

SOFTWARE NOTICE

TRIPLLOT and ACF: General-purpose and metamorphic ACF-AKF-AFM triangular plotting programs for mainframes and microcomputers

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ABSTRACT

Two suites of triangular plotting programs are documented that generate (1) general-purpose A-B-C plots and (2) the specialized ACF, A'KF, and A"FM diagrams used in metamorphic petrology. Each suite consists of versions in FORTRAN for mainframe computers, using the graphics subroutine libraries GKS and GPGS, and versions in Pascal for the Apple® Macintosh® microcomputer, using its own internal graphics routines.

INTRODUCTION

As can be seen by any cursory glance at the literature, triangular diagrams are an essential tool in many branches of earth science (petrology—sedimentary, igneous, and metamorphic—mineralogy, sedimentology, etc.). However, they are rarely programmed by the well-known, proprietary graphics packages (SAS/GRAPH, SYSTAT), whether in mainframe or microcomputer implementations. As a result, several local catalogues of geological computer programs (e.g., Sowerbutts, 1985) indicate the existence of specially written triangular plotting programs for geological use.

Some programs are for the IBM PC or compatible micros, but a further large group are for much less widely distributed machines (e.g., the UK BBC model B); most are written in dialects of BASIC (e.g., Topley and Burwell, 1984) and are therefore of limited portability. Graphics programs are, of course, intrinsically among the least portable of software to begin with, because of the variety and incompatibility of plotting subroutines. The present note therefore advertises a suite of triangular plotting programs that are designed to be as portable as is ever possible with graphics software and, hence, of general use to the geological community. They are portable for the following reasons:

- They are written in standard FORTRAN-77 or Pascal (probably the most portable of major programming languages, and the languages now available on the widest range of computers).

* We would be glad to trade copies of either the mainframe or Macintosh versions of TRIPLLOT or ACF for other geological software. Machine-readable files containing all the necessary documentation are also provided (although, with the Macintosh versions, such documentation should soon prove superfluous). Users wishing to trade are welcome either to contact us first, to negotiate what can be exchanged, or to send examples of their own software on Macintosh 3.5-in. diskettes or IBM-type 5.25-in. floppy disks, which we can return with TRIPLLOT or ACF. Users without software to trade are also welcome to copies, but we would then appreciate it if they send spare disks that we could keep, in lieu of the costs of development, postage, etc. Users are asked not to copy either program to third parties without reference to us.

- The FORTRAN versions rely on two widely distributed libraries of graphics subroutines: (1) a library (Storey, 1984) based on GKS (Graphics Kernel System), the only current international standard and the first internationally portable graphics software (ISO, 1983; Brodlic, 1985), which should be available in most computer centers; (2) GPGS (NORSIGD, 1980), a library very widely used in both Europe and Australasia. These versions have already been run on PDP, GEC, and DEC mainframe computers.

- The Pascal versions are written for the Apple Macintosh, which is rapidly becoming as popular as the IBM PC among professional geologists; the Macintosh standard interface ensures that the programs run on any Macintosh model (Mac 128k, 512k, Plus, SE, or II).

- The programs all produce high-quality graphics output (Fig. 1), suitable for direct publication, and thus improve on previous programs that produce line-printer output suitable only for draft copies (e.g., Blencoe, 1974).

The mainframe and Macintosh versions in a sense represent the possible “extremes” of graphics output available in today’s computing environment: (1) the conventional mainframe environment, requiring line (or full screen) editors, line-by-line program execution, and output to conventional hardware devices (graphics terminal screens, pen or drum plotters); (2) the novel, user-friendly Macintosh interface, based on windows, menus, buttons, and dialogue boxes, with output to a graphics window on the Macintosh itself for subsequent incorporation (via the Macintosh clipboard) into word-processors or more elaborate graphics applications. The mainframe versions also embody two contrasting modes of graphics processing (Table 1): (a) *indirect*, in which the program generates a self-contained *spool file* that can be then used (at any subsequent time) to generate a plot via a device driver, on any device supported by such a driver; (b) *direct*, in which the plot is produced at run-time on any device to which the user is directly linked. Approach (b) has the advantage that the plot is generally produced more quickly; approach (a) is advantageous in that the user need not initially run the program from a graphics terminal, can view the plot on screen prior to producing hard copy, and can produce any number of hard copies (e.g., at different scales and on different devices) from only *one* run of the program.

