PERGAMON

Computers & Geosciences 25 (1999) 909–927

COMPUTERS & GEOSCIENCES

A revised program for microprobe-derived amphibole analyses using the IMA rules ☆

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Received 13 August 1998; received in revised form 7 May 1999; accepted 7 May 1999

Abstract

A Microsoft QUICKBASIC program with the code name NEWAMPHCAL has been written to calculate the structural formulae of amphibole analyses taken from electron-microprobe, and to determine the classification parameters with the prefixes and modifiers according to the procedures proposed by the International Mineralogical Association (IMA) 1997 amphibole nomenclature scheme. The program, which came up with four Al-in hornblende geobarometers, is applicable to plutonic and its associated volcanic rocks including amphibole–biotite–quartz–plagioclase–ortochlase–sphene–FeTi oxides. An amphibole–plagioclase geothermometer for particular calcic amphiboles also is incorporated into the program structure. NEWAMPHCAL has been tested for determination and classification of numerous amphibole analyses compiled from literature. Depending on the evaluations of selected amphibole analyses by using NEWAMPHCAL program, it was determined that approximately 15% amphibole names were changed compared to the author's IMA 1978 findings. The most important variation in amphibole names has been observed in the calcic amphibole group. This program permits the user data entry, their storage, and calculation and plotting of microprobe amphibole analyses. NEWAMPHCAL plots the calculated chemical parameters on one ternary and seventeen different binary diagrams for amphibole classification. This software, with well-designed screen forms, stores all the calculated results in comma delimited ASCII file format and thus permits the user to process the program outputs for further spreadsheet applications. A menu-driven and easy to use program runs on IBM-compatible microcomputers under DOS and Windows systems with the minimum hardware requirements. The compiled form of NEWAMPHCAL takes approximately 398 kilobytes together with the test data.

Keywords: Amphibole; Electron-Microprobe; Classification; Prefix; Modifier; Geobarometry; Geothermometry

1. Introduction

Amphibole group minerals occur in a great variety of igneous and metamorphic rocks with a wide range of pressure and temperature environments. A standard amphibole formulae has the ideal form of $A_{0\text{-}1}B_2C_5T_8O_{22}(OH, F, Cl)_2$, where A = Na, K; B = Na, Li, Ca, Mn, Mg, Fe^{2+}; C = Mg, Fe^{2+}, Mn, Al, Fe^{3+}, Ti; and T = Si, Al. In general, depending on the complex nature of amphibole structure, comparisons of amphibole compositions are carried out following the chemical analyses into the structural formulae.

The IMA amphibole nomenclature scheme (Leake,

☆ Code available at http://www.iamg/org/CGEditor/index.htm

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0098-3004/99/$ - see front matter
PII: S0098-3004(99)00055-2

1978; Rock and Leake, 1984), which is suitable for the computerization of amphibole analysis both from electron-microprobe and wet-chemical analysis was revised by the 1997 IMA report (Leake et al., 1997). The new scheme has over 20 fewer names than the earlier IMA 1978 amphibole nomenclature scheme. Definitions of end-member formulae approved in the IMA 1978 are generally retained in the IMA 1997 report except for extensive modifications in ranges.

A number of programs have been written to classify amphiboles taking into account the IMA 1978 scheme. Mogessie and Tessadri (1982) gave the earliest published program for a Commodore PET 2001 series computer using BASIC programming language. A FORTRAN program with the code name of AMPHTAB was developed by Rock (1987) following the review of the IMA scheme including important corrections, additions, and amendments. Richard and Clarke (1990) gave a compiled program of AMPHIBOL for calculating structural formulae, classifying and plotting chemical analyses of amphiboles according to the IMA guidelines without test data. Mogessie et al. (1990) wrote a HyperCard program on Macintosh computers to determine the name of an amphibole from electron-microprobe analysis according to the IMA 1978 scheme. Currie (1991) developed a BASIC program for calculation of mol fractions of amphibole end-members using the IMA 1978 rules on IBM-compatible computers. Tindle and Webb (1994) have developed PROBE-AMPH, which is a Microsoft Excel spreadsheet program to classify microprobe-derived amphibole analyses with the published four geobarometers for certain calcic amphiboles. A compiled program with the code name AMPHCAL was written by Yavuz (1996) for determining the amphibole name together with the prefix and modifier from electron-microprobe analyses using the IMA 1978 and revised scheme by Rock and Leake (1984). Included with this program also were given published geobarometers and geothermometer. Rao and Rao (1996) developed a simple BASIC program to calculate chemical formulae and assign names to members of the amphibole group. Currie (1997) revised his earlier BASIC computer program according to the IMA 1997 scheme, deleted the calculation of mol fractions from the revised program, and arranged it based on the amphibole names with prefix and modifiers.

NEWAMPHCAL program came up with this paper is the revised form of earlier AMPHCAL program (Yavuz, 1996) and operates according to the IMA 1997 nomenclature scheme. The program developed for amphibole analyses obtained from electron-microprobe and wet chemical analysis. NEWAMPHCAL calculates structural formulae of multiple amphibole analyses, allocates iron from electron-microprobe to Fe^{2+} and Fe^{3+} on the procedure proposed by Droop (1987), produces amphibole names with prefix and modifiers according to the IMA 1997 scheme, and calculates pressures for four geobarometers (Hammarstrom and Zen, 1986; Hollister et al., 1987; Johnson and Rutherford, 1989; Schmidt, 1992) and temperature for geothermometer given by Blundy and Holland (1990). Taking into account the previous users of AMPHCAL program the major oxides, except for Mn_2O_3 and Fe_2O_3, and some minor elements such as Cl, F, and Li are kept in the data entry section of NEWAMPHCAL program. Thus, using the 'Convert.Exe' program, one can convert one's old data file with the extension of 'Amp' to the new file format.

2. Review of the IMA classification scheme for amphiboles

According to the IMA 1978 nomenclature scheme, there were some problems in naming amphibole names of anthophyllite and cummingtonite series from the iron–magnesium–manganese group, because of the overlap of chemical compositions. Thus earlier computer programs for determination of the orthorhombic and monoclinic varieties of the iron–magnesium–manganese were in difficulty, and generally the user was warned to the control of optic determinations for exact amphibole names. In the revised amphibole report of the IMA 1997 scheme, indicated topic has been partly removed at gedrite series depending on the limit for the use of names of end members. The main changes in this group from IMA 1978 are the adoption of divisions at $Mg/(Mg+Fe^{2+})=0.50$, the reduction of modifiers, and the abolition of the tirodite and dannemorite. The most important revision by the IMA 1997 has been carried out in the calcic group. A number of the calcic group amphibole names have been reduced and the boundaries of the group have been revised. Silicic edenite and compound names such as tschermakitic hornblende have been abolished; sadanagaite, which was proposed earlier by Rock and Leake (1984) and cannilloite have been added. There are no important changes in the sodic–calcic amphiboles group compared to the IMA 1978 scheme except for the 50% expansion of the volume occupied by the group. Depending on this revision, a number of previously classified calcic and alkali amphiboles became the sodic–calcic amphibole. The main changes in the sodic amphibole group are revision of the boundary at $Na_B \geq 1.50$ instead of $Na_B \geq 1.34$, the abolition of crossite, and the introduction of nyböite, ferric-nyböite (instead of anophorite), leakeite, ferroleakeite, kornite, and ugarettiite.

Table 1
Prefixes and modifiers for IMA 1997 Amphibole Nomenclature Scheme (Leake et al., 1997)

	Meaning[a]	Applicable to
Prefix		
Alumino	$^{VI}Al > 1.00$	Calcic and sodic–calcic groups only
Chloro	$Cl > 1.00$	All groups
Chromio	$Cr > 1.00$	All groups
Ferri	$Fe^{3+} > 1.00$	All groups except sodic
Fluoro	$F > 1.00$	All groups
Mangano	$1.00 < Mn^{2+} < 2.99$	All groups, except for kozulite and ungarettiite
Permangano	$3.00 < Mn^{2+} < 4.99$	All groups, except for kozulite
Mangani	$Mn^{3+} > 1.00$	All groups, except for kornite and ungarettiite
Potassic	$K > 0.50$	All groups
Sodic	$Na > 0.50$	Mg–Fe–Mn–Li group only
Titano	$Ti > 0.50$	All groups, except for kaersutite
Zinco	$Zn > 1.00$	All groups
Modifer		
Barian	$Ba > 0.10$	All groups
Borian	$B > 0.10$	All groups
Calcian	$Ca > 0.50$	Mg–Fe–Mn–Li group
Chlorian	$0.25 < Cl < 0.99$	All groups
Chromian	$0.25 < Cr < 0.99$	All groups
Ferrian	$0.75 < Fe^{3+} < 0.99$	All groups except sodic
Fluorian	$0.25 < F < 0.99$	All groups
Hydroxylian	$OH > 3.00$	All groups
Lithian	$Li > 0.25$	All groups, but excludes those species defined by the abundance of lithium (e.g., holmquistite)
Manganoan	$0.25 < Mn^{2+} < 0.99$	All groups, but excludes those species defined by the abundance of Mn^{2+}
Manganian	$0.25 < Mn^{3+}$ or $Mn^{4+} < 0.99$	All groups, but excludes those species defined by the abundance of Mn^{3+} (e.g., kornite)
Nickeloan	$Ni > 0.10$	All groups
Oxygenian	$(OH+F+Cl) < 1.00$	All groups, except for ungarettiite
Potassian	$0.25 < K < 0.49$	All groups
Plumbian	$Pb > 0.10$	All groups
Sodian	$0.25 < Na < 0.49$	Mg–Fe–Mn–Li group only
Strontian	$Sr > 0.10$	All groups
Titanian	$0.25 < Ti < 0.49$	All groups
Vanadian	$V > 0.10$	All groups
Zincian	$0.10 < Zn < 0.99$	All groups
Zirconian	$Zr > 0.10$	All groups

[a] Concentrations are expressed in atoms per formula unit.

