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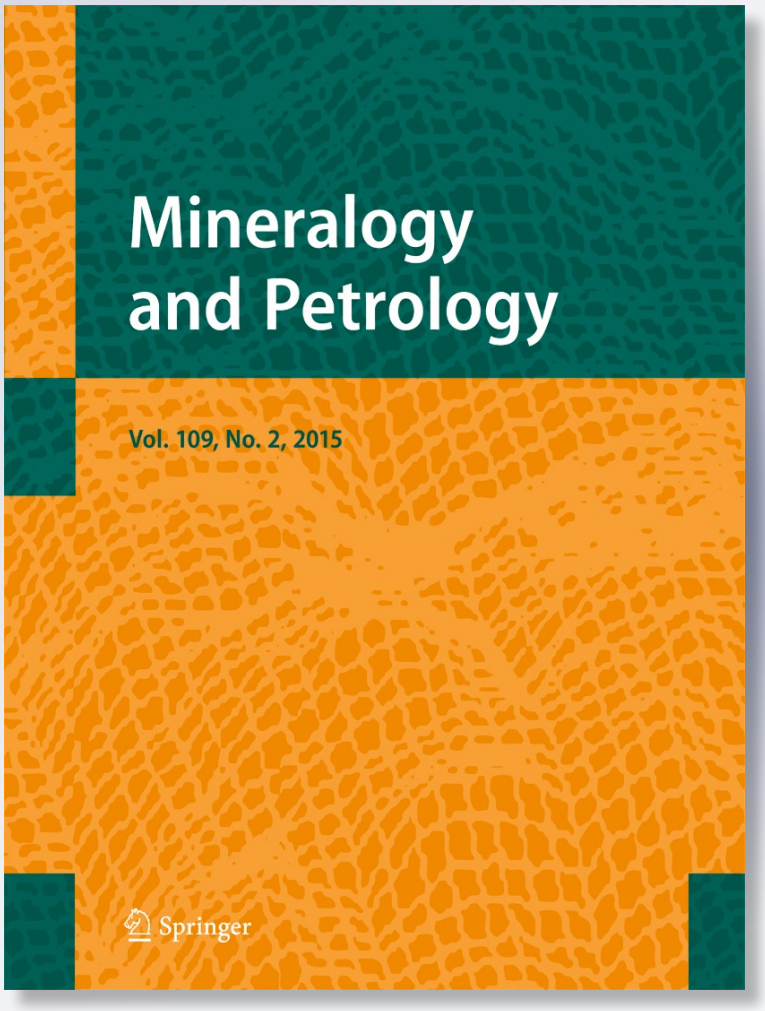

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ORIGINAL PAPER

Determination of the spinel group end-members based on electron microprobe analyses

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Abstract The spinel group minerals have been the focus of many studies, not only because of their economic interest, but also due to the fact that they are very useful as petrogenetic indicators. The application End-Members Generator (EMG) allows to establish, based on electron microprobe analyses (EMPA), the 19 end-members of the spinel group: $MgAl_2O_4$ (Spinel sensu stricto, s.s.), $FeAl_2O_4$ (Hercynite), $MnAl_2O_4$ (Galaxite), $ZnAl_2O_4$ (Gahnite), $MgFe_2O_4$ (Magnesioferrite), Fe_3O_4 (Magnetite), $MnFe_2O_4$ (Jacobsite), $ZnFe_2O_4$ (Franklinite), $NiFe_2O_4$ (Trevorite), $MgCr_2O_4$ (Magnesiochromite), $FeCr_2O_4$ (Chromite), $MnCr_2O_4$ (Manganochromite), $ZnCr_2O_4$ (Zincochromite), $NiCr_2O_4$ (Nichromite), MgV_2O_4 (Magnesiocoulsonite), FeV_2O_4 (Coulsonite), MnV_2O_4 (Vuorelainenite), Mg_2TiO_4 (Qandilite) and Fe_2TiO_4 (Ulvöspinel). EMG is an application that does not require an installation process and was created with the purpose of performing calculations to obtain: cation proportions (per formula unit, p.f.u.), end-members of the spinel group, redistribution proportions for the corresponding end-members in the Magnetite prism or Ulvöspinel prism and a data validation section to check the results. EMG accepts .csv data files and the results obtained can be used to represent a given dataset with the SpinelViz program or any other 2D and/or 3D graph plotting software.

