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SOFTWARE NOTICE

AMPHIBOL: A program for calculating structural formulae and for classifying and plotting chemical analyses of amphiboles

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The AMPHIBOL program

AMPHIBOL is a compiled program that recalculates chemical analyses of amphiboles into their structural formulae and classifies them according to current IMA guidelines. Chemical analyses can be entered directly from the keyboard or imported from a comma-delimited ASCII format file to be saved in an AMPHIBOL file in one of two formats: with Fe^{2+} only (e.g., microprobe data), or with both Fe^{3+} and Fe^{2+}. In cases where Fe^{3+} is not determined, AMPHIBOL will use the charge-balance method

Sample	FE-KATOPHORI						
			Fe2+	15-NK	15-K	13-CNK	AV(2,4)
SiO2	43.14	TSi	7.155	7.499	6.561	6.999	7.249
TiO2	0.00	TAl	0.845	0.501	0.938	1.001	0.751
Al2O3	5.23	TFe3+	0.000	0.000	0.500	0.000	0.000
Cr2O3	0.00	TTi	0.000	0.000	0.000	0.000	0.000
FeO	36.85	SUM IN T	8.000	8.000	8.000	8.000	8.000
MnO	0.00	CAl	0.178	0.572	0.000	0.000	0.286
MgO	0.00	CCr	0.000	0.000	0.000	0.000	0.000
CaO	5.75	CFe3+	0.000	0.000	3.314	1.001	0.500
Na2O	6.36	CTi	0.000	0.000	0.000	0.000	0.000
K2O	0.00	CMg	0.000	0.000	0.000	0.000	0.000
Cl	0.00	CFe2+	4.822	4.428	0.873	3.999	4.214
F	0.00	CMn	0.000	0.000	0.000	0.000	0.000
Total	97.33	CCa	0.000	0.000	0.813	0.000	0.000
-O=Cl,F	0.00	SUM IN C	5.000	5.000	5.000	5.000	5.000
Total	97.33	BMg	0.000	0.000	0.000	0.000	0.000
		BFe2+	0.290	0.929	0.000	0.000	0.464
		BMn	0.000	0.000	0.000	0.000	0.000
		BCa	1.022	1.071	0.124	1.000	1.035
		BNa	0.689	0.000	1.876	1.000	0.500
		SUM IN B	2.000	2.000	2.000	2.000	2.000
		ACa	0.000	0.000	0.000	0.000	0.000
		ANa	1.357	2.144	0.000	1.000	1.572
		AK	0.000	0.000	0.000	0.000	0.000
		SUM IN A	1.357	2.144	0.000	1.000	1.572
		CCl	0.000	0.000	0.000	0.000	0.000
		CF	0.000	0.000	0.000	0.000	0.000
		SUM CATS	16.357	17.144	15.000	16.000	16.572
		SUM OXY	23.001	24.107	23.000	23.000	23.554

METHOD	GROUP	NAME
Fe2+	Sodic-Calcic	Katophorite
15-NK	Fe-Mg-Mn	Grunerite Ferro-Anthophyllite
15-K	Alkali	Riebeckite
13-CNK	Sodic-Calcic	Katophorite
AV. 15-NK & 13-CNK	Calcic	Ferro-Edenite

Fig. 1. Typical output from a dot-matrix printer showing recalculation of the structural formulae and classification of a single amphibole composition (ferrous katophorite). The five recalculation schemes are Fe^{2+}—all Fe as Fe^{2+} using 23 oxygens; 15-NK—total number of cations is 15, excluding the sum of Na and K; 15-K—total number of cations is 15, excluding K; 13-CNK—total number of cations is 13, excluding the sum of Ca, Na, and K; and AV(2,4)—the average of methods 2 (15-NK) and 4(13-CNK).