2.1. Iron partitioning

The most important point in the recalculation of microprobe-derived amphibole analyses is the ferric iron estimation by reason of the $Mg/(Mg+Fe^{2+})$ and Fe^{3+} are the IMA 1997 classification parameters. This topic has been discussed by earlier investigators (Stout, 1972; Robinson et al., 1982; Droop, 1987; Jacobson, 1989; Schumacher, 1991; Holland and Blundy, 1994) and used extensively as empirical estimates in many computer programs (Spear and Kimball, 1984; Mogessie et al., 1990; Yavuz, 1996, 1997, 1999; Yavuz and Öztas, 1997). The estimation of the proportion of Fe^{3+} in the electron-microprobe analysis of amphiboles has been discussed by in detail by Schumacher (1997) following the 'minimum ferric iron' criterion. The ferric iron content of amphibole can be calculated if the chemical analysis is complete, accurate, and the stoichiometry can be assumed. Provided that these conditions are valid for microprobe amphibole analysis, the empirical estimate in fact gives the same result. This study tested the results of ferric iron estimation procedures proposed by Droop (1987) and Schumacher (1997). Evaluations reveal that both pro-

cedures do not show important variation especially in defining the amphibole names.

2.2. Site occupancies of the cations

The proposed nomenclature scheme by the IMA (1997) on amphiboles is based on the chemistry and crystal symmetry, as with the IMA 1978 scheme. The following review outlines the procedure accepted by the IMA (1997) to calculate the standard formulae of wet-chemical or microprobe amphibole analyses.

1. If water and halogen contents are well determined, then the formulae should be calculated to 24 (O, OH, F, Cl);
2. If water and halogen contents are not well established, then the formulae should be calculated to the basis of 23 (O) with 2 (OH, F, Cl);
3. Sum of T to 8.00 using Si, then Al, then Ti. For the sake of simplicity of nomenclature, Fe^{3+} is not allocated to T;
4. Sum of C to 5.00 using excess Al and Ti from (3), and then successively Zr, Cr^{3+}, Fe^{3+}, Mn^{3+}, Mg, Fe^{2+}, Mn^{2+}, any other L^{2+}-type ions including rarer ions of smaller size, such as Zn, Ni, Co, and Li;
5. Sum of B to 2.00 using excess Mg, Fe^{2+}, Mn^{2+}, and Li from (4), then Ca, then Na;
6. Excess Na from (5) is assigned to A, then all K. Total A should be between 0.00–1.00, inclusive, where T is the tetrahedral site, C is the octahedral site, B is the M4-site, and A is the A-site.

2.3. Classification of amphibole groups

The recalculated amphibole analyses are classified into four groups on the occupancy of the B sites:

1. When $(Ca+Na)_B$ is <1.00 and the sum of L-type ions (Mg, Fe, Mn, Li)$_B$ is ≥ 1.00, then the amphibole is a member of the *magnesian–iron–manganese–lithium* group. This group is called as the *iron–magnesium–manganese* in the IMA 1978 nomenclature scheme.
2. When $(Ca)_B$ is ≥ 1.50, then the amphibole is a member of the *calcic* group.
3. When $(Ca+Na)_B$ is ≥ 1.00 and Na_B is in the range of 0.50 to 1.50, then the amphibole is a member of the *sodic–calcic* group.
4. When $Na_B \geq 1.50$, then the amphibole is a member of the *sodic* group. The previous name of this group is called as the *alkali* group by the IMA 1978 scheme.

2.4. Prefixes and modifiers

Compared to modifiers, prefixes show important parts in naming the amphibole group minerals as they denote major substitutions. Consequently, the use of modifiers is optional. In Table 1, modified prefixes and modifiers accepted by the IMA 1997 nomenclature amphibole scheme are shown. NEWAMPHCAL program names most of these prefixes and modifiers in microprobe amphibole analysis depending on its included oxide and element variables.

3. The NEWAMPHCAL program

NEWAMPHCAL is a compiled program developed for the recalculation of electron-microprobe chemical analyses into their structural formulae and classification of them according to the International Mineralogical Association 1997 scheme. This program is the revised form of earlier AMPHCAL program (Yavuz, 1996) taking into consideration the current IMA rules. The process of program can be divided into three categories:

1. Data entry of amphibole analyses;
2. Estimation of chemical analyses;
3. Plotting of recalculated analyses on the classification diagrams.

NEWAMPHCAL is written in QUICKBASIC for using on IBM-compatible computers running under DOS and Windows operating system. The total compiled form of the program with the test data takes approximately 398 kilobytes. It consists of three individual executable programs converting edited oxides to elements on the basis of 23 oxygen, and plotting them on 18 classification diagrams.

3.1. Data entry of amphibole analyses

The 'Amphcal.Exe' program carries out the start-up of NEWAMPHCAL program. This program is used for the data entry of amphibole chemical analyses. Once the 'Amphcal.Exe' is executed the program starts with a similar start-up window on screen presenting program name, author's mailing and e-mail address (Fig. 1A). By pressing any key on keyboard, a new screen design similar to Fig. 1B comes up with the pull-down menu. By pressing the [C] function key on 'Create New File' and selecting this option by pressing Enter key, the program asks the user to enter a file name to store the amphibole analyses. The user of this program can update and enter additional analyses using down and up cursor movement keys on file names, then selecting it by pressing Enter key, and pressing the [U] function key, respectively.

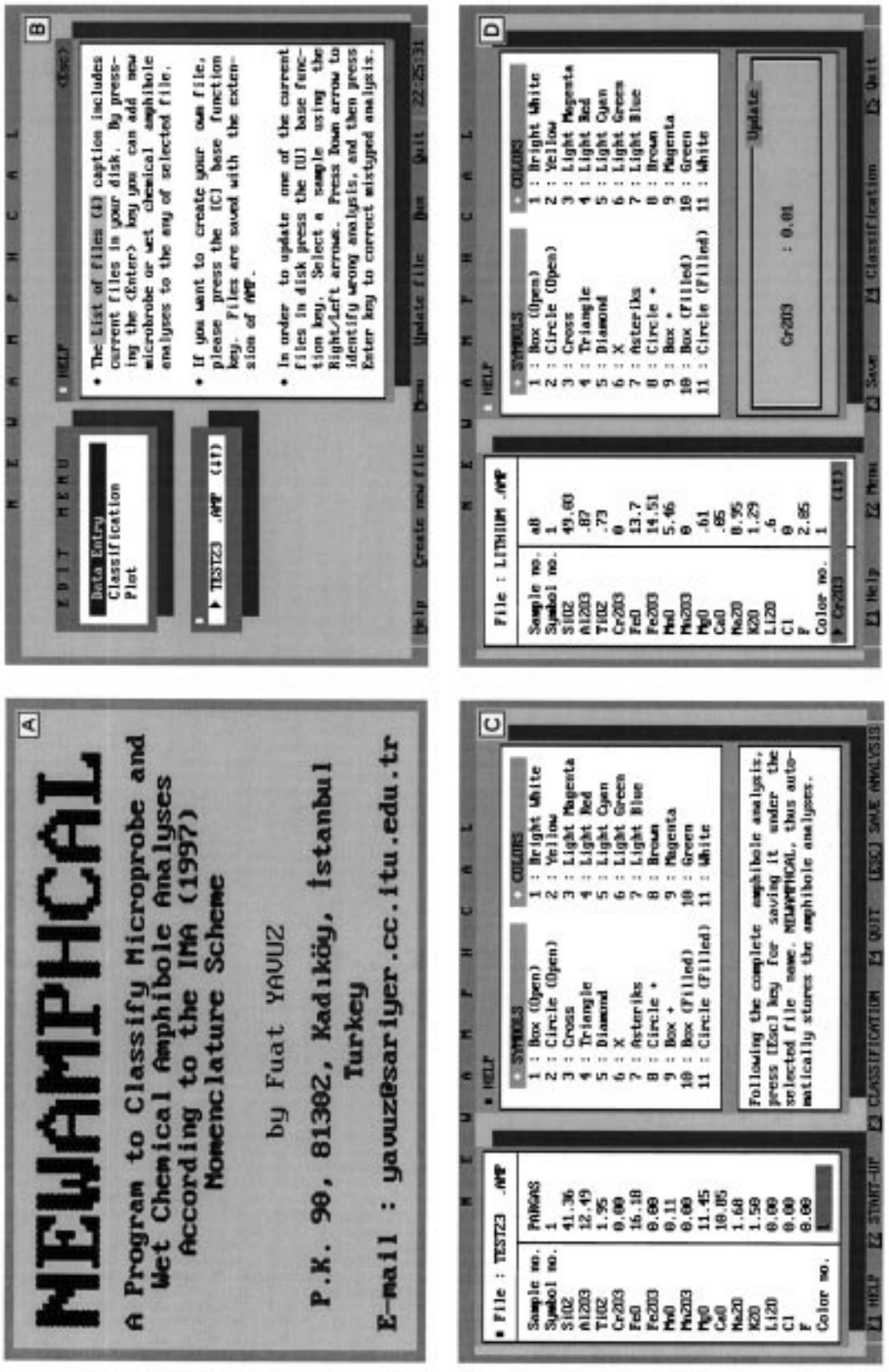

Fig. 1. (A) Start-up window of NEWAMPHCAL by executing 'Amphcal.Exe' program. (B) Edit menu of program with selecting base function options. (C) Input menu format for editing amphibole analysis. (D) Graphic screen output of program to adjust amphibole analysis for selected file name.

