

SOFTWARE NOTICE

MacSuite: An integrated compendium of geoscientific programs for the Apple Macintosh

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ABSTRACT

MacSuite is a compendium of ten programs for geoscience teaching and research, primarily of interest to economic geologists, geochemists, mineralogists, petrologists, and volcanologists, but including several general-purpose programs of much wider application. Capabilities include triangular plots and subplots (general purpose and metamorphic ACF-AKF-AFM); internationally accepted geochemical classification plots (TAS, K_2O-SiO_2); “immobile” trace element plots for discriminating the tectonic setting of igneous rocks and for classifying altered rocks (general purpose and for komatiites, high-Mg basalts, etc., in greenstone belts); “spidergrams” (log-linear normalized multi-element plots); plots of spinel compositions in the oxidized and reduced four-dimensional spinel prisms; general-purpose mineral recalculations; isotopic recalculations for Rb-Sr and Sm-Nd systems; a quiz program for teaching the IUGS QAPF modal classification of igneous rocks; and a general-purpose program to convert standard tab-delimited Macintosh files into fixed-length formats suitable for PC and mainframe programs. File input formats and other operations are standardized. Two programs support color plotting.

GENERAL DESCRIPTION

MacSuite is an integrated suite of ten self-contained Macintosh programs (Table 1) for plotting various diagrams and performing various calculations commonly used in economic ge-

ology, geochemistry, mineralogy, petrology, and volcanology. Some programs offer general-purpose (e.g., triangular) plots that would be of value in many branches of the earth and other sciences as well (e.g., soil sciences, geography). A petrological teaching program is also included.

MacSuite is integrated in the sense that all ten programs work in essentially the same way (using the full Macintosh WIMP interface) and, in particular, accept the same type of input file where appropriate (see below). Any set of data that is suitable for more than one MacSuite program can thus be used freely among different programs without intermediate editing.

Specific capabilities of MacSuite are as follows (see Figs. 1–3 for examples of its plots):

1. triangular plots and subplots, simple or categorized according to several groups of data (Triplot);
2. Eskola's metamorphic ACF, AKF, and AFM plots (ACF);
3. classification and discrimination plots for fresh igneous rocks such as TAS (total alkalis-silica), as recommended by the IUGS subcommission on igneous rock systematics, K_2O-SiO_2 for island-arc volcanic rocks, and Pearce-Cann-Winchester “immobile” trace element plots for discrimination of ancient tectonic settings (Petrograph);
4. classification and discrimination plots for ancient or altered volcanic rocks found in greenstone belts, such as komatiites, high-Mg basalts, and more acidic rocks (MUM);
5. teaching of the IUGS QAPF modal igneous rock classification scheme (Igneous Rock Quiz);

TABLE 1. Outline of the ten programs currently incorporated in MacSuite

Program	Action	Reference	File type used and number of files
ACF	Draws Eskola's metamorphic ACF, AKF, and AFM diagrams	Rock and Carroll (1989a)	Tab-delimited ASCII with labels in first line; one file handled at once
Convert	Mac tab-delimited data files into column-delimited PC-style files	Rock and Wheatley (1989)	Tab-delimited ASCII (Macintosh)/column delimited (fixed length)
Igneous Rock Quiz	Quiz program to test knowledge of IUGS QAPF classification	Rock and Carroll (1989b)	None required; all necessary data contained within program
Isocalc	Initial Rb-Sr and Sm-Nd ratios and ϵ values from measured data	Carroll and Rock (1991)	Data typed directly into program from keyboard
Mintab	Calculates mineral formula units and tabulates formulae	Rock and Carroll (1990)	Tab-delimited ASCII with labels in first line; one file handled at once
MUM	Draws eight classification plots for altered (e.g., Archaean) rocks	—	Tab-delimited ASCII with labels in first line; many files handled at once
Petrograph	Draws TAS and five other rock classification diagrams	—	Tab-delimited ASCII with labels in first line; many files handled at once; color supported
Spider	Draws normalized multielement diagrams (“spidergrams”)	Wheatley and Rock (1988)	Tab-delimited ASCII with labels in first line; one file handled at once
Spineltab	Plots oxidized and reduced spinel prisms (in stereopairs if required)	Williams et al. (1990)	Tab-delimited ASCII with labels in first line; one file handled at once
Triplot	Draws general-purpose triangular diagrams (part or whole)	Rock and Carroll (1989a)	Tab-delimited ASCII with labels in first line; many files handled at once; color supported