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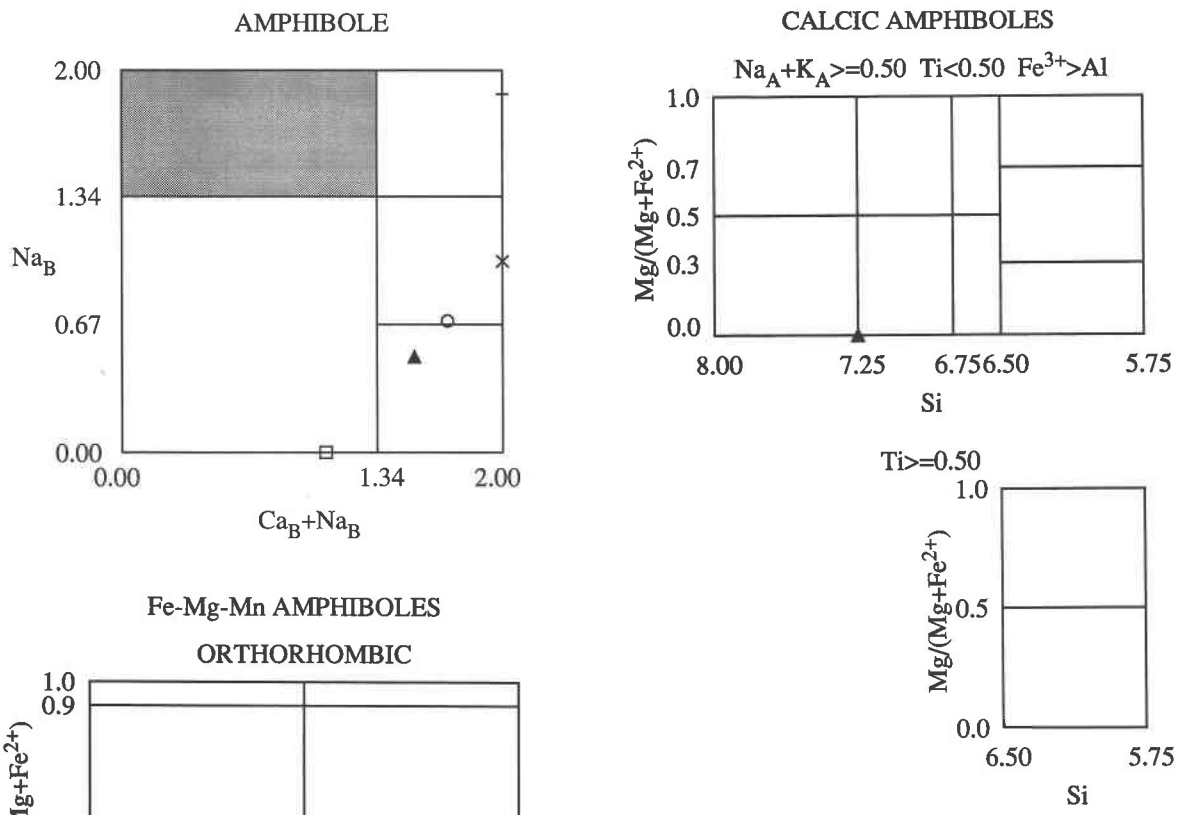


Fig. 2. Laser-printer output for the sample shown in Fig. 1. The following symbols are used in all plots to distinguish each recalculation scheme: circle = all Fe input as Fe^{2+}, or as Fe^{2+} and Fe^{3+}, depending on file structure; square = 15-NK; plus sign = 15-K; diagonal cross = 13-CNK; triangle = average of 15-NK and 13-CNK.