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Introduction

Spinel group minerals are some of the first to crystallize from a siliceous melt and their refractory nature and stability under a wide range of geological conditions, have made them useful indicators of magmatic conditions at the time of their crystallization (Roeder 1994). Therefore, they are of interest as petrogenetic indicators and a very useful prospecting tool in the search for mineral deposits (Irvine 1965, 1967; Dick and Bullen 1984; Sack and Ghiorso 1991b; Groves and Brotherton 1983 and Ahmed et al. 2005; among others).

Based on their properties and utilities, Barnes and Roeder (2001) published a very extensive database of spinel group minerals from different tectonic environments such as: alaskan ultramafic complexes, tholeiitic basalts and boninites, detrital crystals, komatiites, continental mafic-ultramafic intrusions (including layered intrusions), metamorphic spinels, ophiolites – alpine and oceanic peridotites, and mantle – lower crustal xenoliths. In this contribution, the authors propose grouping the spinel minerals in specific fields of the Magnetite prism considering the Cr-Al-Fe^{3+}-Mg-Fe^{2+} ions and some relationships between these cations and TiO_2.

Classic research papers dealing with the spinel group minerals are those of Irvine (1965), Haggerty (1976), Sack and Ghiorso (1991a), Deer et al. (1992) and references therein, which are based on the Magnetite or Ulvöspinel prisms (Fig. 1), known as the modified Johnson spinel prism (Stevens 1944).

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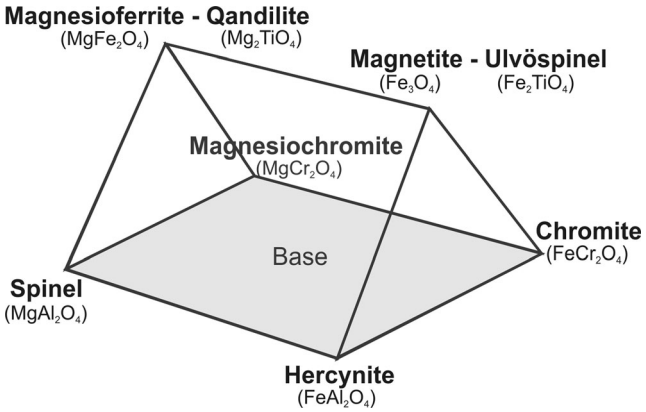

Fig. 1 Magnetite or Ulvöspinel prism (Stevens 1944)

Two of the most serious difficulties when attempting to make these calculations are the fact that this group of oxides: 1) constitute a solid solution with 22 final members and, 2) show bivalent and trivalent cation substitutions, which increases the complexity of the calculations (Barth and Posnjak 1932; Palanche et al. 1944; Haggerty 1976; Deer et al. 1992; Gaines et al. 1997; Bowles et al. 2011).

In order to contribute to the understanding of the complex chemical system of this mineral group it is of uppermost importance to improve the applications devoted to their plotting on 3D graphs based on their chemical composition.

Among the available programs or applications used to establish some end-members of the spinel group, Sack and Ghiorso (1991b) developed a geothermometer based on the Mg-Fe exchange between olivine and spinel (sensu lato, s.l.). In this application the user introduces the composition of spinels (s.l.) expressed as oxides, and the MgO and FeO contents of olivine, and the program returns information about: spinel (s.l.) activity, temperature, olivine end-members and 5 spinel (s.l.) molar fractions ($FeAl_2O_4$- $MgAl_2O_4$- $FeCr_2O_4$- Fe_2TiO_4- Fe_3O_4). The sum of these end-members of the spinel group equals 1.

The program Norm version 4.0 (1993) written by Peter Ulmer allows calculation of some mineral-norms and is based on data inputs as EMMA, SX50 or NST files. This program calculates 11 end-members of the spinel group: Spinel (s.s.) – Hercynite – Galaxite – Magnesioferrite – Magnetite – Jacobsite – Magnesiochromite – Chromite – Manganochromite - Ulvöspinel and Zn-Spinel. The sum of these end-members is approximately 1.

