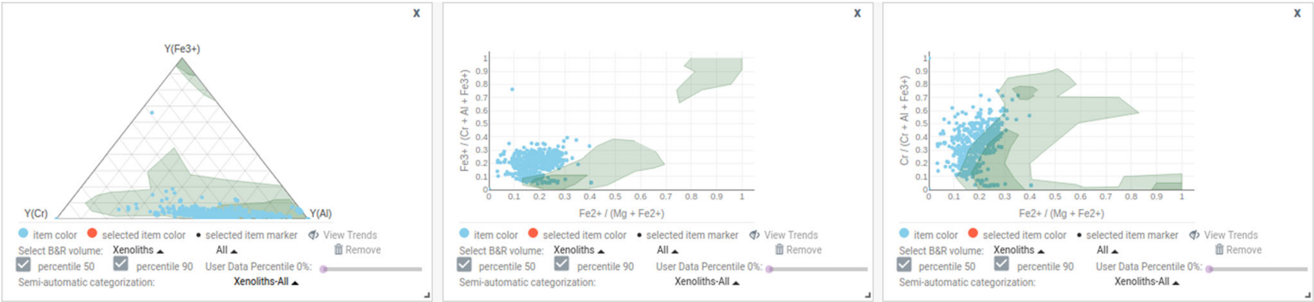

Fig. 5 Barnes and Roeder's contours for Sp-EMX rock xenoliths overlaid with the user-provided data in the projections of the spinel prism. In the triangular projection (**a**), the categorization list is shown (ranking in the first place the Earth's mantle xenoliths). In the rectangular projections (**b**) and (**c**), the semi-automatic categorization also suggests that the best contour for the user data corresponds to Sp-EMX

Implementation

The application is implemented in JavaScript,[1] using React.js[2] for user interface creation, and Highcharts[3] and Plotly[4] for data visualization.

Case study

We evaluate the Spinel Web in one case study conducted with geologists. This case study is based on the Sp-EMX dataset of spinels associated with Earth mantle xenoliths from Patagonia, Argentina. This dataset consists of 748 data samples. Each data sample corresponds to the chemical composition of an analyzed point of the spinel samples and has 73 attributes, including oxide values and end-member values corresponding to each analyzed point. The main goal was to determine the tectonic settings of this set of spinel group minerals. In this particular case, the geologists are aware that the spinels belong to Earth mantle xenoliths, so the goal is to confirm this hypothesis.

Figure 4 shows a screenshot from an analysis session in which the geologists interact with different views of the dataset. They configure the Spinel Web to show the spinel prism and the three projections of the prism at the same time. Then, the experts overlap the Barnes and Roeder's contours, defined for spinels associated with Earth mantle xenoliths, onto the points corresponding to the dataset (as seen in Fig. 5). Indeed, most of the points lie inside the contour, giving the experts positive feedback about their hypothesis. Afterward, the experts activated the semi-automatic categorization provided by Spinel Web. The system searched for the contours that contain most of the samples of the dataset and automatically ranked Barnes and Roeder's contours based on the number of points that they include. Figure 5 shows that, for the three projections, the categorization lists suggest that the best contour for the dataset corresponds to xenoliths, validating the experts' hypothesis.

According to the domain experts, the goals for the case study were effectively achieved using Spinel Web. They also find the interconnection between the different views very useful, specifically the possibility of selecting a subset of data in one view, and identifying that selection in the other views. Finally, the experts valued very positively the availability of the tool on the web. They pointed out the relevance of being able to use the Spinel Web, the only requirements being an Internet connection and a web browser.

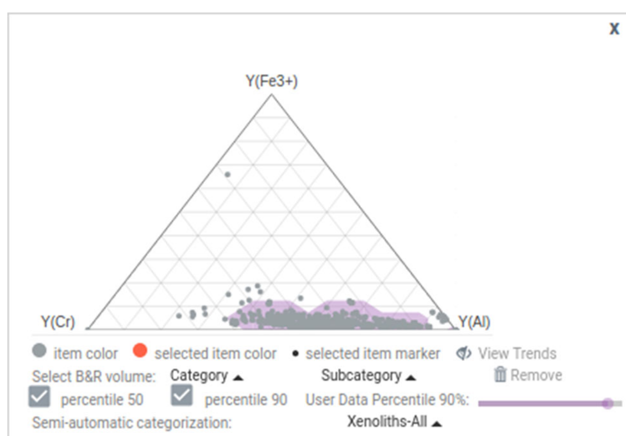

Fig. 6 Contour creation in Spinel Web. The 90th percentile contours (*purple*) for a user-provided dataset have been created. The user can interactively select the percentile of the contour to be generated

[1]https://www.javascript.com/

[2]http://reactjs.org/

[3]https://www.highcharts.com/

[4]https://plot.ly

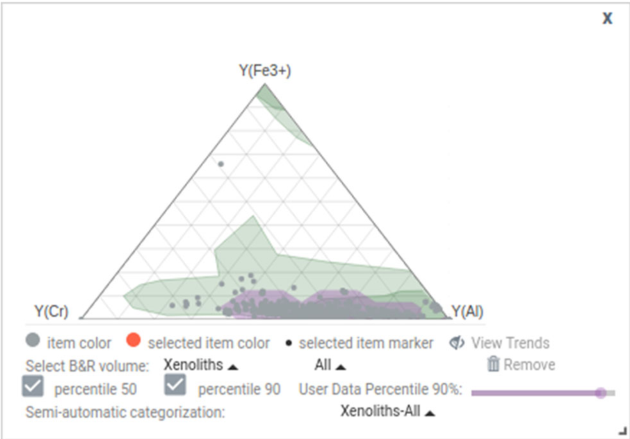

Fig. 7 The 90th percentile contours (*purple*) for user-provided dataset overlapping the 90th percentile Barnes and Roeder's contours for xenoliths

Conclusions

Spinel Web is an online web application for the visualization of the chemical composition of spinel group minerals and their categorization according to the geological setting. It is designed to help geologists in the exploration of the chemical characteristics of the spinel group minerals and to assist the experts in the categorization process. The presented application is freely available and can be accessed from all web browsers.

Spinel Web integrates 2D binary plots, ternary plots, 3D representations of the spinel prisms, and parallel coordinates diagrams in a coordinated-view system. Besides, it supports the semi-automatic, interactive categorization of an arbitrary spinel dataset. All contours are fully integrated and can be depicted in three projections of the 3D spinel prism. This application provides an effective tool for visualizing and interacting with the data to analyze not only tectonic settings but also other possible relationships between the data of the chemical composition of this group of minerals.

Availability and Requirements

Spinel Web is a web application, therefore no installation process is necessary. It can be freely accessed at the website http://vyglab.cs.uns.edu.ar/apps from any browser such as Google Chrome, Internet Explorer, etc.

Supplementary Information The online version contains supplementary material available at (https://doi.org/s12145-020-00542-w).

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Compliance with Ethical Standards

Conflict of interests The authors declare that they have no conflict of interest.

Data Availability Barnes and Roeder's database (Barnes and Roeder 2001a) is available as supplementary data in the corresponding journal webpage (Barnes and Roeder 2001b).

Code Availability The application can be freely accessed at the website http://vyglab.cs.uns.edu.ar/apps from anybrowser. The code is not available at the moment.

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