

A Comprehensive Basic Program for Cation Calculation and Classification of Amphiboles

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ABSTRACT. This paper presents a comprehensive computer program which provides the user with information about the chemically analysed amphiboles. The program is written in BASIC in an interactive style which allows an easy operation using a standard personal computer. The required input is the raw data of mineral analyses, in either oxide or element forms, as obtained from the traditional and instrumental chemical laboratories. The program performs a sequence of tasks which includes; oxide-cation conversion, Fe^{2+}/Fe^{3+} calculations (if required), cation allocation in the different crystal sites, and identification of the amphibole group and mineral. The number of processed elements is 24 which covers all the known relevant elements encountered in amphiboles. The number of tasks and the number of elements included in this program far exceed those considered in any of the previously published programs. Besides, the program allows the user a wide latitude of options with explanations, tables and graphical presentations to help in the selection of appropriate options. The output consists of tables and plots which allow; tracing of the different operations, reliability of calculations, decision making during the execution of the program, as well as standard print forms for publication.

Introduction

In the last few years, the chemical analysis of the different minerals groups (e.g., pyroxenes, amphiboles, ..., etc.) has been subjected to several studies which aim to apply automatic recalculation techniques to analysed data in order to reveal important information about the analysed minerals. This trend is of increasing interest to mineralogists since it offers a quick and cheap way for reliable recalculation of the large number of minerals analyses obtainable by modern automatic analytical techniques.

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Compared with the other mineral groups, the amphiboles have been the subject of relatively extensive investigations, and a number of computer programs dealing with the recalculation of amphiboles analyses have recently been published. These programs generally apply one or more of the different recalculation methods to chemical analyses of amphiboles produced by either wet chemical or instrumental techniques; e.g., electron-probe micro-analysis (EPMA). The recalculation methods include: oxide-element conversion, formula units, Fe^{2+} and Fe^{3+} contents, cation allocation in the crystal structure, and classification of the analysed amphibole. Although many of the published programs are very useful, they have many disadvantages among which are the following:

1. Most programs deal only with a limited number of oxides of the major elements, and neglect minor but sometimes important elements, such as Li, Ni, or Zn and especially F or Cl (e.g., Spear and Kimball, 1984, Richard and Clark, 1990).
2. Most programs are designed for data obtained using EPMA and do not deal with the analyses done by more traditional methods which contain certain important oxides such as Li_2O and H_2O or separate values for Fe_2O_3 and FeO (e.g., Spear and Kimball, 1984, Rock, 1987, Richard and Clark, 1990, and Griffin *et al.* 1991).
3. Some programs are written in high machine language such as FORTRAN which makes them difficult to implement on many machines still in operation in some laboratories (e.g., Spear and Kimball, 1984 and Rock, 1987).
4. Some of the programs are written to deal only with the data form produced by the analytical equipment they are linked with, and do not allow processing of external data.
5. Few of the programs cover most of the known recalculation steps starting from oxide-element conversion to mineral identification (Spear and Kimball, 1984, and Richard and Clark, 1990). Most are designed for partial recalculations (e.g., Afifi and Essene, 1988, and Rock and Carrol, 1990).

The Objective of this work is to provide mineralogists with a comprehensive program which covers all the necessary recalculations for chemically analysed amphiboles, and to avoid all the previously mentioned disadvantages. The present program also allows the mineralogist to identify analytical problems which arise during the automatic recalculations, and provides the necessary comments and illustrations that help in such identification. Moreover, the program provides a tabulated and graphical output of the results that can be used directly for publication.