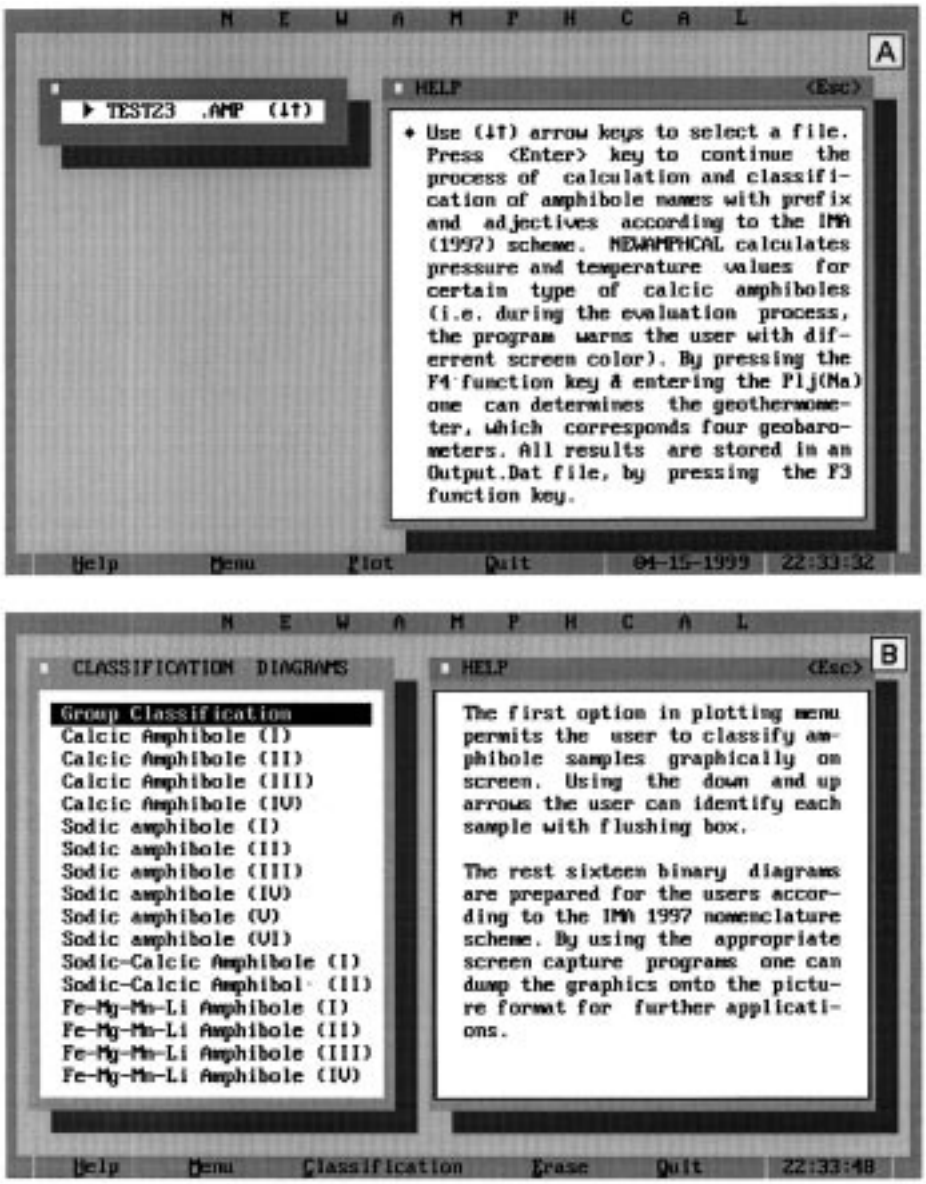

Fig. 2. (A) Start-up window of 'Clasamp.Exe' program with base function keys. (B) Select menu of amphibole classification diagrams by executing 'Ampplot.Exe' program.

Once the [C] function key is selected the screen design similar to Fig. 1C appears on screen. This part of program is used to enter sample identifications, to edit oxide or element analysis from the keyboard, and to add or delete data from file. The [F1] key brings the help menu on screen with symbol and color codes. Eighteen variables are defined by the program for processing such as sample number, symbol number, color number, SiO_2, Al_2O_3, TiO_2, Cr_2O_3, FeO, Fe_2O_3, MnO, Mn_2O_3, MgO, CaO, Na_2O, K_2O, LiO_2, Cl, and F. Entered data for these variables are subsequently stored in sequential (ASCII) files on disk. Eleven different symbol and color shapes are used for different group data set on ternary and binary amphibole classification diagrams. By pressing the [F2] function key on this window (Fig. 1C) and then selecting the [U] base function key (Fig. 1B) the program returns to the other window as shown in Fig. 1D. First selecting oxides or elements with down or up cursor movement keys and then pressing Enter key bring an update window on screen. The user can correct the mistyped amphibole analysis at this part of program process.

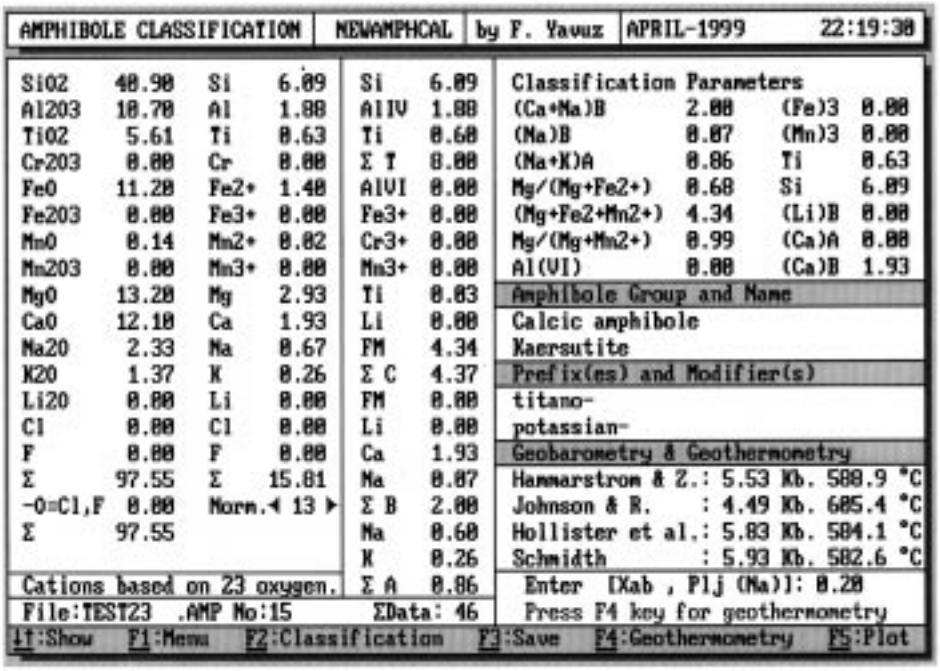

Fig. 3. Calculation and classification of selected amphibole samples by using 'Clasamp.Exe' program (see text for explanations).

Following the correction of mistyped analysis, one can press Enter key for next data operations. By pressing the [F3] function key, one can saves the corrected chemical analyses into the same file name.

3.2. Estimation of chemical analyses

The 'Clasamp.Exe' program can process files, saved on disk with the extension of 'Amp' under the 'Amphcal.Exe' program. This program constitutes the main part of NEWAMPHCAL. Once the user executes the 'Clasamp.Exe', a new screen design similar to Fig. 2A appears. By selecting amphibole file with down arrow key and then pressing Enter key, the program continues to calculate the amphibole analyses and a new screen form comes on screen as shown in Fig. 3. The program presents all the calculated microprobe data together with the classification parameters, amphibole names, Al-in-hornblende geobarometers and geothermometer for certain calcic amphiboles. Pressing down and up arrows brings the next evaluated sample on screen. The function keys at the base of the screen can be used for returning main menu by pressing the [F1] function key, processing another entered microprobe amphibole analysis by pressing the [F2] function key, saving all the calculated results under the 'Output.Txt' file name by pressing the [F3] function key, and plotting binary classification diagrams by pressing the [F5] function key. As earlier stated, NEWAMPHCAL gives temperature values for certain types of calcic amphiboles according to the geothermometer equations proposed by Holland and Blundy (1994). If calculated amphibole analysis is valid for the evaluation, then the screen color changes blue to dark blue during the down cursor movement key. At this part of program, by pressing the [F4] function key brings the 'Enter [X_{ab}, Plj (Na): ■]' message on screen. Following the entrance of recalculated sodium content of plagioclase, the program continues to process and presents the temperature values together with the pressure values as shown in Fig. 2. An example output of calculated test data by NEWAMPHCAL with the 'Example.Amp' file is given in the Appendix. The recalculated sodium content of plagioclase is taken constant 0.25 for calculating the temperature values of certain type calcic amphiboles.