Ganuza et al. (2012) developed the SpinelViz program for the visualization of the spinel group minerals in 2D and 3D. The application projects the spinel (s.l.) geochemical data onto 2D and 3D plots. This program is functional and very useful because it can display mineral composition datasets from different tectonic settings, requiring only that the user previously precomputes the proportions of the end-members for Magnetite or Ulvöspinel prisms. This is not always possible, hindering the use of the application.

Ganuza et al. (2014) introduce a new program called "The Spinel Explorer", which is an interactive visual analysis application for spinel group minerals. The Spinel Explorer includes most of the diagrams commonly used for analyzing spinel group minerals, including 2D binary plots, ternary plots, and 3D Spinel prism plots. Besides those specific plots, the program also employs coordinated multiple views and all views are interactive and linked.

In this contribution we propose an application called EMG (End-Members Generator) that performs calculations to obtain cation proportions per formula unit (p.f.u), end-members of the spinel group, and the redistribution proportions of end-members data required to plot a given dataset in the Magnetite prism or Ulvöspinel prism . This contribution describes the methodology applied to perform the involved calculations and the use of the software application for these determinations. The resulting data provided by EMG allows and facilitates the later utilization and representation of a dataset with the SpinelViz program or any other 2D and 3D plotting program.

The end-members of the spinel group

The spinel group minerals nomenclature is based on the standard chemical formula $X^{2+}Y^{3+}{}_2O_4$. According to Gaines et al. (1997) the spinel group minerals comprise 22 mineral species which are grouped in 5 subgroups as sumarized in Table 1.

The software application presented in this contribution allows the calculation of 19 end-members (Table 1). Only those end-members with Cu, Ge and Co are not determined.

Procedure considerations

The calculations of the spinel end-members were carried out according to the following statements:

1) Determination of cation values from chemical analyses was made according to the atomic weights of Weast (1974, pB1) and based on Spear (1993, Chapter 4) for the calculation of mineral formulae. This last author used the mineral formulae based on 24 cations but for our purpose it has been modified to 3 cations because this is the number adopted by Gaines et al. (1997) to express the 22 end-members that we use. The calculations obtained for cations were checked with de method of Droop (1987), and both methodologies gave the same results.

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Table 1 22 mineral species for the spinel group minerals according to Gaines et al. (1997), including those calculated with EMG

Spinel end-members Subgroups	According to Gaines et al. 1997 Mineral species	Calculate according this work End-member
Aluminum subgroup, XAl_2O_4 (X = Mg, Fe, Mn, Zn)	$MgAl_2O_4$ (Spinel s.s.)	*
	$FeAl_2O_4$ (Hercynite)	*
	$MnAl_2O_4$ (Galaxite)	*
	$ZnAl_2O_4$ (Gahnite)	*
Iron subgroup, $XFe^{3+}{}_2O_4$ (X = Mg, Fe^{2+}, Mn, Zn, Ni, Cu, Ge)	$MgFe_2O_4$ (Magnesioferrite)	*
	Fe_3O_4 (Magnetite)	*
	$MnFe_2O_4$ (Jacobsite)	*
	$ZnFe_2O_4$ (Franklinite)	*
	$NiFe_2O_4$ (Trevorite)	*
	$CuFe_2O_4$ (Cuprospinel)	
	$GeFe_2O_4$ (Brunogeierite)	
Chromium subgroup, XCr_2O_4 (X = Mg, Fe^{2+}, Mn, Zn, Ni, Co)	$MgFe_2O_4$ (Magnesiochromite)	*
	$FeCr_2O_4$ (Chromite)	*
	$MnCr_2O_4$ (Manganochromite)	*
	$ZnCr_2O_4$ (Zincochromite)	*
	$NiCr_2O_4$ (Nichromite)	*
	$CoCr_2O_4$ (Cochromite)	
Vanadium subgroup, XV_2O_4 (X = Mg, Fe^{2+}, Mn)	MgV_2O_4 (Magnesiocoulsonite)	*
	FeV_2O_4 (Coulsonite)	*
	MnV_2O_4 (Vuorelainenite)	*
Titanium subgroup, X_2TiO_4 (X = Mg, Fe^{2+})	Mg_2TiO_4 (Qandilite)	*
	Fe_2TiO_4 (Ulvöspinel)	*