Features of the Program

Chemical analysis of minerals, including amphiboles, was achieved in the past using wet chemical techniques. These techniques are generally used in the quantitative determination of various oxide states of cations and also for determination of H_2O content in hydrous minerals. The inaccuracy of such methods arises from the presence of impurities (*i.e.*, weathering or other alteration products) that generally occur in the analysed mineral since it is difficult, if not possible, to separate a 1/10 to one gram of pure mineral. In the last few decades, the instrumental techniques for mineral analyses, as

optical emission, X-ray fluorescence, atomic absorption, and EPMA have become widespread. These methods allow the quantitative analysis of very small sample sizes and provide increased speed of determination at the expense of some accuracy. Recently, the most commonly used technique is EPMA which provides data in the form of element contents in the analysed mineral. Unfortunately, light elements such as H, Li, Be, B and C can not be detected by EPMA and, in addition, Fe is all presented as Fe^{2+} since the EPMA cannot differentiate between Fe^{2+} and Fe^{3+} . Therefore, a number of recalculations must be applied first to the analysed sample in order to achieve the oxide-element conversion and the calculation of Fe^{2+} , Fe^{3+} concentrations in the sample. Then, the contents of the different elements in the analysed sample are used to calculate the cation formula, to allocate the different elements in the crystal structure, and finally to recognize the type of the amphibole mineral. The present computer program includes a number of subroutines which carry out all these recalculations for amphibole analyses. A brief description of the different recalculation tasks executed by a number of subroutines in the program is provided below.

Selection of Elements

Most of the previous programs, especially those designed for EPMA data, deal only with a limited number of elements which are known to be the major elements in amphibole analyses (Si, Ti, Al, Cr, Fe^{3+} , Fe^{2+} , Mn, Mg, Ca, Na, K). They neglect other minor elements which sometimes occur in amphiboles. The omission of minor elements introduces certain errors, which may reach unacceptable levels in the $\text{Fe}^{2+}/\text{Fe}^{3+}$ ratio and cation distribution among different sites.

A literature survey has been made of the minor elements that may frequently occur in amphiboles. Hawthorne (1981) indicated that the minor elements in amphibole minerals include (Ge, Zn, Ni, Co, B, Be, F, Cl). It was also indicated by Klein and Hurlbut (1985) that Phosphorus (P) may also occur where it substitutes silicon in some minerals. Accordingly, the minor elements considered in this program are Ge, P, Be, Zn, Ni, Co, Li, F, Cl, OH. This list of minor elements covers all the analyses made by either wet or instrumental chemical techniques and exceeds all the minor elements included in any other program for amphibole recalculations. The final sequence of the major and minor elements in the present program is; Si, Ti, Al, Ge, P, B, Cr, Fe^{3+} , Fe^{2+} , Co, Ni, Mn, Mg, Zn, Be, Ca, Li, Na, K, F, Cl, OH^+ , OH^- and H_2O .

Oxide-Element Conversion

This process is quite essential for the subsequent recalculations applied to amphibole minerals since the contents of all elements are required to compute the Fe^{2+} and Fe^{3+} concentrations, the cation formula, and the cation allocation in the crystal structure. The method of Oxide-Element conversion described in Klein and Hurlbut (1985) was considered in the present program. Subroutine OXEL is designed to allow conversion from oxides to elements and from elements to oxides as well. This process allows the user to deal with the different forms of analyses received from wet chemical and instrumental laboratories.

Ferrous / Ferric Computation

EPMA cannot distinguish the two oxidation states of iron in a mineral. EPMA software generally treats all the Fe present as Fe^{2+} . However, because many kinds of mineral (amphiboles included) contain iron in both oxidation states, the EPMA analyses of such minerals generally have to be recalculated using stoichiometric criteria in order to estimate the Fe^{3+} content in the absence of an independent Fe^{3+} analysis by wet chemistry or Mossbauer spectroscopy. The methods of recalculation for amphibole minerals are numerous (e.g., Stout, 1972, Robinson *et al.* 1981, and Droop, 1987) but they all require a reliable estimate of oxygen value generally called the oxygen base (O_b) which is actually the anhydrous oxygen equivalent (AOE). The oxygen base for amphibole is considered as 24 for analysis which contains H_2O and/or F and Cl, otherwise the oxygen base is considered as 23.

Recalculation of microprobe data for minerals with F and Cl as well as H_2O^+ presents a problem for any mineral recalculation program. A typical EPMA analysis with F or Cl but no H_2O^+ ideally needs to be calculated to a variable oxygen base, depending on how much F or Cl is actually present that is, O_b is considered 23 when (F + Cl) value is near zero, while $O_b = 24$ when (F + Cl) value approaches 2.0.