3.3. Plotting of recalculated analyses on the classification diagrams

Executing of 'Ampplot.Exe' program creates Cal1, Cal2, Cal3, Cal4 (i.e., for calcic group), Alk1, Alk2, Alk3, Alk4, Alk5, Alk6 (i.e., for sodic group), Sc1, Sc2 (i.e., for sodic–calcic group), Feg1, Feg2, Feg3, Feg4 (i.e., for Fe–Mg–Mn–Li group), and Amph data files with the extension of 'Dat' each time on disk for the magnesian–iron–manganese–lithium, calcic, sodic–calcic, and sodic group amphibole analyses. The 'Amplot.Exe' program for plotting samples uses these files. Once the 'Amplot.Exe' program is executed, a

Table 2
Representative amphibole analyses selected from literature and their comparison with respect to amphibole names, prefix, and modifiers by NEWAMPHCAL (IMA 1997 scheme) and earlier form of AMPHCAL (IMA 1978 scheme) computer programs

	1	2	3	4	5	6	7	8	9
SiO_2	44.22	56.01	52.50	55.27	55.74	44.89	57.14	59.06	32.10
TiO_2	0.00	0.14	0.00	0.00	0.00	0.67	0.00	0.20	3.20
Al_2O_3	23.79	2.96	1.60	0.34	0.23	17.91	1.94	12.38	22.00
Cr_2O_3	0.00	0.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FeO	9.21	7.01	27.22	4.52	7.09	13.31	11.12	10.84	13.70
Fe_2O_3	0.20	0.15	0.09	0.00	0.00	0.67	0.01	2.36	0.00
MnO	0.16	0.01	0.80	16.62	14.73	0.37	0.11	0.25	0.10
Mn_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MgO	20.69	27.94	14.70	19.18	18.55	18.09	26.82	8.82	8.00
CaO	0.62	1.68	0.60	1.19	1.40	0.40	0.63	0.21	12.50
Na_2O	0.00	0.56	0.10	0.26	0.08	1.45	0.27	0.11	0.70
K_2O	0.00	0.19	0.00	0.00	0.02	0.05	0.06	0.05	3.80
Li_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.00
Total	98.89	96.87	97.61	97.38	97.81	97.81	97.99	94.46	96.10
Amphibole group & name with prefix and modifiers given by authors	Fe–Mg–Mn *Gedrite* (Deer et al., 1962)	Fe–Mg–Mn *Anthophyllite* (Deer et al., 1962)	Fe–Mg–Mn *Anthophyllite* (Deer et al., 1962)	Fe–Mg–Mn *Tirodite* (Rock and Leake, 1984)	Fe–Mg–Mn *Tirodite* (Rock and Leake, 1984)	Fe–Mg–Mn *Gedrite* (Deer et al., 1962)	Fe–Mg–Mn *Anthophyllite* (Hawthorne, 1983)	Fe–Mg–Mn *Holmquistite* (Deer et al., 1962)	Calcic *Magnesio sadanagaite* (Shimazaki et al., 1984)
Amphibole group & name with prefix and modifiers by AMPHCAL	Fe–Mg–Mn *Magnesio, Cummingtonite* or *Gedrite*	Fe–Mg–Mn *Magnesio, Cummingtonite* or *Antophyllite*	Fe–Mg–Mn *Dannemorite*	Fe–Mg–Mn *Tirodite*	Fe–Mg–Mn *Tirodite*	Fe–Mg–Mn *Gedrite* or *Cummingtomite*	Fe–Mg–Mn *Magnesio, Cummingtonite* or *Anthophyllite*	Fe–Mg–Mn *Cummingtonite* or *Anthophyllite*	Calcic *Potassium, Titanian, Magnesio, Sadamagaite*
Amphibole group & name with prefix and modifiers by NEWAMPHCAL	Fe–Mg–Mn–Li *Gedrite*	Fe–Mg–Mn–Li *Cummingtonite* or *Anthophyllite*	Fe–Mg–Mn–Li *Grunerite* or *Ferroanthophyllite*	Fe–Mg–Mn–Li *Mangano cummingtonite*	Fe–Mg–Mn–Li *Mangano, Cummingtonite*	Fe–Mg–Mn–Li *Sodian Gedrite*	Fe–Mg–Mn–Li *Cummingtonite* or *Anthophyllite*	Fe–Mg–Mn–Li *Cummingtonite* or *Anthophyllite*	Calcic *Potassic Titanian, Magnesio, Sadanagaite*
	10	11	12	13	14	15	16	17	18
SiO_2	30.20	54.90	39.83	39.52	53.00	40.90	48.40	41.36	48.10
TiO_2	4.00	0.21	2.56	0.24	0.07	5.61	0.33	1.95	0.10
Al_2O_3	24.80	1.20	14.98	18.05	2.97	10.70	11.54	12.49	11.05
Cr_2O_3	0.00	0.50	0.00	0.00	0.01	0.00	0.00	0.00	0.00
FeO	15.20	2.80	3.78	3.23	9.21	11.20	3.59	12.36	1.65
Fe_2O_3	0.00	0.50	7.66	0.00	1.88	0.00	1.44	4.25	0.67
MnO	0.10	0.08	0.00	0.37	0.25	0.14	0.07	0.11	0.00
Mn_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MgO	6.60	25.30	14.44	17.87	17.30	13.20	18.03	11.45	20.60
CaO	12.30	12.70	12.39	15.78	13.70	12.10	10.70	10.85	12.50
Na_2O	1.00	0.60	2.27	1.46	0.30	2.33	2.52	1.68	2.54
K_2O	3.70	0.00	1.25	0.23	0.06	1.37	0.60	1.50	1.24
Li_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	0.00	0.00	0.00	3.20	0.00	0.00	0.00	0.00	0.00
Total	97.90	98.79	99.16	99.95	98.75	97.55	97.22	98.00	98.45

