

SOFTWARE NOTICE

SPINEL and SPINELTAB: Macintosh programs to plot spinel analyses in the three-dimensional oxidized (magnetite) and reduced (ulvöspinel) prisms

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ABSTRACT

SPINEL and SPINELTAB accept analyses of spinels for nine major and minor oxides, recalculate microprobe data where possible to 32 O atoms, eight divalent, and 16 trivalent cations, and plot their positions in the oxidized magnetite or reduced ulvöspinel prisms. Any angle of view can be chosen by the user, enabling stereographic pairs to be produced. Plots can be copied to the clipboard for editing in other Macintosh graphics applications. SPINEL is a self-contained variant, allowing data entry, editing, and printing within the program, whereas SPINELTAB accepts standard Macintosh tab-delimited input files, generated by other spreadsheet or word-processing applications. Both versions are otherwise functionally identical.

INTRODUCTION

The general spinel formula is MR_2O_4 , where M covers any of a wide range of divalent cations (Mg, Fe, Zn, etc.) and R a similar medley of trivalent cations (Al, Fe, Cr, etc.) and also Ti^{4+} . The complexity of element substitutions and the lack of any official IMA nomenclature for minor substitutions make summarizing their chemistry by name or on two-dimensional plots extremely difficult. As a result, it is now common to plot spinels in either or both of the oxidized magnetite (Fe_3O_4 - $MgFe_2^{3+}O_4$ - $MgAl_2O_4$ - $Fe^{2+}Al_2O_4$ - $Fe^{2+}Cr_2O_4$ - $MgCr_2O_4$ = Mt-Mf-Sp-Her-Chr-Pc) or reduced ulvöspinel (MgTit-Usp-Sp-Her-Chr-Pc) prisms, which provide a reasonably easily interpretable three-dimensional view on two-dimensional paper (Fig. 1). Such plots are now extremely widespread, notably in the literature on diamond exploration, where spinel compositions are a critical factor in assessing the economic potential of kimberlitic bodies. They are, however, difficult to generate by hand and are an obvious candidate for computerization.

We are aware of no other published program to plot spinel analyses, and the present article therefore offers one for the Macintosh range of microcomputers, which are particularly suited to graphical output such as Figure 1.¹

¹ Executable copies are available from the authors in exchange for other software. Please send disks with the software you are prepared to exchange. We will return your disks with a copy of whichever version you specify (SPINEL or SPINELTAB), a machine-readable copy of the appropriate documentation (or reprint), and a comprehensive test file of data from Deer et al. (1962). Users not able to exchange software are asked to send a small contribution (say US\$10) in exchangeable form, to cover costs. We regret we are unable to deal with requests that only enclose a single disk. We ask users to refrain from copying either program to third parties without reference to us and to cite this paper when the programs are used in their published work. Suggestions for improvements are welcomed.

PROGRAM DETAILS

Two versions of SPINEL are available, differing only in their manner of data storage and input and in other respects identical. Both are written as stand-alone applications in Microsoft QuickBASIC v1.0, run on all Macs from 512 to Iix, and employ the exceptionally user-friendly Mac interface. Both have been tested not only under a wide range of system configurations (up to System 6.0.3 under Multifinder), but also on a large data base of several hundred spinel analyses. A 400k disk drive is adequate to use either variant; a hard disk is not necessary, though useful.

By means of a series of standard dialog boxes, both versions allow the user the following options: (1) to select either or both of the oxidized and reduced spinel prisms for plotting; (2) to enlarge or shrink the plot; (3) to choose the angle of view of the plot in terms of its horizontal rotation and forward tilt, allowing stereographic pairs to be produced by repeating the same plot with about 3° horizontal rotation between the two projections (Fig. 1); (4) to distinguish up to five distinct groups of spinel analyses by means of different symbols (specified in the input file by the numbers 1, 2, 3, 4, and 5 against each analysis); for clarity, resulting plots use solid symbols for the upper (oxidized) prism and open symbols for the lower (reduced) prism (Fig. 1); (5) to print out the calculated cationic proportions on which a plot is based.