The $\text{Fe}^{2+}/\text{Fe}^{3+}$ conversion is achieved in the program using subroutine FERRIC where the recalculation is based on the method suggested by Droop (1987). The Fe^{3+} content (F) is given by the equation

$$F = 2X(1 - T/S)$$

where X is oxygen base (O_b) and is defined in the equation as the AOE = 23,

T is the ideal number of cations per formula unit,

S is the observed total cation per X oxygen.

The ideal number of cations (T) is automatically calculated in the program using the criteria described by Hawthorne (1981) where the amphiboles are divided into four groups according to the relative occurrence of Ca and Na in the M4 site. The basis of classification and the ideal cation number selection is provided in Table 1.

TABLE 1. Basis for selection of the amphibole group and the ideal cation number (after Hawthorne, 1981).

Occurrence of Ca, Na in Site M4	Amphibole group	Ideal cation no. (T)	Indices of elements* required to get (S)
(Ca + Na) < 1.34	Fe-Mg-Mn	15	from 1 to 16
(Ca + Na) >= 1.34 and Na < 0.67	Calcic	13	from 1 to 15
(Ca + Na) >= 1.34 and 0.67 <= 1.34	Sodic-Calcic	13	from 1 to 15
Na >= 1.34	Alkali	16	from 1 to 9

* This indices of elements, are their orders in the sequence of elements described in page 5. (e.g., the indices of Si and K are 1 & 19, respectively).

The selection of the amphibole group by the user allows the program to recognize which elements in the sample that must be added together to obtain the value of S .

Then this value is compared with the corresponding ideal cation number (T). Finally, the content of Fe^{3+} is calculated from the previous equation and consequently the program modifies the values Fe^{2+} and FeO according to the relative frequency of each cation using the method described by Droop (1987). In case of wet chemical analyses, where the content of Fe^{2+} and Fe^{3+} are determined, the program does not recalculate their contents.

Cation Distribution in the Different Sites

The calculation of the element content using oxide-element conversion (Subroutine OXEL) and the modifications introduced in the Fe^{2+} and Fe^{3+} concentration using Subroutine (FERRIC) provide the user with the most reliable frequency of the occurrence of each element in the analysed mineral. The adjusted values of the element content is then distributed in the different sites of the crystal structure of the investigated amphibole mineral. Subroutine (CATDIST) performs this complicated process according to cation distribution form compiled by Mogessie *et al.*, (1990). This form which is accepted by the International Mineral Association (IMA) considers the major element group and a minor group which do not include some of the minor elements considered in this program. Therefore, an extensive work has been achieved to match the additional minor elements in the convenient sites according to the distributions suggested by many authors (e.g., Hawthorne, 1981; Robinson *et al.* 1982; Klein and Hurlbut, 1985). On the other hand, the general site-formula of amphiboles {A (O-1) B (2) C (5) T (8) O (22)} {OH, F, Cl} (2), accepted by IMA is replaced by the modified form suggested by some of the previous authors that divides the T and C-sites into separate sites. The relationship between the two forms, the number of cations in each site, and its crystal form is described in Table 2. Therefore, the program distributes the cation in six sites instead of the four sites, which are generally considered by most of the mineralogists in order to reveal a more detailed crystal description.

TABLE 2. Description of the different sites in amphibole minerals.

Site IMA	Site in program	Coordination number	No. of cations	Elements included in program
A	A	12	1	Na, K
B	M4	6-8	2	Fe2, Mg, Mn, Co, Ni, Zn, Ca, Li, Na
C	M1, M3	6 (Octahed)	3	Fe2, Mg, Mn, Co, Ni, Zn, Li,
	M2	6 (Octahed)	2	Al, Ti, Cr, Fe3, B
T	T1	4 (tetrahed)	4	Si, Ge, Be, Al, Fe3, Ti
	T2	4 (tetrahed)	4	Si, Ge