2) After cation determination, the Fe^{3+}/Fe^{2+} ratio estimation was carried out according to the stoichiometric methodology of Droop (1987) and the spinel (s.l.) data published by this author was used as a reference to make all calculations described in this manuscript. The users can choose if they want the program to provide the stoichiometric calculation of Fe_2O_3 and FeO.
3) In case that the user has previously determinated Fe_2O_3 and FeO by another methodology, the EMG can also be used to provide the 19 end-members.
4) The sum of the 19 end-members is 8 because we consider the presence of oxygen in the standard chemical formula $X^{2+}Y^{3+}{}_2O_4$. In the spinel group minerals oxygen is the only anion present in the crystalline framework and considering the formula unit as XY_2O_4, the total cation charge is 8 and this number is twice the number of oxygen in the formula unit. For this reason the sum of the end-members considering the formula unit based on 4 oxygens and 3 cations is restricted by the total cation charge of 8.
5) To plot the data in the Magnetite or Ulvöspinel prisms, recalculation of the end-members must be made and the normalizations must be equal to 1. Afterwards the users can plot their data with the SpinelViz program for visualization in 2D and 3D, or directly use ternary and binary diagrams to plot the dataset (2D).

In order to choose which prism should be used to plot the data, we have introduced 2 conditions:

A) If $Fe_2O_3 > 2TiO_2$ wt.%, the data should be plotted in the Magnetite prism. This condition is ruled by the following comparison:

Fe_3O_4 (Magnetite)$\equiv Fe_2TiO_4$ (Ulvöspinel)
$FeO \cdot Fe_2O_3 \equiv 2\ FeO \cdot TiO_2$
$Fe_2O_3 \equiv 2\ TiO_2$

B) If $Fe_2O_3 < 2TiO_2$ wt.% the data should be plotted in the Ulvöspinel prism according to the equation indicated above.

If Fe_2O_3 and TiO_2 wt.% are both equal to 0, the dataset will be plotted on the base of the prism. In this particular case, data could be plotted in both prisms since they both have the same end-members on the base (Fig. 1), a quite uncommon situation. Namely, when the program was checked with the dataset from different tectonic settings (26.000 data) compiled by Barnes and Roeder (2001), only 150 data have both Fe_2O_3 and TiO_2 equal to 0. Users can choose one prism or the other to plot their data, depending on the convenience of visualizing the whole dataset in the Magnetite prism or in the Ulvöspinel prism although

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they must check the end-members obtained after the calculations, to know which prism they should use to represent their dataset.

6) EMG incorporates a "Data Validation" option which allows users to verify if the calculations of their data are well computed. The data validation is accomplished considering 29 ratios between the following end-members: $FeAl_2O_4/MgAl_2O_4$; $FeFe_2O_4/MgFe_2O_4$; $FeCr_2O_4/MgCr_2O_4$; FeV_2O_4/MgV_2O_4; $MnAl_2O_4/FeAl_2O_4$; $MnFe_2O_4/FeFe_2O_4$; $MnCr_2O_4/FeCr_2O_4$; MnV_2O_4/FeV_2O_4; $MnAl_2O_4/MgAl_2O_4$; $MnFe_2O_4/MgFe_2O_4$; $MnCr_2O_4/MgCr_2O_4$; MnV_2O_4/MgV_2O_4; $MgCr_2O_4/MgAl_2O_4$; $FeCr_2O_4/FeAl_2O_4$; $MnCr_2O_4/MnAl_2O_4$; $MgFe_2O_4/MgAl_2O_4$; $FeFe_2O_4/FeAl_2O_4$; $MnFe_2O_4/MnAl_2O_4$; $MgFe_2O_4/MgCr_2O_4$; $FeFe_2O_4/FeCr_2O_4$; $MnFe_2O_4/MnCr_2O_4$; $Mg_2TiO_4/MgAl_2O_4$; $Fe_2TiO_4/FeAl_2O_4$; $MgV_2O_4/MgAl_2O_4$; $FeV_2O_4/FeAl_2O_4$; $MnV_2O_4/MnAl_2O_4$; $MgFe_2O_4/MgV_2O_4$; $FeFe_2O_4/FeV_2O_4$; $MnFe_2O_4/MnV_2O_4$. Examples are provided in the Electronic Supplementary Data.