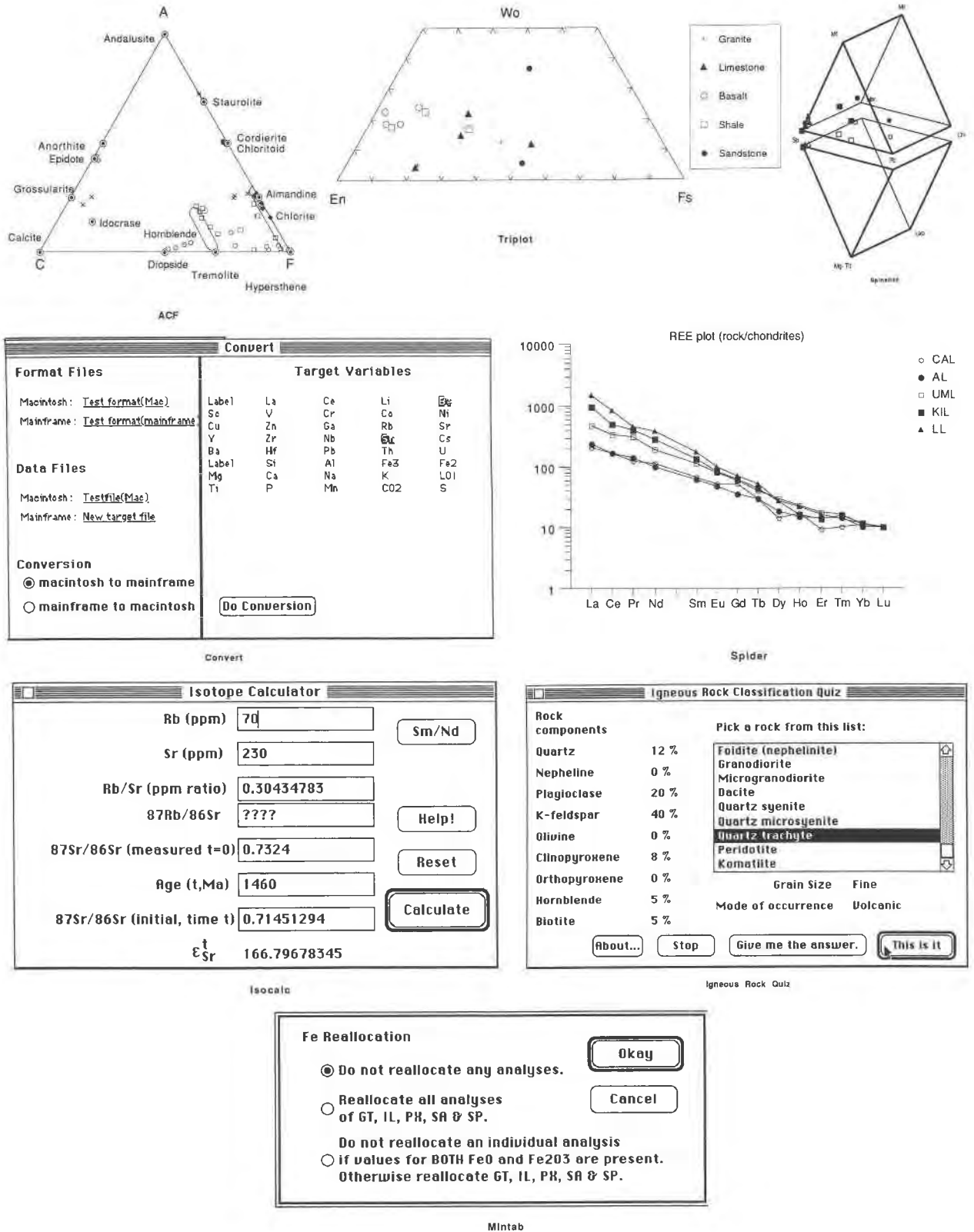


Fig. 1. Examples of diagrams and screens generated by the eight previously described programs. Diagrams are shown for the six programs where diagrams represent the final product; in the case of Mintab and Convert, the final product is a recalculated or converted data file, so screens shown during the operation of the program are shown instead.