Amphibole group & name with prefix and modifiers given by authors	Calcic *Sadanagaite* (Shimazaki et al., 1984)	Calcic *Tremolite* (Deer et al., 1962)	Calcic *Basaltic, Hornblende* (Deer et al., 1962)	Calcic *Fluor Cannilloite* (Hawthorne et al., 1996)	Calcic *Actinolite* (Tindle and Webb, 1994)	Calcic *Potassian, Kaersutite* (Tindle and Webb, 1994)	Calcic *Hornblende* (Hawthorne, 1983)	Calcic *Potassian, Tschermakite* (Hawthorne, 1983)	Calcic *Pargasite* (Deer et al., 1962)
Amphibole group & name with prefix and modifiers by AMPHCAL	Calcic *Titanium, Potassium, Alumino, Sadanagaite*	Calcic *Tremolitic, Hornblende*	Calcic *Titanian, Magnesio hastingsite*	Calcic *Fluor Subsilisic, Tschermakite*	Calcic *Actinolite*	Calcic *Potassian, Titanian, Kaersutite*	Calcic *Magnesio hornblende*	Calcic *Potassian, Ferroan Pargasite*	Calcic *Edenitic, Hornblende*
Amphibole group & name with prefix and modifiers by NEWAMPHCAL	Calcic *Alumino Potassic, Titanian, Sadanagaite*	Calcic *Magnesio hornblende*	Calcic *Titanian, Magnesio hastingsite*	Calcic *Fluoro, Cannilloite*	Calcic *Actinolite*	Calcic *Titano Potassian, Kaersutite*	Calcic *Magnesio hornblende*	Calcic *Potassian, Pargasite*	Calcic *Edenite*
	19	20	21	22	23	24	25	26	27
SiO_2	41.63	47.40	37.20	53.80	52.67	53.73	58.88	57.74	53.84
TiO_2	0.87	0.31	1.36	0.10	3.53	0.41	0.00	0.01	0.16
Al_2O_3	13.13	12.10	12.13	1.37	1.72	2.72	0.00	0.37	12.92
Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FeO	11.00	8.88	22.44	0.00	2.41	4.70	0.00	0.01	5.03
Fe_2O_3	2.20	6.46	8.34	1.89	0.58	4.72	0.17	0.29	0.00
MnO	0.16	0.18	1.14	8.69	0.06	0.00	0.00	2.40	0.02
Mn_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MgO	11.86	10.70	1.42	18.45	21.32	20.60	24.24	23.67	14.21
CaO	12.33	7.20	7.36	5.43	6.95	2.73	7.00	9.01	2.33
Na_2O	1.55	4.50	4.22	5.63	3.64	7.42	7.20	3.14	9.26
K_2O	2.83	0.28	2.43	1.72	5.70	1.82	0.00	0.67	0.14
Li_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F	1.78	0.00	0.00	0.36	1.29	0.92	4.74	0.37	0.00
Total	99.34	98.01	98.04	97.44	99.87	99.77	102.23	97.68	97.91
Amphibole group & name with prefix and modifiers given by authors	Calcic *Potassic, Pargasite* (Robinson et al., 1997)	Sodic–calcic *Barroisite* (Tindle and Webb, 1994)	Sodic–calcic *Ferri Potassian, Taramite* (Deer et al., 1962)	Sodic–calcic *Richterite* (Deer et al., 1962)	Sodic–calcic *Richterite* (Deer et al., 1962)	Sodic–calcic *Potassian, Magnesio, Katophortie* (Deer et al., 1962)	Sodic–calcic *Richterite* (Deer et al., 1962)	Sodic–calcic *Richterite* (Deer et al., 1962)	Alkali *Nyböite* (Ungaretti et al., 1981)
Amphibole group & name with prefix and modifiers by AMPHCAL	Calcic *Potassium, Ferroan Pargasite*	Sodic–calcic *Barroisite*	Sodic–calcic *Ferri Taramite*	Sodic–calcic *Manganese, Potassian, Richterite*	Sodic–calcic *Potassium, Titanian, Magnesio katophorite*	Alkali *Potassian, Anophorite,* (*Magnesio Arfvedsonite*)	Sodic–calcic *Fluor Magnesio katophorite*	Calcic *Subcalcic, Tremolite*	Alkali *Nyböite* (*Eckermannite*)
Amphibole group & name with prefix and modifiers by NEWAMPHCAL	Calcic *Potassic fluorian, Pargasite*	Sodic–calcic *Barroisite*	Sodic–calcic *Ferri Taramite*	Sodic–calcic *Potassian, Richterite*	Sodic–calcic *Potassic Titanian, Fluorian, Magnesiokatophorite*	Sodic–calcic *Potassian Ferrian, Fluorian, Magnesiokatophorite*	Sodic–calcic *Fluoro Magnesio katophorite*	Sodic–calcic *Winchite*	Sodic *Nyböite*
	28	29	30	31	32	33	34	35	36
SiO_2	54.56	59.30	57.20	50.45	55.80	50.66	48.56	51.12	51.91
TiO_2	0.23	0.25	2.20	0.14	0.03	0.00	0.67	0.68	0.41
Al_2O_3	8.29	8.66	0.38	1.96	1.27	0.00	1.41	1.13	1.86
Cr_2O_3	0.00	0.00	3.50	0.00	0.00	0.00	0.00	0.00	0.00

(continued on next page)

FeO	10.31	8.05	0.44	17.90	0.00	0.00	18.43	8.87	6.45	
Fe_2O_3	7.94	5.21	0.00	17.52	12.23	0.50	12.58	16.73	6.77	
MnO	0.13	0.12	0.05	1.40	0.00	12.42	3.38	4.51	3.82	
Mn_2O_3	0.00	0.00	0.00	0.00	3.86	24.35	0.00	0.00	0.00	
MgO	8.74	9.37	20.90	0.05	10.96	1.46	1.23	2.02	13.36	
CaO	0.81	1.24	3.70	0.08	0.50	0.18	0.45	0.15	6.64	
Na_2O	6.71	6.11	8.30	6.80	9.69	9.13	8.26	9.22	4.60	
K_2O	0.14	0.55	1.20	1.48	1.12	0.76	1.15	1.19	0.82	
Li_2O	0.00	0.00	0.00	0.00	0.00	0.02	0.21	0.99	0.11	
Cl	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
F	0.00	0.00	0.00	2.58	1.08	0.00	1.90	2.87	2.91	
Total	97.06	98.86	97.87	98.88	96.54	99.48	98.23	99.48	99.66	
Amphibole group & name with prefix and modifiers given by authors	Alkali *Crossite* (Deer et al., 1962)	Alkali *Glaucophane* (Deer et al., 1962)	Alkali *Eckermannite* (Tindle and Webb, 1994)	Alkali *Fluor Riebeckite* (Hawthorne, 1983)	Sodic *Leakeite* (Hawthorne et al., 1992)	Sodic *Ungarettite* (Hawthorne et al., 1995)	Sodic *Arfvedsonite* (Hawthorne et al., 1993)	Sodic *Ferro Fluor, Leakeite* (Hawthorne et al., 1993)	Sodic *Magnesio Ferri, Fluor Katophorite* (Hawthorne et al., 1993)	
Amphibole group & name with prefix and modifiers by AMPHCAL	Alkali *Crossite*	Alkali *Glaucophane*	Cannot classify	Alkali *Fluor Potassian, Ferro glaucophane*	Cannot classify	Alkali *Alumino Kozulite*	Cannot classify	Alkali *Fluor Kornite*	Sodic–calcic *Fluor Barroisite*	
Amphibole group & name with prefix and modifiers by NEWAMPHCAL	Sodic *Magnesio riebeckite*	Sodic *Glaucophane*	Sodic *Chromian, Richterite*	Sodic *Fluoro Potassian, Riebeckite*	Sodic *Fluorian Leakeite*	Sodic *Ungarettite*	Sodic *Fluorian Arfvedsonite*	Sodic *Fluoro Ferro Leakeite*	Sodic–calcic *Richterite*	

pull-down (Fig. 2B) menu appears on screen showing the plot types of one ternary and 17 binary diagrams. Using the down and up cursor movement keys on pull-down menu and selecting one of them by pressing the Enter key, the program loads appropriate file with the extension of 'Dat', and then brings the selected amphibole classification diagram on screen.

In order to show the program outputs on amphibole classification diagrams, this study has compiled representative amphibole analyses from literature. A list of these analyses together with the evaluations by authors, the earlier form of AMPHCAL program, and its new version of NEWAMPHCAL are given in Table 2. The discrimination of amphibole groups can be plotted on binary $Ca+Na_B$ vs Na_B and ternary $(Ca+Na_B)-(Fe^{2+}+Fe^{3+})-Na_B$ diagrams (Fig. 4A and B). Using the classification parameters of $Ca+Na_B$ and Na_B, Mogessie et al. (1990), plotted the 57 amphibole analyses on this diagram. Taking into account the revision at Na_B contents between the calcic, sodic–calcic and sodic amphiboles, NEWAMPHCAL plots the recalculated chemical analyses of amphibole samples with the revised form as shown in Fig. 4A. Once the graphic is on screen, the user can identify each sample with the flushing green box by pressing the down arrow key. Using the Esc key, the program brings the next ternary amphibole group classification diagram on screen, which is given, in this study. One also can determine the amphibole name in each group by pressing the down arrow key as shown in Fig. 4B. The amphibole name presented on this diagram is the graphical illustration of 'Amph.Dat' created under the 'Clasamp.Exe' program. By pressing the Esc key, the program returns the plotting menu (Fig. 2B). Plots of amphibole analyses on different diagrams have been shown in Fig. 5A–D for the calcic type, in Fig. 6A–D for the sodic type, in Fig. 7A and B for the iron–magnesium–manganese–lithium, and in Fig. 7C and D for the sodic type. 'Ampplot.Exe' program plots these diagrams using the Cal1.Dat, Cal2.Dat, Cal3.Dat, Cal4.Dat, Alk1.Dat, Alk2.Dat, Alk3.Dat, Alk4.Dat, Sc1.Dat, Sc2.Dat, Feg1.Dat, Feg2.Dat, Feg3.Dat, and Feg4.Dat files created each time under the 'Clasamp.Exe' program. It means that NEWAMPHCAL automatically classifies the amphibole analyses for graphical outputs.

4. Discussion

NEWAMPHCAL is the new version of AMPHCAL (Yavuz, 1996) program running under DOS and Windows operating systems for the amphibole formulae calculation and classification proposed by the

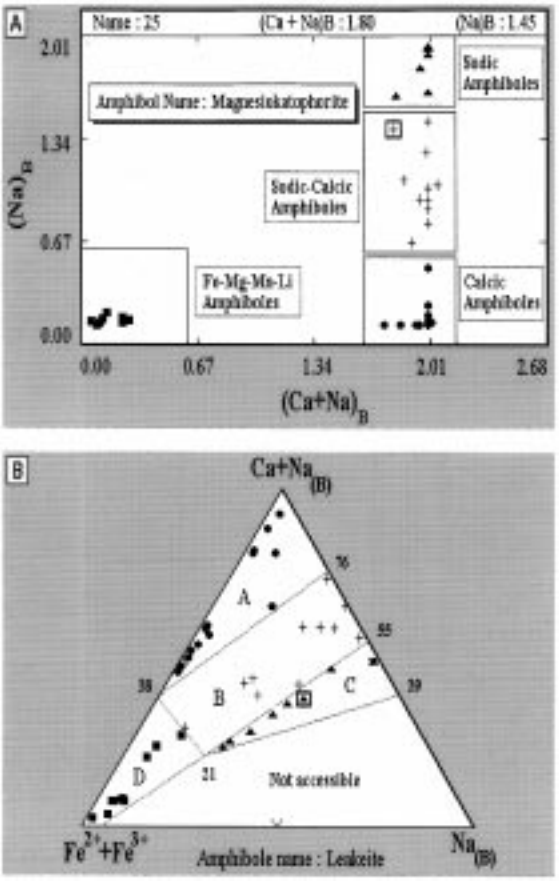

Fig. 4. (A) Plot of classification parameters on binary $(Ca+Na)_B$ vs $(Na)_B$ diagram for amphibole group discrimination using selected amphibole analyses from literature. (B) Plot of recalculated analyses on ternary $(Ca+Na)_B-(Fe^{2+}+Fe^{3+})-Na_B$ group classification diagram. A = calcic amphibole field; B = sodic–calcic amphibole field; C = sodic amphibole field; D = Fe–Mg–Mn–Li amphibole field. Sample in box shows the amphibole name in which selected by the down arrow key.