The ratios mentioned above, have been considered for the data validation provided that for the calculated final end-members of a given spinel group mineral, the ratios between each pair of divalent cations (Fe, Mg, Mn, Zn, Ni) in each spinel subgroup will provide the same numerical value. Likewise, the ratios between each pair of trivalent cations (Al, Fe^{3+}, Cr, V, Ti) for each divalent cation will also be a constant numerical value.

In case that, for example, there is no Cr in the sample, the end-members with Cr will be equal to 0 and the same will happen concerning the ratios in the data validation. Moreover, if the spinel group mineral analyzed is a pure end-member all ratios in the data validation will be equal to 0.

Application description

EMG.exe should be copied in a folder of the users computer. Once the interface of the application is loaded, EMG is ready to be used. The user interface of the application is very simple (Fig. 2) and .csv (Comma Separated Value format) files can be loaded using the corresponding button.

The .csv source file must contain the wt.% oxides values in columns, the first column containing the sample name and the next columns the oxides (Table 2). The first row of the file is reserved for labels and the first cell of the first row for the word "Sample". The following rows must contain a label for each oxide. It is not required that the oxides follow a fixed order or all to be present. EMG considers the SiO_2, TiO_2, Al_2O_3, Cr_2O_3, V_2O_3, Fe_2O_3, FeO, MnO, MgO, CaO, ZnO, NiO, Na_2O and K_2O oxides, if any of these is not present in the input file a warning message is displayed and the computation proceeds assuming the value zero for the missing oxides.

If the user has previously determined the values of Fe_2O_3 and FeO, both oxides must be included but we strongly recommend to use the data obteined with EMPA for the calculations. Each data sample corresponds to a row in the .csv file, which means that for a twenty samples dataset the file must contain at least 21 rows. The labels corresponding to the oxides in the first row of the file are detailed Table 2.

If the user wants that EMG calculates Fe_2O_3 from FeO, in the column of Fe_2O_3 they must type 0.

EGM performs the corresponding calculations and provides the results in a new output .csv file. In addition, it allows calculations for the stoichiometric discrimination between Fe_2O_3 and FeO (wt.%), the cation proportions (p.f.u.), the end-members of the spinel group, recalculation of the end-members to the Magnetite prism or Ulvöspinel prism, and to perform a data validation. The data validation conducts a test to verify if the data introduced have been correctly calculated. In case the format of the file is correct, a "Selection" window is shown (Fig. 3) allowing the user to select which of those results should be included in the .csv output file. Once the selection is made, the application generates a new file containing the results of the calculations choosen by the user, and saves it in the same directory as the source file. In addition, EMG allows the user to obtain the results in separated files. If this option is selected, the application will generate a general file containing a compilation of the results of all calculations requested for the user, and one particular file for any selected item containing the results of that calculation in particular.

Table 3 is showing the results of 18 end-members data take from the Handbook of Mineralogy (Anthony

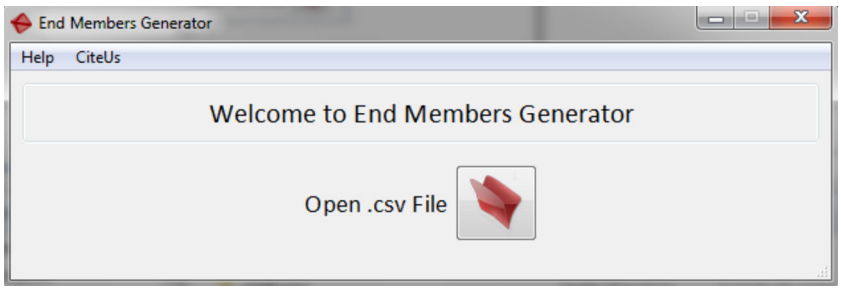

Fig. 2 EMG user interface

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Table 2 Oxide labels for .csv input files