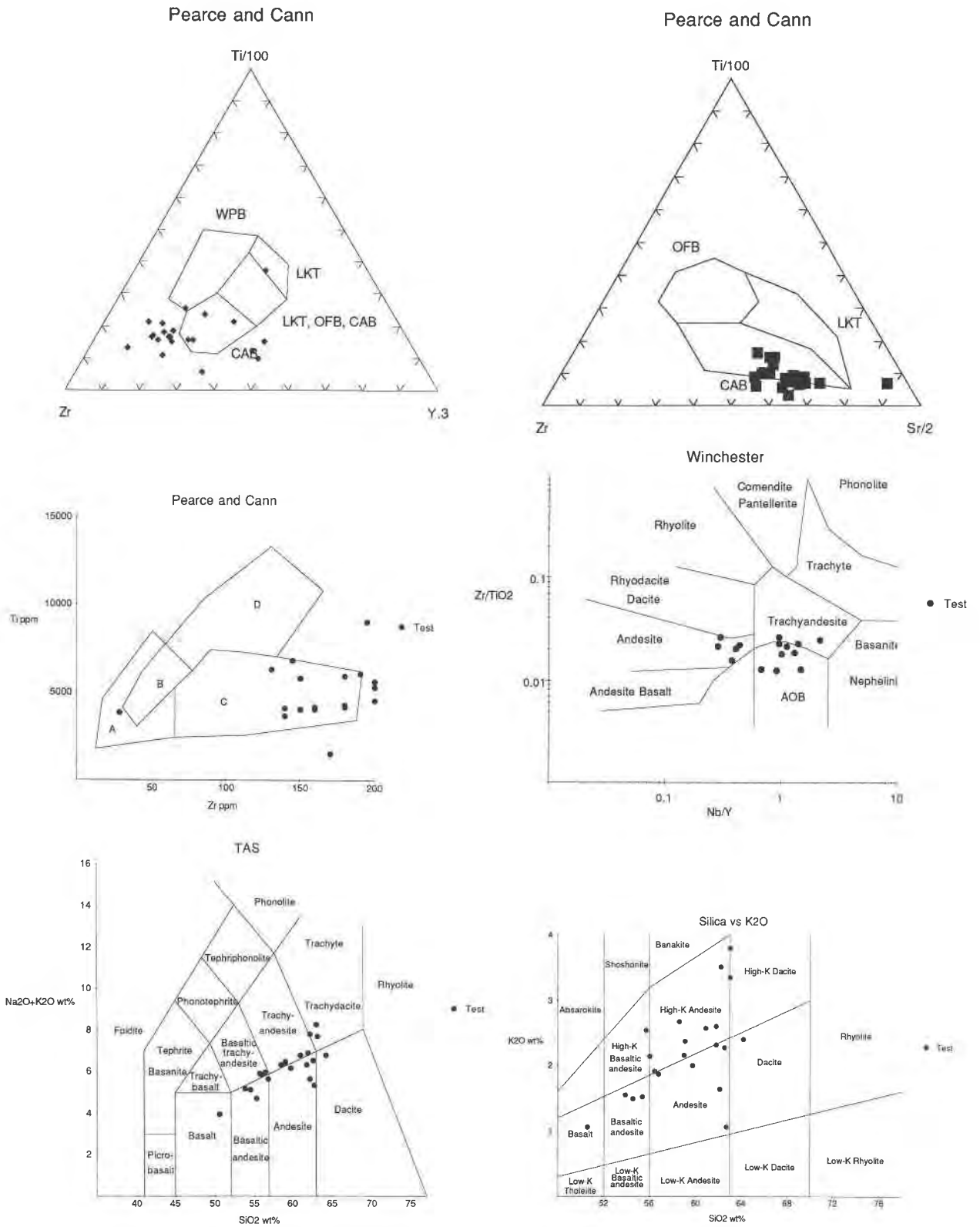


Fig. 2. Examples of the six diagrams currently generated by Petrograph. See text for explanation.