IMA 1997 amphibole nomenclature scheme. The program is written in QUICKBASIC and consists of three executable programs. It is an easy program to use with pull-down menus and base function keys. The program allows the user data input, their storage, calculation of chemical analyses and plotting of classification parameters on 18 different diagrams. The calculated results can be exported to spreadsheet and editing programs such as EXCEL and Microsoft WORD for Windows applications. This software, which is controlled by several error codes, warns the user while it continues to process, and thus shows limited unexpected program termination. The program gives a message 'NEWAPHCAL cannot classify' if amphibole analysis is not appropriate to process. The performance of NEWAMPHCAL was checked by calculating selected representative amphibole analyses from literature (Deer et al., 1962; Ungaretti et al., 1981; Hawthorne, 1983; Rock and Leake, 1984; Shimazaki et al., 1984; Hawthorne et al., 1992, 1993, 1995; Tindle and Webb, 1994; Currie, 1997; Robinson et al., 1997).

The advantage of this program can be stated as the input of multiple amphibole data for the user under the defined file name, automatic saving of edited analyses with restricted data base functions, calculation and classification of amphibole analyses together with the prefixes and modifiers, determination of four Al-in-hornblende geobarometer including one geothermometer for the certain calcic type amphiboles, and plotting of recalculated analyses on various diagrams. In this study, I have used the classification parameters of $Ca+Na_B$ and Na_B on ternary $(Ca+Na_B)-(Fe^{2+}+Fe^{3+})-Na_B$ diagram (Fig. 4B) to separate four amphibole analyses onto the each amphibole groups. The given diagram also is harmonious with the binary amphibole plot by Mogessie et al., (1990). Following the primary divisions at $Na_B < 0.50$ and $Na_B \geq 1.50$, instead of $Na_B < 0.67$ and $Na_B \geq 1.34$ between the calcic, sodic–calcic and sodic amphiboles, the binary $Ca+Na_B$ vs Na_B group classification diagram (Fig. 4A) is redrawn according to the IMA 1997 rules. If microprobe iron contents are given as total FeO, then the program makes ferric and ferrous iron separation according to the procedure given by Droop (1987). This calculation scheme gives a similar result compared to the 'minimum ferric iron' criterion outlined by Schumacher (1997).

In this paper, the printouts of screen images were converted to 'Pcx' file formats using the memory resident screen capture program of PCXDUMP. Following some adjustments on figures they were sent to a Microsoft WORD editor for quality printouts. A compiled version of the program takes approximately 398 kilobytes and can be obtained by anonymous FTP from the server IAMG.ORG.

Acknowledgements

I would like to give special thanks to J. Schumacher for the improvement of ternary diagram and A. Mogessie for valuable comments on the earlier form of this manuscript.

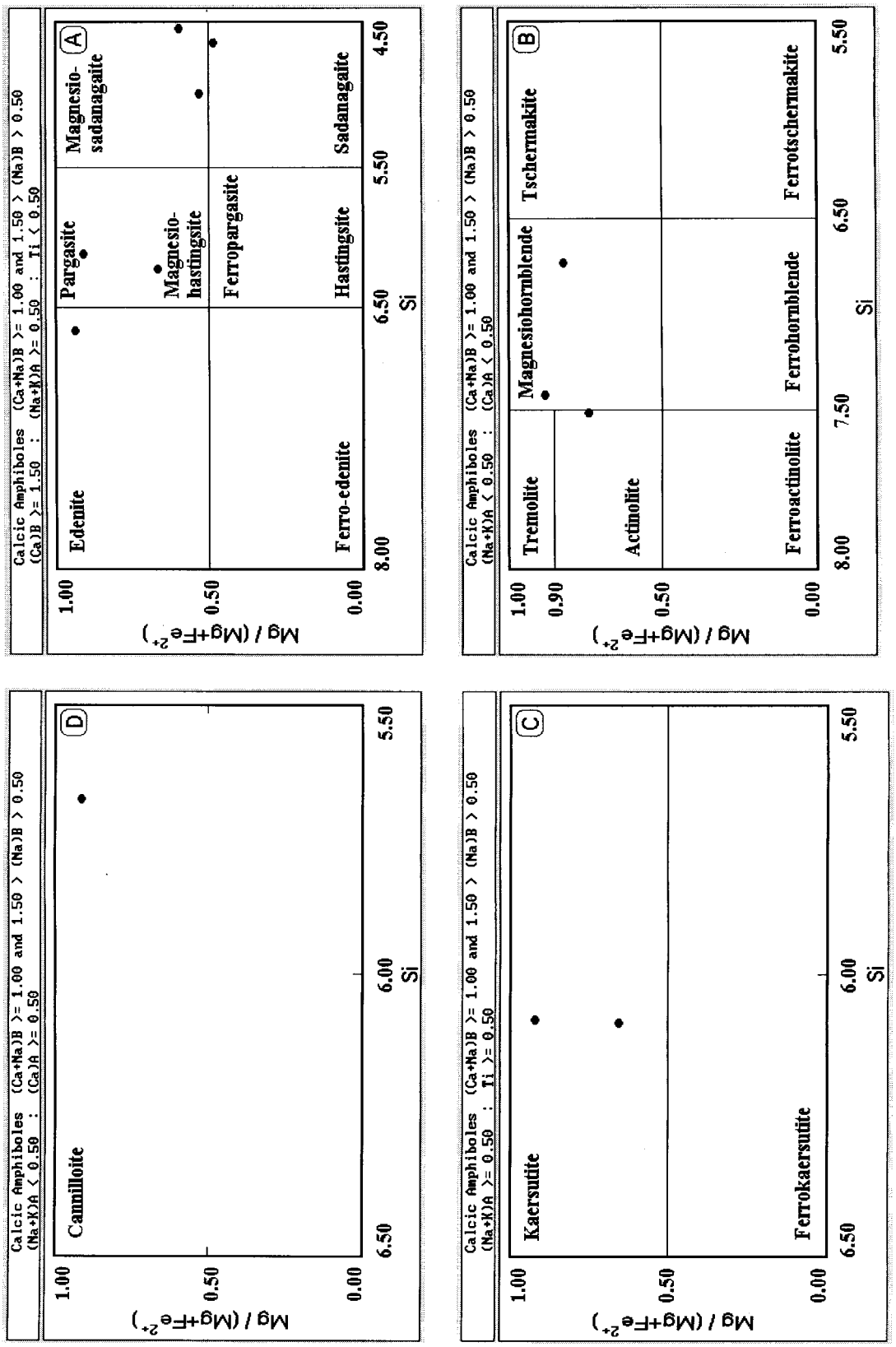

Fig. 5. (A–D) Distribution of selected amphibole samples in Test23.Amp file on calcic classification diagrams together with classification parameters.