Amphibole Classification

The subroutine (MNRLID) was specially designed to provide the mineral name according to the classification of the IMA (Leak, 1978; Mogessie *et al.*, 1990). In this respect, the ninety one amphiboles included in the IMA sheet are classified in four groups, but the identification of any investigated amphibole still requires the determination of several parameters. Most of these parameters are automatically determined by the subroutine through the scanning of the stored results of cation distribution. This criterion is used to determine the name of the investigated amphibole in

three of the four amphibole-groups, (Table 1). For the fourth group (Fe-Mn-Mg group), the mineral identification requires additional information about the investigated mineral such as the Li content and the crystal form (orthorhombic or monoclinic). Unfortunately, in most analyses (e.g., EPMA), the Li content is not detected and the exact crystal form is not previously known. In this case, the program suggests four names for the investigated amphibole, from which the selection of the appropriate name remains the responsibility of the mineralogist. If either Li-content or crystal form is known, the number of suggested mineral names decreases to two and if both pieces of information are available ofcourse the mineral name can be determined.

Program Operation

The present program is a menu-driven interactive program written in Basic which allows easy operation and widespread use on most types of personal computers. The input/output (I/O) data and the calculation tasks are accomplished by means of a set of subroutines specially designed for these purposes. The tasks in this program can be divided into three main groups; the input group, the computation group, and the output group. The selection of each group is available through the main menu, while the selection of any of the tasks included in each group is available through one of the three menus assigned for each group. A brief description of the different functions executed using the main menu and the three relevant menus is explained below.

Main Menu

This Menu (Fig. 1) displays four options which allow the user to utilize one of three relevant menus (an input menu, a calculation menu, and an output menu) and an additional option to allow program termination. The sequence of operations must start with the input menu then the calculation menu and finally the output menu. This is designed to warn the user if the sequence of operation is incorrect and to allow him to restart the proper operation.

Data Input Menu

This menu provides the user with five options (Fig. 2) which allows him to input his data and to check if the input data are in the proper form to pass to the calculation menu. The different options provided by this menu are to input from keyboard, to input from an ASCII disk file, to edit and correct the input data, to save the input data on a disk file and to check the input data before operating the calculation menu. The last option displays the input data for the last check and to return back to the main menu.

Computation Menu

This menu (Fig. 3) allows the user four options to perform a number of operations which include; oxide-element conversion, Fe^{2+} and Fe^{3+} corrections if necessary, cation distribution, amphibole group, and name of the investigated mineral. The operations must be executed in the previously mentioned sequence, especially in the case of analyses performed utilizing instrumental techniques (e.g., EPMA) that require corrections for Fe^{2+} and Fe^{3+} contents. For wet chemical analyses, where Fe^{2+} and Fe^{3+} contents

PROGRAM AMPHIBOLE

This program allows the user to do the following jobs:

- 1- To calculate Fe^{+++} concentrations in the amphibole minerals using microprobe or chemical analyses.
- 2- To calculate the cation distribution in the different sites.
- 3- To determine the amphibole mineral group, the mineral name and location within this group.
- 4- The program provides tables and plots which precisely describe the results.

MAIN MENU

- 1- Input data MENU
- 2- Calculation MENU
- 3- Output MENU
- 4- QUIT

Enter your choice [DEF.=] : ?

FIG. 1. Main Menu of Program AMPHBL 94.

A - DATA INPUT MENU

- 1- Input from a keyboard
- 2- Input from a disk file
- 3- Edit input data
- 4- Store input data in a disk file
- 5- Check input data and MAIN MENU

Enter your choice [DEF=5] : ?

FIG. 2. Data Input Menu.