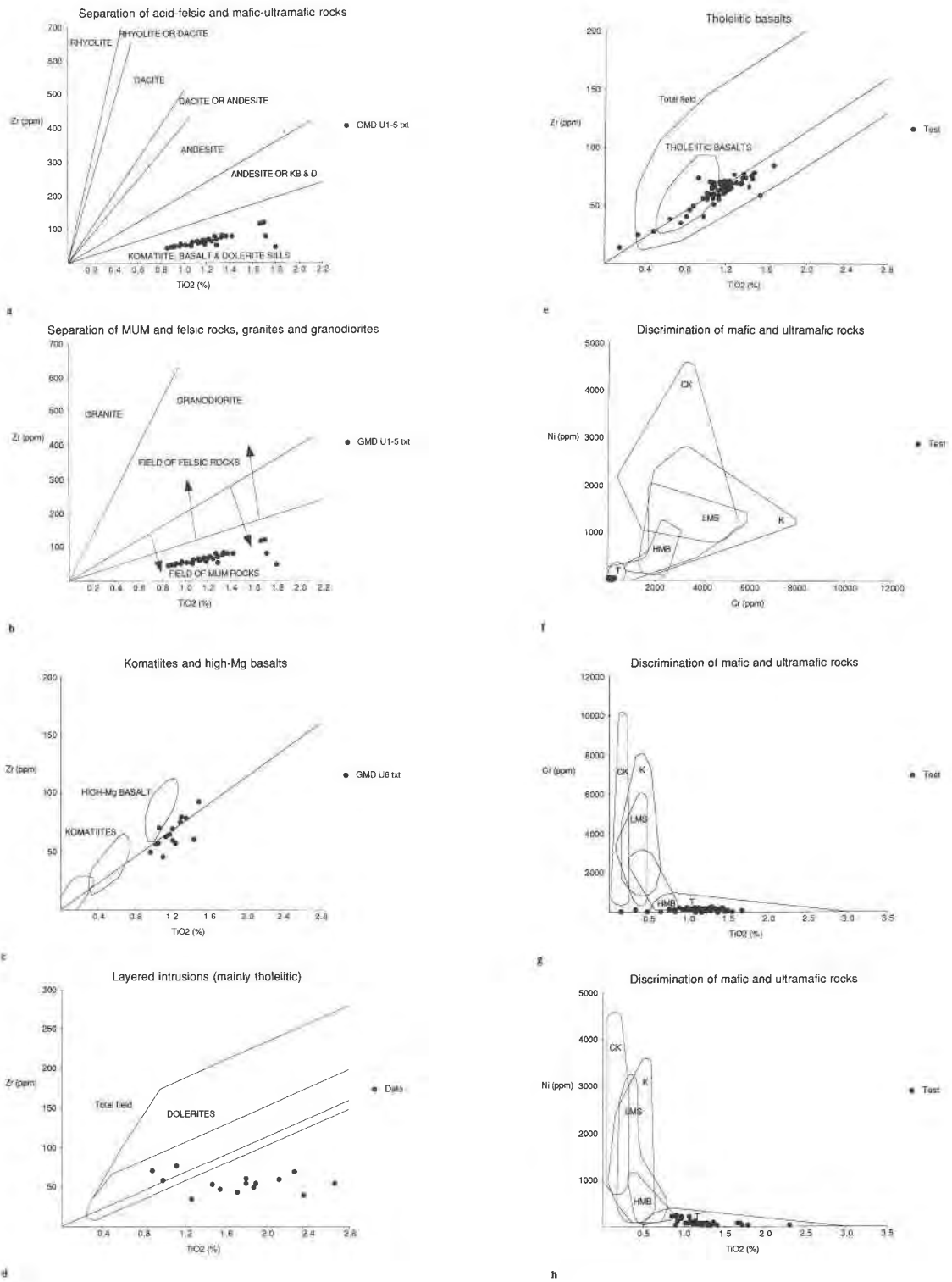


Fig. 3. Examples of the eight diagrams currently generated by MUM. See text for explanation.

6. recalculation of Rb-Sr and Sm-Nd present-day isotopic ratios to initial ratios and ϵ values (Isocalc);

7. "spidergrams," i.e., log-normalized multielement geochemical plots (Spider);

8. recalculation of many types of mineral analyses to formula units, with reallocation of Fe to $\text{Fe}^{3+}/\text{Fe}^{2+}$ and other adjustments (Mintab);

9. plotting of spinel analyses in the reduced or oxidized four-dimensional spinel prisms (Spinelab);

10. universal conversion of Macintosh-style, tab-delimited files to fixed-length, column-delimited (Fortran) styles more suited to many PC and mainframe computer programs (Convert).

INPUT AND OUTPUT

The eight programs that require input all accept the same, standard Macintosh file format, namely, a tab-delimited TEXT (ASCII) file with an initial label line indicating the names of the variables. Such a file is standard input to Macintosh data-processing software and is thus readily generated by all the major Macintosh editing, word-processing, statistical, and spreadsheet applications (e.g., Edit; MacWrite; Microsoft Excel, File, or Word; QUED; Statview; Systat, Wingz). For a printed example of this type of file, see Table 2 of Wheatley and Rock (1988). Variables can be in any order and may include variables not needed by a particular program—each program incorporates algorithms to recognize those variables that are needed and those that are not and to reorder them as required.

The user does, of course, need to provide a file with data that are intrinsically suitable for the program being employed (e.g., spinel analyses for Spinelab, geochemical data for Spider). Warning messages and error traps are nevertheless included in each program to recognize unsuitable data files. Data editing (as opposed to plot editing) within the programs is not implemented, but program Convert allows files generated on other platforms (including mainframes and PCs) to be converted for use with MacSuite (or, for that matter, most other Macintosh applications).