Sample	SiO_2	TiO_2	Al_2O_3	Cr_2O_3	V_2O_3	Fe_2O_3	FeO	MnO	MgO	CaO	ZnO	NiO	Na_2O	K_2O	Total
Droop 1987 data	0	0	61.99	0	0	0	24.68	0.11	13.7	0	0	0	0	0	100.48
Coulsonite pure end-member	0	0	0	0	67.6	0	32.4	0	0	0	0	0	0	0	100
Magnesiochromite pure end-member	0	0	0	79.04	0	0	0	0	20.96	0	0	0	0	0	100
Chromite pure end-member	0	0	0	67.9	0	0	32.1	0	0	0	0	0	0	0	100
Zincochromite pure end-member	0	0	0	65.13	0	0	0	0	0	0	34.87	0	0	0	100
Spinel pure end-member	0	0	71.67	0	0	0	0	0	28.33	0	0	0	0	0	100
Magnesiocoulsonite pure end-member	0	0	0	0	78.81	0	0	0	21.19	0	0	0	0	0	100
Hercynite pure end-member	0	0	58.66	0	0	0	41.34	0	0	0	0	0	0	0	100
Gahnite pure end-member	0	0	55.61	0	0	0	0	0	0	0	44.39	0	0	0	100
Trevorite pure end-member	0	0	0	0	0	68.13	0	0	0	0	0	31.87	0	0	100
Magnetite pure end-member	0	0	0	0	0	68.97	31.03	0	0	0	0	0	0	0	100
Magnesioferrite pure end-member	0	0	0	0	0	79.85	0	0	20.15	0	0	0	0	0	100
Ulvöspinel	0	35.73	0	0	0	0	64.27	0	0	0	0	0	0	0	100
Jacobsite	0	0.38	8.15	0	0	59.5	0.5	32.1	0.03	0	0	0	0	0	100.66
Franklinite	0	0.7	1.25	0	0	63.9	3.6	0.6	0	0	30.25	0	0	0	100.3
Manganochromite	0	0	0	62.3	1.7	0	9.4	24	0	0	1.7	0	0	0	99.1
Galaxite	0.96	0	45.71	0	0	0	16.36	34.03	1.5	0	0	0	0	0	98.56
Qandilite	0	26.63	5.67	0	0	26.62	11.98	0	29.11	0	0	0	0	0	100.01
Vuorelainenite	0	0	0	4.7	63.3	0	7.6	22	0	0	2.4	0	0	0	100
Coulsonite 2	0	5.29	0	0.12	59.6	0	33.1	0	0	0	0	0	0	0	98.11

et al. 2001–2005) to test the program. The only end-member which is not included is Nichromite because this mineral is not listed in the Handbook of Mineralogy and according to the data from the webpage http://webmineral.com/, this end-member has not only Ni but also Co and EMG does not calculate end-members with Co, as already indicated.

Important considerations to use EMG

To use the EMG application some important considerations must be taken into account:

1) The sample name must be listed in the first column of the .csv file.