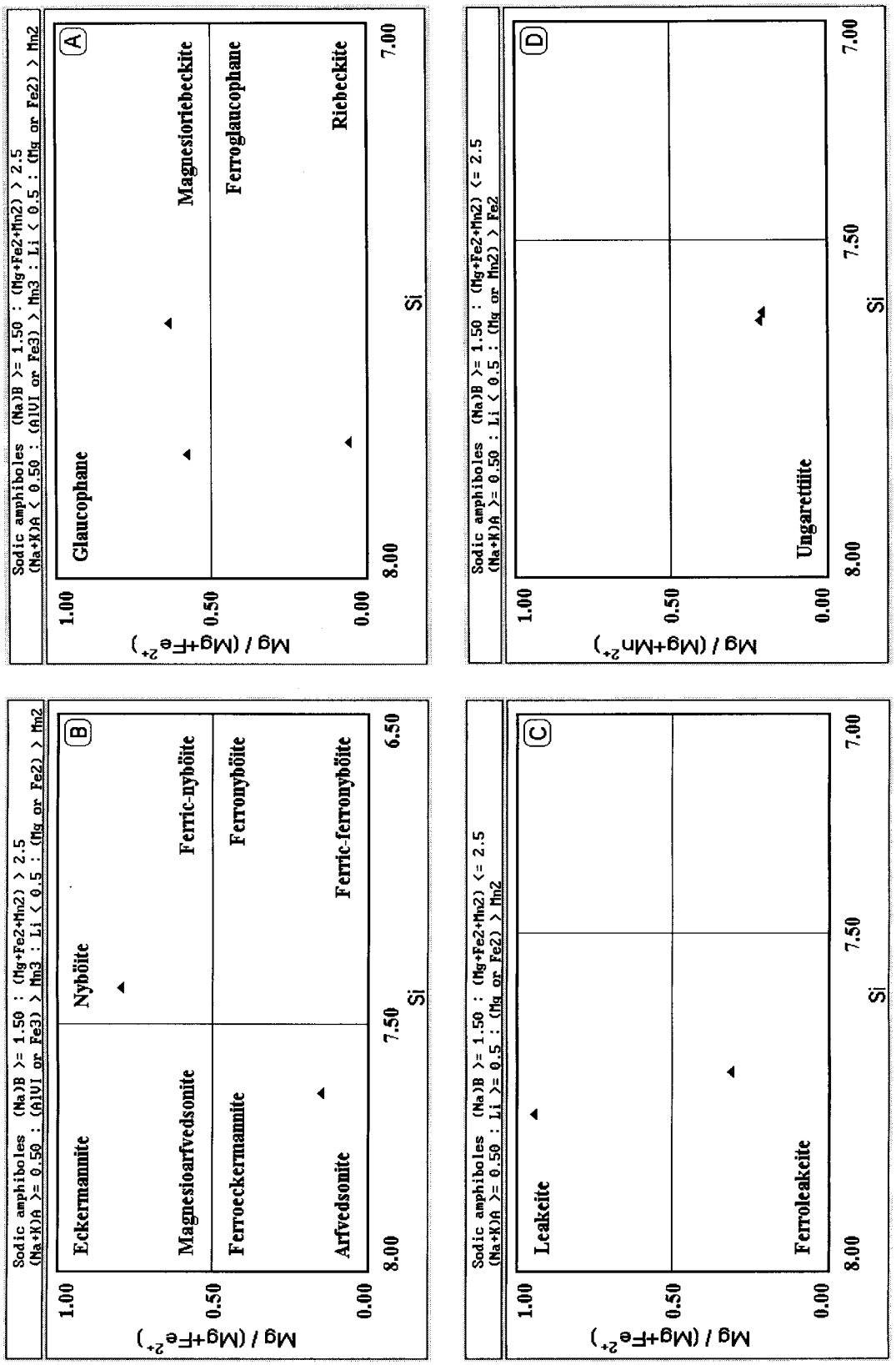

Fig. 6. (A–D) Distribution of amphibole samples in Test23.Amp file on sodic classification diagrams.

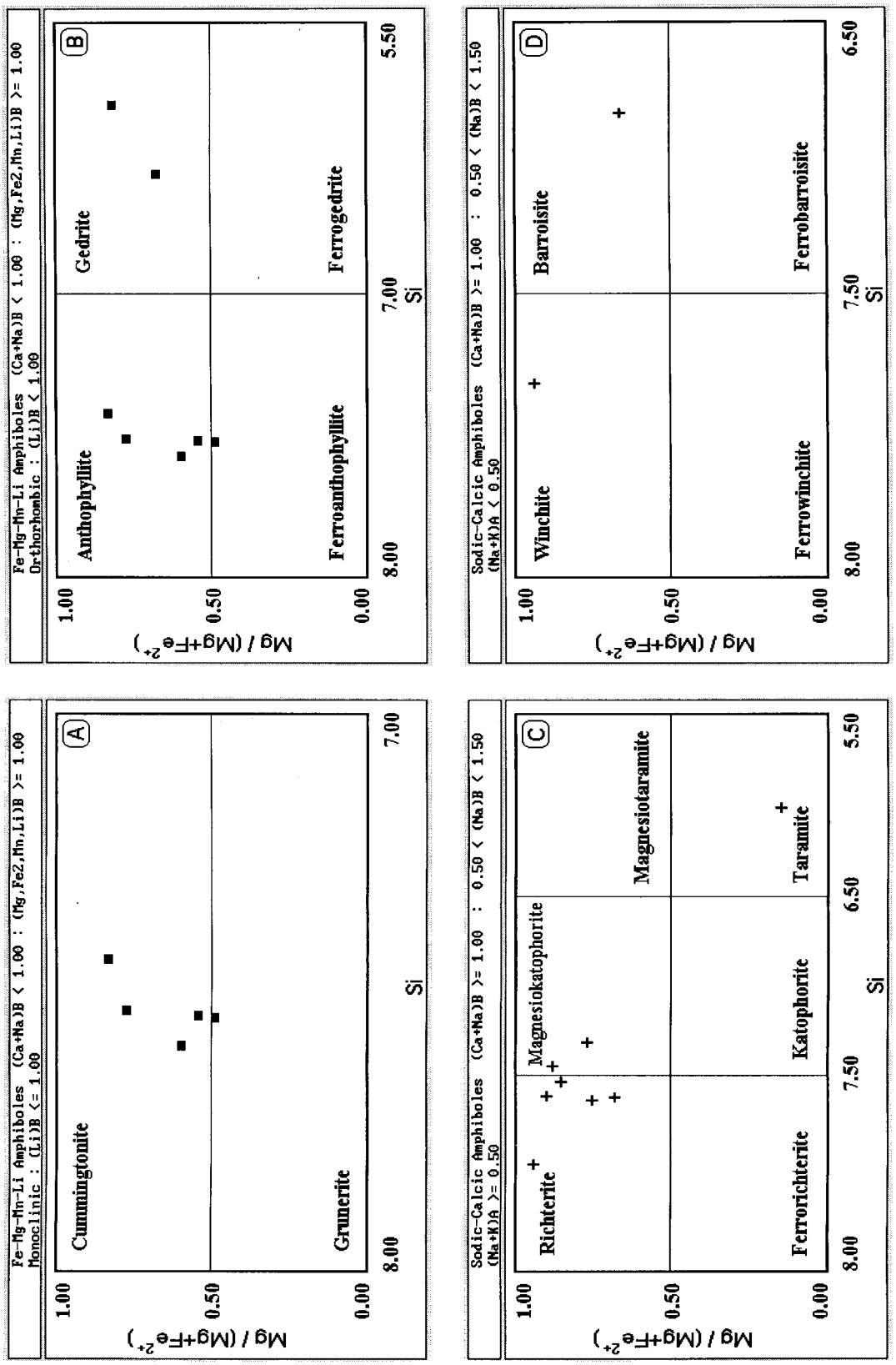

Fig. 7. (A and B) Distribution of amphibole samples on Fe–Mg–Mn–Li amphibole classification diagrams. (C and D) Amphibole samples on sodic–calcic amphibole classification diagrams.

Appendix A

The calculated results of (Example.Amp) file by NEWAMPHCAL 04-19-1999 22:31:46 are shown below.

Sample	SiO_2	Al_2O_3	TiO_2	Cr_2O_3	FeO	Fe_2O_3	MnO	Mn_2O_3	MgO
1	44.22	23.79	0.00	0.00	9.39	0.00	0.16	0.00	20.69
2	56.01	2.96	0.14	0.22	7.14	0.00	0.01	0.00	27.94
3	52.50	1.60	0.00	0.00	27.30	0.00	0.80	0.00	14.70
4	55.27	0.34	0.00	0.00	4.52	0.00	16.62	0.00	19.18
10	30.20	24.80	4.00	0.00	15.20	0.00	0.10	0.00	6.60
12	39.83	14.98	2.56	0.00	10.67	0.00	0.00	0.00	14.44
15	40.90	10.70	5.61	0.00	11.20	0.00	0.14	0.00	13.20
16	48.40	11.54	0.33	0.00	5.06	0.00	0.07	0.00	18.03
19	39.90	14.35	4.65	0.00	0.67	0.00	0.08	0.00	14.52
20	47.40	12.10	0.31	0.00	14.69	0.00	0.18	0.00	10.70
21	37.20	12.13	1.36	0.00	29.94	0.00	1.14	0.00	1.42
22	53.80	1.37	0.10	0.00	1.70	0.00	8.69	0.00	18.45
23	52.67	1.72	3.53	0.00	2.93	0.00	0.06	0.00	21.32
28	53.84	12.92	0.16	0.00	5.03	0.00	0.02	0.00	14.21
29	54.56	8.29	0.23	0.00	17.45	0.00	0.13	0.00	8.74
30	59.30	8.66	0.25	0.00	12.74	0.00	0.12	0.00	9.37
32	50.45	1.96	0.14	0.00	33.66	0.00	1.40	0.00	0.05