All graphical output is especially designed (using Postscript commands) for maximum quality on LaserWriters and has been routinely employed by the authors in books and papers published in international journals, obviating the need for expensive manual drafting of plots. Large numbers of diagrams generated in MacSuite programs can be found, for example, in Rock (1991). Color is supported by Triplot and Petrograph. Plots are generated in standard Macintosh PICT format and can be pasted using the clipboard into dedicated graphics programs such as SuperPaint or MacDraw, or saved as separate PICT files. Several programs also have internal plot-editing capabilities.

IMPROVEMENTS TO EARLIER PROGRAM VERSIONS

Earlier versions of eight programs in MacSuite have already been described in this or other journals (Table 1), and interested readers can therefore refer to these previous accounts for details. However, the new versions offered in MacSuite do offer major improvements, for example, in the following ways:

1. Spider now allows the user to preselect and interactively change up to ten spidergrams to appear on one plot (spider diagram). This allows large data-sets to be browsed in batches of chosen size, for example, the first three can first be plotted in one spider diagram, then the next seven, and so on. Plot symbols can also now be changed retrospectively.

2. Triplot now supports color, subplots, and category plots. Color plotting, of course, requires a color monitor or printer. Subplots allow any portion of a standard triangle to be plotted

(e.g., the pyroxene quadrilateral in Fig. 1). In category plots, different symbols can be used for different groups of samples (Fig. 1), simply using any text column in a single input file containing a finite number of categories (grouping words). Separate groups of data can thus be plotted together by using either separate input files and overlaying them successively, or by using a single input file once only.