Both programs deliberately lack internal options to edit or print spinel prism plots, because these are automatically copied

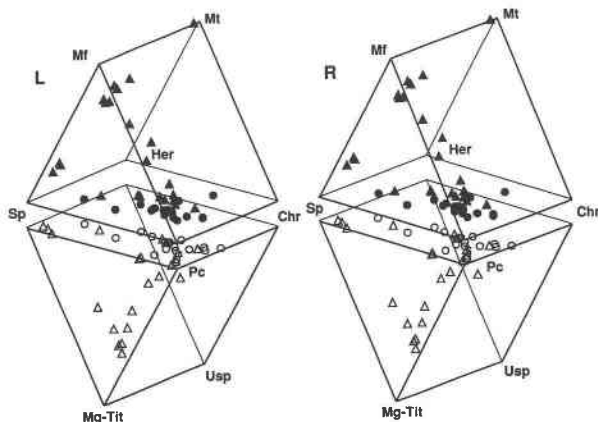


Fig. 1. Stereographic pair of plots from SPINEL and SPINELTAB printed on an Apple LaserWriter. Data from Deer et al. (1962). Chr = chromite ($FeCr_2O_4$); Her = hercynite ($FeAl_2O_4$); Mt = magnetite (Fe_3O_4); Mf = magnesioferrite ($MgFe_2O_4$); Mg-Tit = magnesiotitanite (Mg_2TiO_4); Pc = picrochromite ($MgCr_2O_4$); Sp = spinel ($MgAl_2O_4$); Usp = ulvöspinel (Fe_2TiO_4).

DATA ENTRY/EDIT		Sample I.D.:	<input type="text" value="UMI/01"/>
<input type="text" value="0.05"/>	SiO ₂	<input type="button" value="Enter this sample"/> <input type="button" value="Cancel"/> <input type="button" value="Sample entry finished"/>	
<input type="text" value="0.09"/>	TiO ₂		
<input type="text" value="14.46"/>	Al ₂ O ₃		
<input type="text" value="55.05"/>	Cr ₂ O ₃		
<input type="text" value="3.59"/>	Fe ₂ O ₃		
<input type="text" value="12.02"/>	FeO		
<input type="text" value="0"/>	ZnO		
<input type="text" value="0.24"/>	MnO		
<input type="text" value="14.5"/>	MgO		
<input type="text" value="2"/>	Plot Symbol (1-3)		

Fig. 2. Data-entry box from SPINEL. The tab key or mouse is used to move between fields, in the usual Macintosh fashion.

during execution to the Macintosh clipboard as PICT files, from which they are readily pasted for printing or subsequent editing in innumerable Macintosh graphics or word-processing applications (MacWrite, MacDraw, SuperPaint, etc). They can also be saved as PICT files. Best results for printing on a LaserWriter will be obtained using MacDraw or other object-oriented applications.

Both programs can cope with up to nine major and minor oxides (Fig. 2). If one of the iron oxides in a particular spinel analysis is entered as 0.0 (as with microprobe data), both attempt to recalculate to eight divalent and 16 trivalent cations per 32 O atom formula unit, essentially the same procedure as used in MINTAB (Rock and Carroll, 1990). For the purposes of formula-unit calculation, SiO₂ is grouped with TiO₂, MnO with FeO, and ZnO with MgO. [SiO₂ present as contaminant rather than actually substituted in a spinel should not, of course, be entered at all, and this may include Si determined by an energy-dispersive analyzer as a result of internal fluorescence in the Si(Li) detector]. Although it would have been possible to include NiO, CoO, Mn₂O₃, and other oxides, the intrinsic value of the oxidized and reduced spinel prisms as plots decreases as these additional components increase; the range of nine used here was felt to be an adequate compromise.

Details of the differences between SPINEL and SPINELTAB now follow.

SPINEL: Editing version

This version is more suitable for users who need a completely stand-alone, self-contained version that requires no use of other Macintosh applications. By means of a standard Macintosh-style data-entry box (Fig. 2), the user can create new input files of

spinel analyses, edit old ones (adding, amending, or deleting analyses), or print out a file. However, the internal format used to store files, though transparent to the user within SPINEL itself, is for various reasons delimited by a carriage return; this means that SPINEL files will not always be easily imported into other Macintosh applications such as Excel or MacWrite, which expect tab-delimited data.