Sample	CaO	Na_2O	K_2O	Li_2O	Cl	F	Total	O = F, Cl	Total
1	0.62	0.00	0.00	0.00	0.00	0.00	98.87	0.00	98.87
2	1.68	0.56	0.19	0.00	0.00	0.00	96.63	0.00	96.63
3	0.60	0.10	0.00	0.00	0.00	0.00	97.60	0.00	97.60
4	1.19	0.26	0.00	0.00	0.00	0.00	97.38	0.00	97.38
10	12.30	1.00	3.70	0.00	0.00	0.00	97.90	0.00	97.90
12	12.39	2.27	1.25	0.00	0.00	0.00	98.39	0.00	98.39
15	12.10	2.33	1.37	0.00	0.00	0.00	97.55	0.00	97.55
16	10.70	2.52	0.60	0.00	0.00	0.00	97.25	0.00	97.25
19	12.14	1.90	2.31	0.00	0.00	0.00	90.52	0.00	90.52
20	7.20	4.50	0.28	0.00	0.00	0.00	97.36	0.00	97.36
21	7.36	4.22	2.43	0.00	0.00	0.00	97.20	0.00	97.20
22	5.43	5.63	1.72	0.00	0.00	0.36	97.25	0.15	97.10
23	6.95	3.64	5.70	0.00	0.00	1.29	99.81	0.54	99.27
28	2.33	9.26	0.14	0.00	0.00	0.00	97.91	0.00	97.91
29	0.81	6.71	0.14	0.00	0.00	0.00	97.06	0.00	97.06
30	1.24	6.11	0.55	0.00	0.00	0.00	98.34	0.00	98.34
32	0.08	6.80	1.48	0.00	0.00	2.58	98.60	1.09	97.51

Sample	Si	Al_{IV}	Al_{VI}	Ti	Cr	Fe^{3+}	Fe^{2+}	Mn^{2+}	Mn^{3+}
1	5.94	2.06	1.70	0.00	0.00	0.36	0.69	0.02	0.00
2	7.68	0.32	0.15	0.01	0.02	0.00	0.82	0.00	0.00
3	7.84	0.16	0.12	0.00	0.00	0.01	3.40	0.10	0.00
4	7.99	0.01	0.05	0.00	0.00	0.00	0.55	2.03	0.00
10	4.62	3.38	1.08	0.46	0.00	0.34	1.60	0.01	0.00
12	5.79	2.21	0.36	0.28	0.00	0.41	0.88	0.00	0.00

15	6.09	1.88	0.00	0.63	0.00	0.00	1.40	0.02	0.00
16	6.74	1.26	0.63	0.03	0.00	0.00	0.59	0.01	0.00
19	6.09	1.91	0.67	0.53	0.00	0.00	0.09	0.01	0.00
20	6.83	1.17	0.88	0.03	0.00	0.70	1.07	0.02	0.00
21	6.00	2.00	0.30	0.16	0.00	1.01	3.03	0.16	0.00
22	7.62	0.23	0.00	0.01	0.00	0.00	0.20	1.04	0.00
23	7.45	0.29	0.00	0.38	0.00	0.00	0.35	0.01	0.00
28	7.38	0.62	1.47	0.02	0.00	0.00	0.58	0.00	0.00
29	7.69	0.31	1.07	0.02	0.00	1.09	0.97	0.02	0.00
30	8.00	0.00	1.41	0.03	0.00	0.12	1.35	0.01	0.00
32	7.97	0.03	0.34	0.02	0.00	1.25	3.20	0.19	0.00

Sample	Mg	Ca	Na	K	Li	Cl	F	Tot. cat.	$(Na)_B$
1	4.14	0.09	0.00	0.00	0.00	0.00	0.00	15.00	0.00
2	5.71	0.25	0.15	0.03	0.00	0.00	0.00	15.15	0.03
3	3.27	0.10	0.03	0.00	0.00	0.00	0.00	15.03	0.00
4	4.13	0.18	0.07	0.00	0.00	0.00	0.00	15.02	0.05
10	1.50	2.00	0.30	0.72	0.00	0.00	0.00	16.03	0.02
12	3.13	1.93	0.64	0.23	0.00	0.00	0.00	15.87	0.00
15	2.93	1.93	0.67	0.26	0.00	0.00	0.00	15.81	0.07
16	3.74	1.60	0.68	0.11	0.00	0.00	0.00	15.38	0.40
19	3.30	1.98	0.56	0.45	0.00	0.00	0.00	15.59	0.02
20	2.30	1.11	1.26	0.05	0.00	0.00	0.00	15.42	0.89
21	0.34	1.27	1.32	0.50	0.00	0.00	0.00	16.09	0.73
22	3.90	0.82	1.55	0.31	0.00	0.00	0.16	15.68	1.04
23	4.50	1.05	1.00	1.03	0.00	0.00	0.58	16.04	1.00
28	2.90	0.34	2.46	0.02	0.00	0.00	0.00	15.80	1.66
29	1.84	0.12	1.83	0.03	0.00	0.00	0.00	14.98	1.83
30	1.92	0.18	1.63	0.10	0.00	0.00	0.00	14.75	1.63
32	0.01	0.01	2.08	0.30	0.00	0.00	1.29	15.39	1.99

Sample	$(Na+K)_A$	$(Ca)_A$	$(Ca)_B$	$(Ca+Na)_B$	Mg/(Mg+Mn)	$(Mg+Fe^{2+}+Mn)$	$(Li)_B$	$Mg/(Mg+Fe^{2+})$
1	0.00	0.00	0.09	0.09	1.00	4.85	0.00	0.86
2	0.15	0.00	0.25	0.28	1.00	6.53	0.00	0.87
3	0.03	0.00	0.10	0.10	0.97	6.77	0.00	0.49
4	0.02	0.00	0.18	0.24	0.67	6.71	0.00	0.88
10	1.00	0.12	2.00	2.02	0.99	3.12	0.00	0.48
12	0.87	0.00	1.93	1.93	1.00	4.01	0.00	0.78
15	0.86	0.00	1.93	2.00	0.99	4.34	0.00	0.68
16	0.38	0.00	1.60	2.00	1.00	4.34	0.00	0.86
19	1.00	0.00	1.98	2.00	1.00	3.40	0.00	0.97
20	0.42	0.00	1.11	2.00	0.99	3.39	0.00	0.68
21	1.09	0.00	1.27	2.00	0.69	3.52	0.00	0.10
22	0.82	0.00	0.82	1.86	0.79	5.14	0.00	0.95
23	1.03	0.00	1.05	2.05	1.00	4.85	0.00	0.93
28	0.83	0.00	0.34	2.00	1.00	3.48	0.00	0.83
29	0.03	0.00	0.12	1.96	0.99	2.82	0.00	0.66
30	0.10	0.00	0.18	1.81	0.99	3.28	0.00	0.59
32	0.39	0.00	0.01	2.00	0.06	3.40	0.00	0.00

Sample	Amphibole group	Amphibole name
1	Fe–Mg–Mn–Li amphibole	Gedrite
2	Fe–Mg–Mn–Li amphibole	Cummingtonite/anthophyllite
3	Fe–Mg–Mn–Li amphibole	Grunerite/ferroanthophyllite
4	Fe–Mg–Mn–Li amphibole	Manganocummingtonite
10	Calcic amphibole	Sadanagaite
12	Calcic amphibole	Magnesiohastingsite
15	Calcic amphibole	Kaersutite
16	Calcic amphibole	Magnesiohornblende
19	Calcic amphibole	Kaersutite
20	Sodic–calcic amphibole	Barroisite
21	Sodic–calcic amphibole	Taramite
22	Sodic–calcic amphibole	Richterite
23	Sodic–calcic amphibole	Magnesiokatophorite
28	Sodic amphibole	Nyböite
29	Sodic amphibole	Magnesioriebeckite
30	Sodic amphibole	Glaucophane
32	Sodic amphibole	Riebeckite

Sample	Prefixes	Modifiers
1	–	–
2	–	–
3	–	–
4	–	–
10	alumino-potassic-	titanian-
12	–	titanian-
15	titano-	potassian-
16	–	–
19	titano-	potassian-
20	–	–
21	ferri-	–
22	–	potassian-
23	potassic-	titanian-fluorian-
28	–	–
29	–	–
30	–	–
32	fluoro-	potassian-

Sample	Hammerstrom and Zen	Johnson and Rutherford	Hollister et al.	Schmidt (Kb)
1	0.00	0.00	0.00	0.00
2	0.00	0.00	0.00	0.00
3	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00
12	9.00	9.72	7.40	9.21
15	5.53	5.83	4.49	5.93
16	5.60	5.91	4.55	6.00
19	9.06	9.79	7.45	9.27
20	0.00	0.00	0.00	0.00

21	0.00	0.00	0.00	0.00
22	0.00	0.00	0.00	0.00
23	0.00	0.00	0.00	0.00
28	0.00	0.00	0.00	0.00
29	0.00	0.00	0.00	0.00
30	0.00	0.00	0.00	0.00
32	0.00	0.00	0.00	0.00

Sample	Temperature 1 (°C)	Temperature 2 (°C)	Temperature 3 (°C)	Temperature 4 (°C)
1	0.00	0.00	0.00	0.00
2	0.00	0.00	0.00	0.00
3	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00
12	580.29	568.82	605.44	576.87
15	635.01	630.18	651.47	628.65
16	633.87	628.91	650.51	627.58
19	579.30	567.72	604.62	575.94
20	0.00	0.00	0.00	0.00
21	0.00	0.00	0.00	0.00
22	0.00	0.00	0.00	0.00
23	0.00	0.00	0.00	0.00
28	0.00	0.00	0.00	0.00
29	0.00	0.00	0.00	0.00
30	0.00	0.00	0.00	0.00
32	0.00	0.00	0.00	0.00

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