We do not here offer programs for the IBM PC, primarily because we are aware that perfectly good commercial or university-generated packages already exist, but also because there are some advantages in the mainframe and Macintosh environments that are not shared by the PC.

SOFTWARE DESCRIPTION

Both suites of programs TRIPLLOT and ACF are available in *two* mainframe versions (using GKS-like and GPGS libraries) and

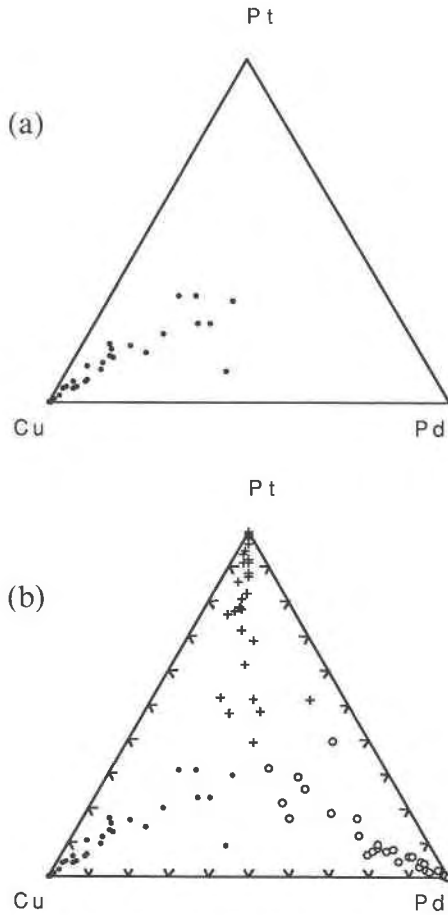


Fig. 1. Examples of general-purpose triangular diagrams generated by the Macintosh version of TRIPLOTT. Plots can be unadorned, as in (a), or have tick marks, as in (b). Full triangular grid lines can also be drawn. Plot (b) illustrates an overlay of the same data plotted three times (rotated through 60°) using different symbols each time. Subregions can also be plotted.

one Macintosh version. The mainframe versions should be portable to any mainframe environment supporting GKS or GPGS—with very minor changes to the FORTRAN code (specifically the logical unit numbers). Implementation on machines supporting different graphics libraries would however require rewriting the graphics subroutine calls. The Macintosh version is, of course, usable on Macintoshes only. All versions incorporate numerous error-trapping routines, both during option-setting and run-time. The interfaces of TRIPLOTT and ACF have been made as similar as possible, bearing in mind their distinct purposes. For example, overlaying of different suites of rocks (with different symbols) can be executed with both programs on a single plot (Figs. 1, 2). Input files can include sample numbers, but need not do so. Table 1 shows where the mainframe and Macintosh versions differ.

TRIPLOT: A general-purpose triangular plotting program

This program can produce a general *A-B-C* triangular plot from an input file whose size (columns by rows) is unlimited by TRIPLOTT itself. The user selects any 3 variables from this input file and assigns them to the *A, B, C* apices in any order. The program automatically calculates the sum $[A + B + C]$ and plots the points in the conventional way. If the user wishes to specify the input variables, this can be done by providing an initial line in the input file, giving the names of the variables present, whereupon TRIPLOTT labels the three apices accordingly. If the user does not specify the input variables, however, TRIPLOTT simply generates a plot labeled “Apex 1,” “Apex 2,” “Apex 3.”

TRIPLOT deals with missing data case-by-case: each analysis is plotted as long as values are supplied for all 3 chosen variables. Analyses are not rejected in their entirety during file input if missing values are encountered for any variable; that is, the same analysis can be used with a later set of three variables if it cannot be used with an earlier set. On the other hand, if several sets of 3 variables are used to plot different triangular diagrams from one data-file, an individual analysis will only appear on those plots for which values of all 3 variables are provided. This procedure ensures that maximum information within the data-file is plotted for different combinations of variables.