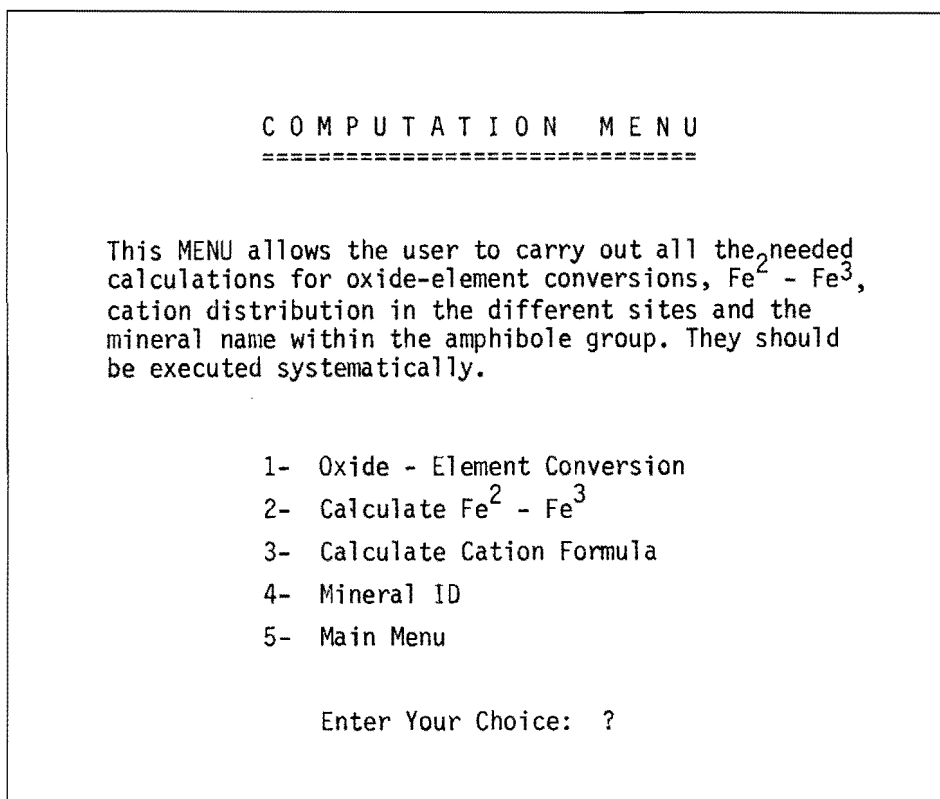


FIG. 3. Computation Menu.

are determined, the execution will not change the pre-determined Fe^{2+} and Fe^{3+} values. A screen display of the mineral name and amphibole group is generally provided during the execution of the last operation of the computation menu.

Data Output Menu

The data output menu (Fig. 4) allows the user a number of options to obtain the recalculation results together with the input analysis of the investigated amphibole. The output can be either displayed on the screen or obtained as a hard copy using a line printer. The screen display allows the user to review the output data and decide if a hard copy is required. The hard copy includes tables and plots produced in a format which can be directly used in publications. They provide the results of all calculations of the investigated unknown mineral, the suggested amphibole group, the mineral identification, and, in addition, they demonstrate the location of the investigated mineral within the amphibole group.

Two examples were selected from a previous publication (Droop, 1987) where microprobe analyses of two amphibole minerals were recalculated by the present program as unknown minerals. The results are illustrated in Fig. 5 and 6. The results of Fe^{2+} and

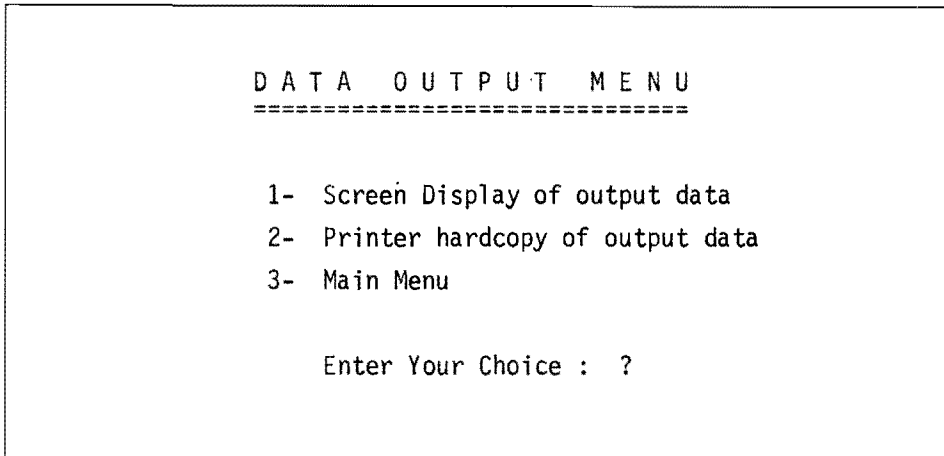


FIG. 4. Data Output Menu.