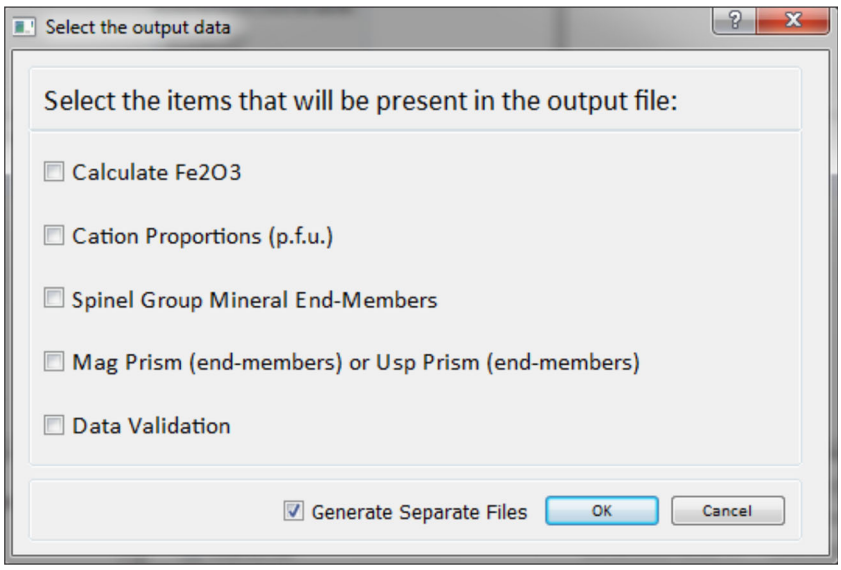

Fig. 3 Selection window

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Table 3 Different end-members data results taken from the Handbook of Mineralogy (Anthony et al. 2001–2005) and data from Droop (1987), all of them used to test EMG

Sample	$MgAl_2O_4$	$FeAl_2O_4$	$MnAl_2O_4$	$ZnAl_2O_4$	$MgFe_2O_4$	$FeFe_2O_4$	$MnFe_2O_4$	$ZnFe_2O_4$	$NiFe_2O_4$	$MgCr_2O_4$
Droop 1987 data	4.118	3.539	0.019	0	0.174	0.149	0.001	0	0	0
Coulsonite pure end-member	0	0	0	0	0	0	0	0	0	0
Magnesiochromite pure end-member	0	0	0	0	0	0	0	0	0	8
Chromite pure end-member	0	0	0	0	0	0	0	0	0	0
Zincochromite pure end-member	0	0	0	0	0	0	0	0	0	0
Spinel pure end-member	8	0	0	0	0	0	0	0	0	0
Magnesiocoulsonite pure end-member	0	0	0	0	0	0	0	0	0	0
Hercynite pure end-member	0	8	0	0	0	0	0	0	0	0
Gahnite pure end-member	0	0	0	8	0	0	0	0	0	0
Trevorite pure end-member	0	0	0	0	0	0	0	0	8	0
Magnetite pure end-member	0	0	0	0	0	8	0	0	0	0
Magnesioferrite pure end-member	0	0	0	0	8	0	0	0	0	0
Ulvöspinel	0	0	0	0	0	0.002	0	0	0	0
Jacobsite	0.002	0.021	1.389	0	0.011	0.1	6.476	0	0	0
Franklinite	0	0.028	0.005	0.205	0	0.903	0.152	6.697	0	0
Manganochromite	0	0	0	0	0	0.079	0.315	0.019	0	0
Galaxite	0.438	0.605	5.643	0	0.086	0.119	1.109	0	0	0
Qandilite	0.929	0.215	0	0	2.786	0.643	0	0	0	0
Vuorelainenite	0	0	0	0	0	0	0	0	0	0
Coulsonite 2	0	0	0	0	0	0	0	0	0	0

Sample	$FeCr_2O_4$	$MnCr_2O_4$	$ZnCr_2O_4$	$NiCr_2O_4$	MgV_2O_4	$FeV2O_4$	MnV_2O_4	Mg_2TiO_4	Fe_2TiO_4
Droop 1987 data	0	0	0	0	0	0	0	0	0
Coulsonite pure end-member	0	0	0	0	0	8	0	0	0
Magnesiochromite pure end-member	0	0	0	0	0	0	0	0	0
Chromite pure end-member	8	0	0	0	0	0	0	0	0
Zincochromite pure end-member	0	0	8	0	0	0	0	0	0
Spinel pure end-member	0	0	0	0	0	0	0	0	0
Magnesiocoulsonite pure end-member	0	0	0	0	8	0	0	0	0
Hercynite pure end-member	0	0	0	0	0	0	0	0	0
Gahnite pure end-member	0	0	0	0	0	0	0	0	0
Trevorite pure end-member	0	0	0	0	0	0	0	0	0
Magnetite pure end-member	0	0	0	0	0	0	0	0	0
Magnesioferrite pure end-member	0	0	0	0	0	0	0	0	0
Ulvöspinel	0	0	0	0	0	0	0	0	7.998
Jacobsite	0	0	0	0	0	0	0	0	0.001
Franklinite	0	0	0	0	0	0	0	0	0.01
Manganochromite	1.414	5.63	0.348	0	0	0.039	0.156	0	0
Galaxite	0	0	0	0	0	0	0	0	0