TABLE 1. General comparison of mainframe and Macintosh versions

	Mainframe versions	Macintosh version
Language	FORTRAN-77	Lightspeed Pascal
Provided as	Raw code; requires compiling and linking	Stand-alone application
Input data-matrix	Standard FORTRAN format with data-items either in predetermined columns (fixed format) or separated by commas or spaces (free format)	Macintosh ASCII format with tab-delimited items (e.g., Edit or MacWrite “textonly” files)
Maximum size for input file	Unlimited number of cases (analyses); variables limited only by length of FORMAT statement	Limited by available RAM only
Differentiating groups of data (cases) by different symbols	Codes included in input file for each case (e.g., “2” plots “x,” “8” plots “+”); all records plotted together; changing symbols requires editing of input file and cannot be done from within program <i>except</i> where one symbol is used for all cases; one run of program required for multiple symbol plot	Each group of cases is plotted separately—input from a new file and superimposed on one plot; symbols can be allocated at run time and changed without editing input files; multiple plot needs multiple runs
Graphics library	GKS	GPGS (Macintosh QuickDraw)
Original implementation	GEC-4090 operating RS 4000+; also PDP11/70; being ported to VAX	DEC-10 operating TOPS 10 (Macintosh OS)
Graphics output	To spool file for subsequent hard-copy production via device driver; user need not be connected to graphics device at run-time	Direct to Macintosh screen; plots are object-oriented (as in MacDraw), not bit-mapped (as in MacPaint)

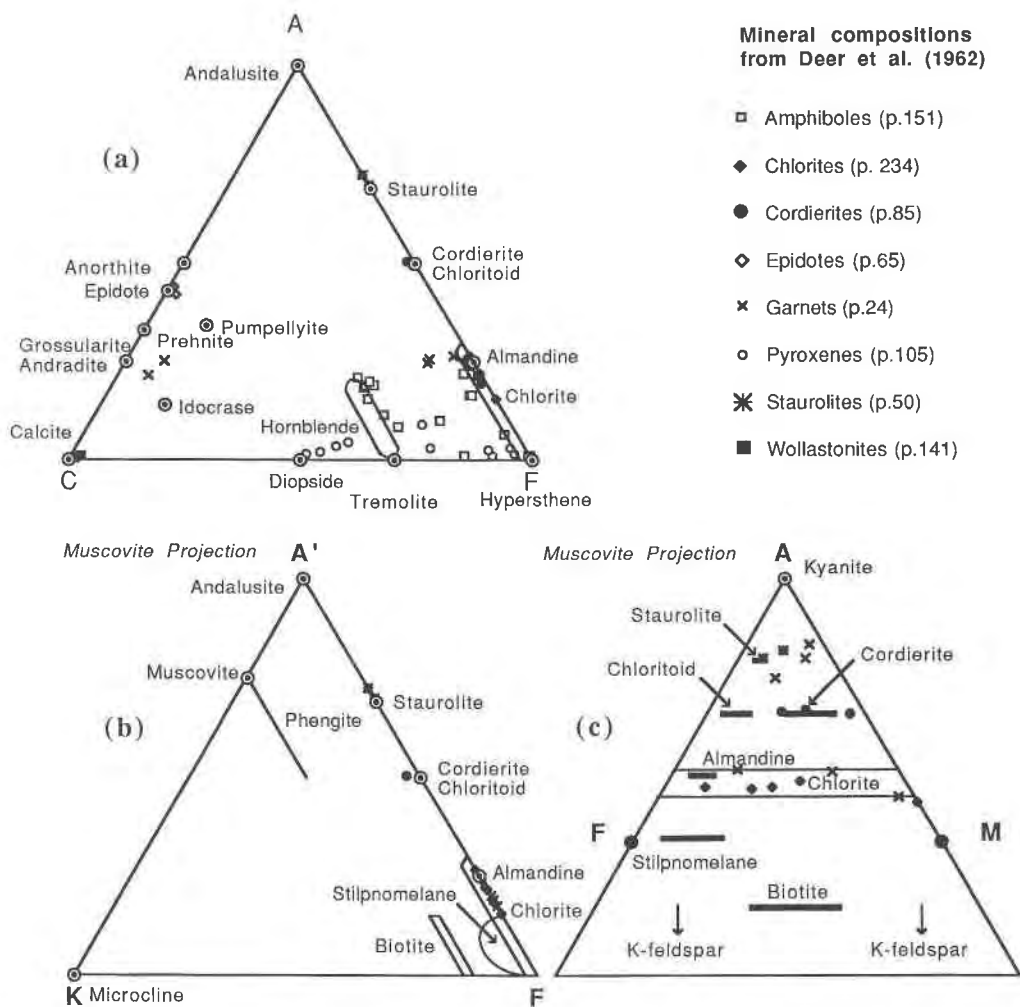


Fig. 2. Examples of (a) ACF, (b) A'KF, and (c) A''FM plots generated by the Macintosh version of ACF. As in Fig. 1, 10% tick marks and 10% grid lines can be optionally added. The positions of only a few minerals are shown, to avoid congestion; many other minerals can be plotted at will from within the program. Positions of representative natural mineral analyses are shown from Deer et al. (1962), to confirm that the “real” analyses are correctly positioned by ACF near to the theoretical “ideal” compositions. In (c), the plotted garnets cover a wide area because they are actually solid solutions between almandine, pyrope, and grossular, the latter two not being conventionally shown on AFM plots.