NEW PROGRAMS

Two programs (Petrograph and MUM) have not been documented previously, and geological aspects of these are therefore detailed below.

Petrograph

Given appropriate data, Petrograph can plot six different classification diagrams, here (Fig. 2) shown in black and white but also available in color, given suitable hardware: (1) three "immobile" trace element diagrams developed by Pearce and Cann (1973) for discriminating the tectonic settings of volcanic rocks, based on Ti, Sr, Y, Zr, and Nb; (2) a diagram developed by Winchester and Floyd (1976) and Floyd and Winchester (1975) for classifying volcanic rocks based on immobile elements (Ti, Y, Zr, Nb) when their major element chemistry has been substantially modified from primary compositions; (3) the TAS [total alkalis-silica, i.e., $(\text{Na}_2\text{O} + \text{K}_2\text{O})$ vs. SiO_2] diagram recommended by the IUGS Subcommittee on the Systematics of Igneous Rocks (Le Bas et al., 1986) for the universal chemical classification of unaltered fine-grained (e.g., volcanic) rocks; (4) the SiO_2 - K_2O diagram originally developed by Peccerillo and Taylor (1976) for the classification of island-arc volcanic rocks and subsequently adopted widely by volcanic petrologists.

As these diagrams are already in widespread use, they require no further explanation here.

MUM

MUM (mafic-ultramafic) can plot eight more specialized diagrams, originally developed by Archaean geologists in Western Australia for the discrimination and classification of altered ancient volcanic rocks such as komatiites, high-Mg basalts, and tholeiites. See Figure 3 for examples and Hallberg (1985) for discussion. These diagrams are again based on immobile elements: Ti, Zr, Cr, and Ni, of which Ti and Zr are essentially immobile even in very weathered rocks, whereas Cr and Ni are immobile in fresh rocks, slightly immobile in slightly weathered rocks, and variably mobile in very weathered rocks. We believe these diagrams are fully applicable to similar ancient MUM rocks in greenstone belts throughout the world and probably to certain other geological settings as well.

The full range of diagrams offered is as follows: Figure 3a: Zr vs. TiO_2 plot, with fields defined that separate mafic-ultramafic rocks from acidic-felsic volcanic rocks; Figure 3b: Zr vs. TiO_2 plot, with fields defined that broadly separate andesites, dacites and rhyolites, and granites and granodiorites; Figure 3c: Zr vs. TiO_2 plot, with fields defined that separate komatiites, high-Mg basalts, and tholeiitic rocks (both volcanic and from layered intrusions); Figure 3d: Zr vs. TiO_2 plot, with fields defined that separate various units in layered mafic-ultramafic intrusions; Figure 3e: Zr vs. TiO_2 plot, with fields defined that separate various kinds of tholeiitic basalts; Figure 3f: Cr vs. Ni plot, with fields defined that separate komatiites, tholeiites, etc.; Figure 3g: Cr vs. TiO_2 plot, with fields defined that separate komatiites, tholeiites, etc.; Figure 3h: Ni vs. TiO_2 plot, with fields defined that separate komatiites, tholeiites, etc.

Figures 3f–3h should be used with great caution in highly altered or weathered rocks, but they are useful in conjunction with Figures 3a–3e to distinguish komatiites, high-Mg basalts, high-Mg layered sills, tholeiitic basalts, and layered tholeiitic sills. Sedimentary, pyroclastic, and volcanoclastic rocks will reflect the nature of the precursor volcanism and should plot in the relevant field, especially on plot Figure 3a.

Broad fields for Figures 3a–3e were derived from Hallberg (1985) and checked using the data from the sources below. Figures 3f–3h were constructed from scratch using the following data sources.

Cumulative komatiites: 33 from Kambalda (Leshner, 1983); 18 from Mount Monger (Williams, 1971); seven from Kalgoorlie-Kambalda (Perriam, 1985).