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Table 3 (continued)

Sample	$FeCr_2O_4$	$MnCr_2O_4$	$ZnCr_2O_4$	$NiCr_2O_4$	MgV_2O_4	$FeV2O_4$	MnV_2O_4	Mg_2TiO_4	Fe_2TiO_4
Qandilite	0	0	0	0	0	0	0	2.785	0.643
Vuorelainenite	0.138	0.405	0.039	0	0	1.887	5.532	0	0
Coulsonite 2	0.015	0	0	0	0	7.372	0	0	0.614

2) The values of wt.% oxides obtained with an EMPA (in any order), must be listed in columns to the right side of the sample name column.
3) The values of wt.% oxides that must be introduced are SiO_2, TiO_2, Al_2O_3, Cr_2O_3, V_2O_3, Fe_2O_3, FeO, MnO, MgO, CaO, ZnO, NiO, Na_2O and K_2O. Other oxides analyzed by the users will not be considered in the calculations.
4) If the introduced data include some amount of wt.% SiO_2, after the program has performed the discrimination between Fe^{2+} and Fe^{3+} cations and all the other normalization calculations, the total wt.% of the all oxides will sum more than 100 wt.%.
5) Since the stoichiometric methodology of Droop (1987) has been adopted, if the result of the following equation Fe^{3+} (F=2X(1 - T/S)) is negative, EMG will consider all iron as Fe^{2+}, and in this case Fe^{3+} and Fe_2O_3 will be equal to 0 in the final result.
6) Although the program can discriminate between the two prisms commonly used (Magnetite and Ulvöspinel prisms), it is very important to analyze the results considering the 19 the end-members.
7) According to the previous consideration, when the introduced values of MnO, V_2O_3, NiO and ZnO are greater than 0.45 wt.%, the program will not give values for any of the prisms because the proportion of some of the end-members ($MnAl_2O_4$ - $ZnAl_2O_4$ - $MnFe_2O_4$ - $ZnFe_2O_4$ - $NiFe_2O_4$ - $MnCr_2O_4$ - $ZnCr_2O_4$ - $NiCr_2O_4$ - MgV_2O_4 - FeV_2O_4 - MnV_2O_4) could be higher than 5 %, introducing an error in the plotted dataset. For this reason, if the users have mineral analyses with V_2O_3, MnO, NiO and/or ZnO contents≥0.45 wt.%, we recommend not to use any of the prisms to plot the data (examples in Electronic Supplementary Data).
8) This program does not perform the calculation for end-members with Cu, Co or Ge. Nonetheless, the users can request from the authors the calculation of end-members including these cations.

Conclusions

The spinel group minerals are very important because their composition is related to the tectonic environment to which they belong and particularly the 8 spinel end-members which are part of the Magnetite or Ulvöspinels prisms. Up to now there was no simple application to calculate the end-members of this group of minerals.

This manuscript presents an easy to use and free application software called End-Members Generator, which allows the determination of 19 spinel end-members proportions, calculation of Fe_2O_3 based on FeO (wt.%) and calculation of the

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cation proportions (p.f.u.), based on electron microprobe analyses. EMG also gives a validation data section and allows to recalculate the proportion of the spinel end-members for the Magnetite or Ulvöspinel prisms.

With the determination of 19 spinels end-members it is possible to evaluate if it is appropiate to use the Magnetite or the Ulvöspinel prisms depending on the most abundant end-members present in a given set of samples. Moreover, in case the analyses can be recalculated to plot on some of the prisms, the user has the opportunity to visualize the results on 3D prism as well as 2D plots.

Technical information

The application was implemented in C++ and Qt, using the qtCreator (Nokia 2008) and can be freely downloaded at the VyGLab website (http://vyglab.cs.uns.edu.ar). The users are kindly requested to give appropiate credit to this article in their publications if EMG has been used to perfom calculations.

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