Fe³⁺ corrections are the same, but the present program also calculated the cation formula and accordingly identified the minerals as gedrite and ferroan-pargasitic hornblende. In addition to the table presentation of the cation distribution in the output, it is also possible to obtain the distribution in a form of equation from Fig. 7a and 7b.

Conclusion

The computer program discussed in this paper provides the most comprehensive program that can be easily operated in the laboratories of mineral analysis. The program covers all the known operations used in the recalculation of amphiboles.

The advantages of this program over the previously published software can be summarized as follows:

1. The program covers all the known operations required for the recalculation of amphibole minerals.
2. This program considers all the reported minor element lists as well as all the element substitutions.
3. The program allows oxide-element and element-oxide conversions to provide the user with wide latitude of information that can be used for many purposes.
4. The cation distribution can be provided in either a table or equation forms.
5. The output tables and plots precisely describe the results and allow the user to check the recalculations. In addition, they are designed in a form which can directly utilized for publications.

RESULTS OF AMPHIBOLE ANALYSIS

A- Sample ID:

Area : DROOP
Location : AMPHIBOLE2

Sample No. : P.434
Date : 12/1/1415

B- Element Analysis

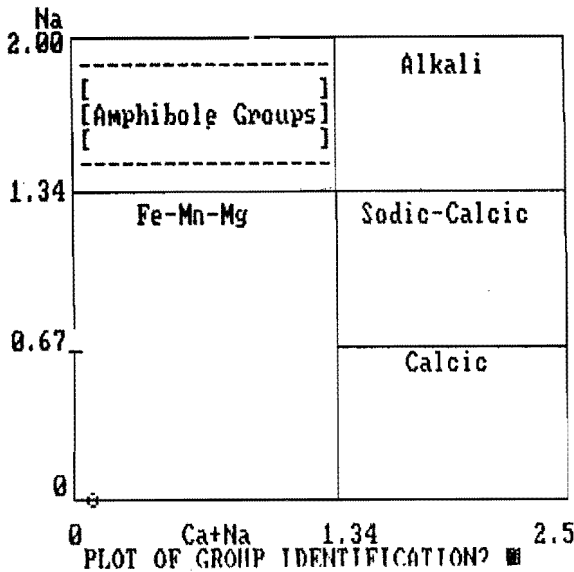
(Table) : Oxide - Cation and Fe2/Fe3 conversion Table

Oxide name	Weight %	Molec. prop.	Cation no.	Calcul. oxygen	Corr. cation	Modified cation
SiO2	43.4300	0.7228	0.7228	1.4456	6.1552	6.1438
TiO2	0.2000	0.0025	0.0025	0.0050	0.0213	0.0213
Al2O3	18.2600	0.1791	0.3582	0.5373	3.0500	3.0444
Fe2O3	0.8002	0.0000	0.0000	0.0000	0.0000	0.0852
FeO	12.1300	0.1789	0.1789	0.1789	1.5230	1.4350
MnO	0.2100	0.0030	0.0030	0.0030	0.0252	0.0252
MgO	19.6700	0.4880	0.4880	0.4880	4.1559	4.1482
CaO	0.6400	0.0114	0.0114	0.0114	0.0972	0.0970
Na2O	1.9700	0.0318	0.0636	0.0318	0.5413	0.5403
TOTALS	97.2300		1.8283	2.7010	15.5692	15.5403

C: MINERAL FORMULA

(Table) : Cation distribution in the different sites

Elem. name	Site T2	Site T1	Site M2	Sites M1,3	Site M4	Site A
Si	4.0000	2.1438				
Ti			0.0213			
Al		1.8562	1.1882			
Fe3			0.0852			
Fe2			0.1805	0.7676	0.4869	
Mn			0.0032	0.0135	0.0085	
Mg			0.5217	2.2189	1.4075	
Ca					0.0970	
Na					0.0000	0.5403
TOTALS	4.0000	4.0000	2.0000	3.0000	2.0000	0.5403



MINERAL IDENTIFICATION
The investigated mineral is
Gedrite

FIG. 5. A table-graph list of the analysis and calculation of a Fe-Mn-Mg amphibole mineral.