ACF: A program to plot metamorphic ACF, A'KF and A''FM diagrams

This program generates Eskola's ACF, A'KF and Thompson's A''FM plots, where, in ACF,

$$A = Al_2O_3 + Fe_2O_3^* - Na_2O - K_2O;$$

$$C = CaO - 3.3P_2O_5;$$

$$F = [FeO^* + MnO + MgO];$$

in A'KF,

$$A' = Al_2O_3 + Fe_2O_3^* - Na_2O - K_2O - CaO^*$$

$$K = K_2O;$$

$$F = [FeO^* + MnO + MgO];$$

and in A''FM,

$$A'' = [Al_2O_3 - \mu K_2O] / [Al_2O_3 - \mu K_2O + MgO + FeO]$$

$$M = MgO / [MgO + FeO^*]$$

and all oxides are expressed molecularly. CaO* is the CaO combined in epidote and anorthite, but not that in carbonates, sphene, or wollastonite, FeO* is the FeO in silicates but not in magnetite or ilmenite, Fe₂O₃* excludes that in hematite, and $\mu = 3$ or 1 for projections through muscovite or K-feldspar, respectively, both of which are implemented (Winkler, 1976).

For all three types of figure, Fe_{total} can be partitioned between Fe₂O₃ and FeO according to the user's choice of Fe³⁺/Fe_{total} ratio. This partitioning may be confined to analyses that lack a figure for one of the two oxides or may be performed on *all* analyses input. CaO can be corrected for its proportion in sphene, and/or FeO for its proportion in ilmenite, by assigning the proportion of TiO₂ in the two minerals. CaO* can also be corrected for its proportion in calcite by either leaving or removing CO₂. Corrections for epidote, grossular, margarite, paragonite, etc. are not, however, incorporated, partly because they are infrequently called for in the literature, partly because the necessary modal information is so rarely available, and partly because the extra “precision” is rarely justified.

Inputting the raw data necessarily takes a slightly different form with ACF than with TRIPLLOT, since to calculate ACF, A'KF or A"FM coordinates requires that a value for each of several *specific* oxides be provided. If the input file consists of raw data alone, ACF assumes that the oxides have been arranged in the following default order: SiO₂, Al₂O₃, Fe₂O₃, FeO, MgO, CaO, Na₂O, K₂O, H₂O, TiO₂, P₂O₅, MnO, CO₂. Alternatively, as with TRIPLLOT, the user can provide an input file in which any other order of elements is defined by a set of oxide labels in the first line. Of course, if the input file is *not* in the above default order, and the user does not provide a label line, the resulting plot will be incorrect (unlike TRIPLLOT, where it will be correct but unlabeled).

Missing values also perform require a more complicated approach than with TRIPLLOT, for if the "essential" oxides are missing, calculations clearly cannot be completed. However, restricting what is taken to be "essential" too far can be self-defeating (for example, if Na₂O is defined as "essential," ACF will reject any analysis of, say, a chlorite, epidote, or garnet since Na₂O is not generally analyzed for in these phases). For simplicity, therefore, ACF restricts its definitions of the "essential" oxides to Al₂O₃, MgO, and *either* Fe₂O₃ *or* FeO. If one of these is missing for a particular analysis, warning messages are printed and that analysis is skipped.

Calculations are aborted with analyses that yield inadmissible negative values for any of the three coordinates, and warning messages are provided (negative A in ACF or A' in A'KF are commonplace, for example, when allowing for CO₂ in carbonate-rich rocks).

As well as rock or mineral analyses, the positions of up to 30 "ideal" metamorphic minerals can be plotted from within Mac-

intosh ACF (Fig. 2). Tie-lines have not been implemented, partly because copying plots into object-oriented graphics software such as MacDraw®, MacDraft®, or Superpaint® for subsequent editing is so quick and simple, and partly because the number of permutations of tie-lines between all the different possible minerals is too large for simple automation.

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