SPINELTAB: Non-editing version compatible with other Macintosh applications

Unlike SPINEL, SPINELTAB has no internal data entry, editing, or printing capabilities but instead accepts a type of input file that is more compatible not only with other major Macintosh applications, but also with our own recently described programs (Wheatley and Rock, 1988; Rock and Carroll, 1989, 1990). It is thus more useful for those who wish to perform mineral recalculations in MINTAB as well as spinel plots, or intend to store their data in other Macintosh spreadsheet or data-base applications (e.g., Cricket Graph, Excel, Statview, 4th Dimension).

SPINELTAB uses tab-delimited ASCII files (a universal Mac standard), in which rows represent samples (spinel analyses) and columns represent variables (oxides), and in which the first line must be a series of tab-delimited labels indicating the order of these variables (see below and Table 1). Such files are readily generated, either directly by typing data into simple text editors such as Edit; or indirectly by entering data into spreadsheet or data-base applications, and then saving the file in ASCII format (usually referred to in Save or Save As menu options as "text" or "textonly"). For full instructions on how to do this, see the appropriate application manuals, including that for TRIPLOT (Rock and Carroll, 1989). Neither SPINEL nor SPINELTAB will accept the program-specific binary format files produced as default by major Mac applications (these are usually termed "normal," or "full document" files in the Save and Save As options).

SPINELTAB recognizes the same nine oxides as SPINEL (Fig. 2). The first (label) line of the input file must consist of a tab-delimited string of at least four of these five identifiers: TiO₂, Al₂O₃, MgO, and at least one of FeO or Fe₂O₃. ZnO, MnO, SiO₂, and Cr₂O₃ will be recognized if present, but are not essential. These oxides can be in any order: SPINELTAB will rearrange them during processing. Identifiers must, however, be specified exactly as in Figure 2, e.g., SiO₂, not SIO₂, sio₂, SiO₂, slo₂, Si, or SI (subscripts cannot of course be used). Subsequent rows of actual data must of course conform to the oxide order and combination preset in the label line and must consist of tab-delimited columns of real decimal numbers indicating percentages (e.g., 35.64). If a tenth column headed "Symbol" is identified as present by the label line of the input file, it should contain the numbers 1-5 only, and will be used as in Figure 2

Table 1. Typical input data-file for SPINELTAB (same spinel analysis as in Fig.2)

Label	Δ	SiO ₂	Δ	Al ₂ O ₃	Δ	Fe ₂ O ₃	Δ	FeO	Δ	MgO	Δ	TiO ₂	Δ	MnO	Δ	ZnO	Δ	Cr ₂ O ₃	Δ	Symbol	↵	Label line	
DHZ	2	Δ	0.05	Δ	14.46	Δ	3.59	Δ	12.02	Δ	14.5	Δ	0.24	Δ	0.09	Δ	0.0	Δ	55.05	Δ	2	↵	Spinel 1
etc.																						Spinel 2	

Note: Δ represents a tab character, ↵ a carriage-return. Variable order in the first line can be amended at will, as long as subsequent rows are in the same order. Leading zeros and spaces are allowed in the data rows, but spaces and case variations (SIO₂ etc.) are *not* allowed in the label line.

to distinguish the plotting symbol for up to five groups of spinel analyses on the same plot (as in Fig. 1). Any other variables (columns) not among those specifically recognized will be ignored. This allows input of preexisting data files into SPINELTAB without any editing; sample numbers or other identifiers (e.g., "Label" in Table 1) will simply be ignored.

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REFERENCES CITED

- Deer, W.A., Howie, R.A., and Zussman, J. (1962) Rock-forming minerals. Longman's, London.
- Rock, N.M.S., and Carroll, G.W. (1989) TRIPLLOT and ACF: General-purpose and metamorphic ACF-AKF-AFM triangular plotting programs for mainframes and microcomputers. *American Mineralogist*, 74, 277-280.
- (1990) MINTAB: A general-purpose mineral recalculation and tabulation program for Macintosh microcomputers. *American Mineralogist*, 75, 424-430.
- Wheatley, M.R., and Rock, N.M.S. (1988) SPIDER: A Macintosh program to generate normalized multielement "spidergrams." *American Mineralogist*, 73, 919-921.

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