Komatiites: 42 from Kambalda (Leshner, 1983); 36 from Kalgoorlie-Kambalda (Perriam, 1985); 25 from Mount Monger (Williams, 1971);

High-Mg basalts: 16 from Yakabindie area (Naldrett and Turner, 1977); 14 from Mount Monger (Williams, 1971); six from Leonora-Laverton area (Hallberg, 1985) plus miscellaneous samples from Kambalda-Kalgoorlie area (about 20);

Layered high-Mg sills: 26 from Mount Monger (Williams, 1971); 11 from Mount Scholl (Mathison and Marshall, 1981); 17 from Langenbeck (Jones, 1971); two from Mount Thirsty (Whitfield, 1973) plus check samples from Wadda Wadda Hill and Fields Find;

Tholeiitic basalts: 20 from Yakabindie (Naldrett and Turner, 1977); 13 from Kambalda (Wong, 1986); nine from Kambalda (Leshner, 1983); eight from Norseman-Wiluna Belt (Hallberg, 1970); eight from Leonora-Laverton (Hallberg, 1985) plus other data from the footwall to nickel deposits (e.g., Groves and Hudson, 1981);

Layered tholeiitic sills: 122 from Golden Mile Dolerite (UWA unpublished data); 13 from Langenbeck (Jones, 1971).

FUTURE DEVELOPMENTS

We intend to add programs to future versions of MacSuite to improve its coverage and to upgrade the existing ten programs. Suggestions from users for improvements and additions are welcomed. Among improvements under development are the addition of category plots (as already available in Triplot) to Petrograph and MUM. The following are among other programs already written that we are considering integrating fully into the compendium: Crystal, a program to draw molecular structures; Gresens, a program to perform Gresens-type metasomatic volume-change calculations that are useful in, for example, the study of ore bodies; DIM (diamond indicator minerals), a program to classify garnets, clinopyroxenes, and orthopyroxenes according to cluster analysis groups (e.g., Dawson and Stephens, 1975), which are used in exploration as predictors for the presence of diamond; Harker, a program to plot Harker silica variation diagrams in petrology; MacIGBA, a program to decode and interrogate the international igneous rock database IGBA, which currently contains geochemical and petrographical data for some 16000 samples worldwide; Pxtab and Amphtab, programs for the tabulation and classification of pyroxenes and amphiboles according to IMA nomenclature (Rock, 1987, 1990); and various programs to perform quantitative calculations on igneous fractionation processes.

AVAILABILITY

MacSuite is now available from Rockware, Suite 595, 4251 Kipling Street, Wheat Ridge, Colorado 80033, U.S.A. (fax 303-423-6171), for US\$200, or direct from the first author in ex-

change for an equivalent sum in convertible funds (e.g., dollar draft, recognized international bank check). A complete manual and example test datasets are included. Full backup services and accessibility to upgrades are available for purchasers of the complete compendium. We are also prepared to consider making available a limited number of copies of individual programs from MacSuite, for \$25 per program, by direct application to the first author. We greatly regret, however, that we cannot offer individual purchasers a manual, backup services, or upgrades and emphasize that we can no longer accept personal checks (because of previous bad experiences!) or disks in lieu of costs (due to viruses such disks have frequently carried in the past).

We have "gone commercial" in this way very reluctantly and only following the precedent established by well-known Macintosh programs that evolved from freeware into shareware or commercial products after extensive development (e.g., Red Ryder, Stuffit). We have also done so only after earlier versions of MacSuite programs were freely distributed to over 150 institutions worldwide. Unfortunately, the number of requests we have been receiving has reached unmanageable proportions, and few requests have offered anything in exchange, in a situation where we are now required to cover commercial programming costs. Because we have received no notification of problems or bugs with any of these programs, and yet they have been used by others to generate plots and diagrams in the published literature, we feel sure that they have been more than adequately β tested. Costs recovered from the sale of MacSuite will be invested in future upgrades.

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