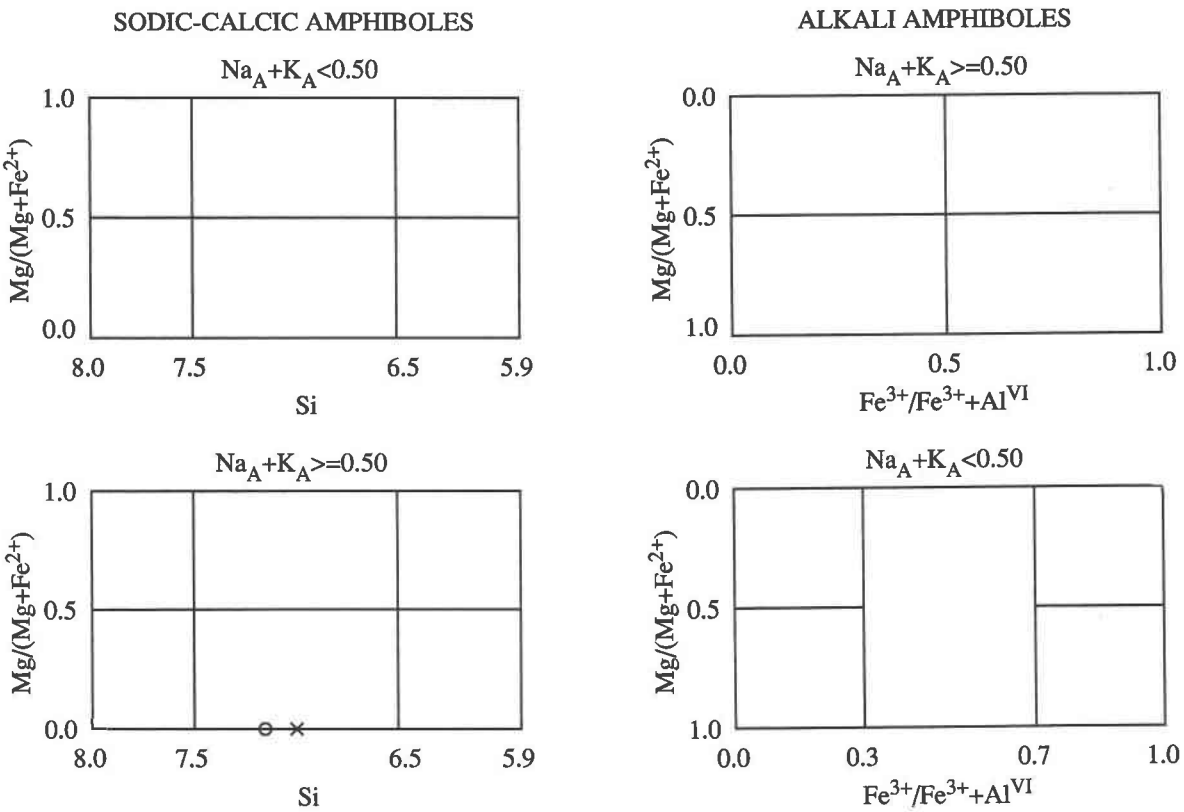
described by Robinson et al. (1981) to estimate the Fe^{3+} content. A printed output can be produced that contains five recalculation schemes (Fig. 1) and the appropriate nomenclature for each recalculation. Also, the results can be presented graphically on the screen or printed on a dot matrix printer or a POSTSCRIPT laser printer (Fig. 2). Finally, the raw data and one selected recalculation scheme can be exported to an ASCII format file for processing with other software.

The distribution disk contains the following files, both for executing the program and for testing all end-members for the elements normally determined by electron microprobe: AMPHIBOL.BAT (the batch file), AMPHY87.EXE (the main program compiled for a system that uses a math coprocessor), AMPHN87.EXE (the main program compiled for a system that does not have a math coprocessor), README.AMP (operating instructions), and eight test-data files—CALCIC1.DAT, CALCIC2.DAT, FEMG.DAT, ALKALI1.DAT, ALKALI2.DAT, SODIC1.DAT, SODIC2.DAT, and ROBINSON.DAT.

AMPHIBOL is menu-driven and is extremely easy to use. Instructions are generally displayed on the screen, and the README.AMP file contains a complete set of instructions for running all aspects of the program.

The test-data files contain all the stoichiometric end-members currently accepted by IMA (Leake and Winchell, 1978). End-member chemical compositions were calculated from their stoichiometric formulae (Hawthorne, 1981).

The sample number, oxide values, and recalculated results from one selected recalculation scheme can be exported in ASCII format. The output will contain the following variables: sample$, SiO_2, TiO_2, Al_2O_3, Cr_2O_3, FeO, Fe_2O_3 (if entered), MnO, MgO, CaO, Na_2O, K_2O, Cl, F, total, $-O \equiv$ (Cl,F), total, TSi, TAl, TFe^{3+}, TTi, sum in T, CAl, CCr, CFe^{3+}, CTi, CMg, CFe^{2+}, CMn, CCa, sum in C, BMg, BFe^{2+}, BMn, BCa, BNa, Sum in B,



ACa, ANa, AK, sum in A, CCl, CF, sum cations, and sum oxygens.

AMPHIBOL is not copy protected.

Hardware requirements

The AMPHIBOL software requires an IBM or a fully compatible computer with a color graphics card and DOS version 2.0 or later. In order to produce screen dumps, the GRAPHICS.COM file must be copied from DOS onto the AMPHIBOL distribution disk, and an EPSON or EPSON-compatible printer is needed to print screen dumps of the graphs displayed by the software. Access to a POSTSCRIPT laser printer will enable production of high-quality diagrams suitable for publication.

Ordering instructions

Please send a formatted 5.25″ or 3.5″ floppy disk, a self-addressed return mailer, and $2 Canadian (or a Universal Postal Union coupon for that amount) to Linda Richard.

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References cited

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