RESULTS OF AMPHIBOLE ANALYSIS

A- Sample ID:

Area : DROOP
Location : AMPHIBOLE 1

Sample No. : A
Date : 14/1/1414

B- Element Analysis

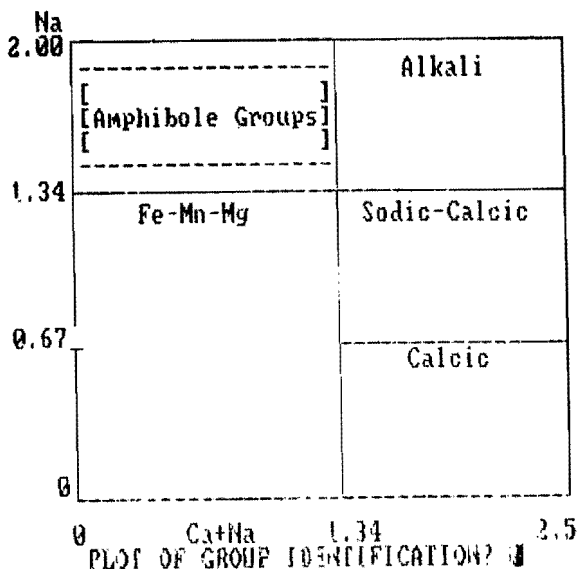
(Table) : Oxide - Cation and Fe2/Fe3 conversion Table

Oxide name	Weight %	Molec. prop.	Cation no.	Calcul. oxygen	Corr. cation	Modified cation
SiO2	42.8900	0.7138	0.7138	1.4277	6.4562	6.4130
TiO2	1.8000	0.0225	0.0225	0.0451	0.2038	0.2024
Al2O3	11.5500	0.1133	0.2266	0.3398	2.0491	2.0354
Fe2O3	2.7396	0.0000	0.0000	0.0000	0.0000	0.3083
FeO	12.4348	0.2082	0.2082	0.2082	1.8833	1.5624
MgO	11.1200	0.2759	0.2759	0.2759	2.4954	2.4787
CaO	11.4900	0.2049	0.2049	0.2049	1.8531	1.8407
Na2O	1.8700	0.0302	0.0603	0.0302	0.5456	0.5421
K2O	1.0600	0.0113	0.0225	0.0113	0.2036	0.2022
TOTALS	96.7400		1.7348	2.5430	15.6901	15.5850

C: MINERAL FORMULA

(Table) : Cation distribution in the different sites

Elem. name	Site T2	Site T1	Site M2	Sites M1,3	Site M4	Site A
Si	4.0000	2.4130				
Ti			0.2024			
Al		1.5870	0.4483			
Fe3			0.3083			
Fe2			0.4025	1.1599		
Mg			0.6385	1.8401		
Ca				0.0000	1.8407	
Na					0.1593	0.3828
K						0.2022
TOTALS	4.0000	4.0000	2.0000	3.0000	2.0000	0.5850



MINERAL IDENTIFICATION
The investigated mineral is
Ferroan-Pargasitic-Hornblen

FIG. 6. A table-graph list of the analysis and calculation of a Calcic amphibole mineral.

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-----
IN SITE T2  TOTAL CATIONS= 4  CHEM. FORM IS
T2=4.0000Si
-----
IN SITE T1  TOTAL CATIONS= 4  CHEM. FORM IS
T1=2.1438Si+1.8562Al
-----
IN SITE M2  TOTAL CATIONS= 2  CHEM. FORM IS
M2=0.0213Ti+1.1882Al+0.0852Fe3+0.1805Fe2+0.0032Mn+0.5217Mg
-----
IN SITE M13 TOTAL CATIONS= 3  CHEM. FORM IS
M13=0.7676Fe2+0.0135Mn+2.2189Mg
-----
IN SITE M4  TOTAL CATIONS= 2  CHEM. FORM IS
M4=0.4869Fe2+0.0085Mn+1.4075Mg+0.0970Ca+0.0000Na
-----
IN SITE A1  TOTAL CATIONS= .540329  CHEM. FORM IS
A1=0.5403Na
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D- MINERAL IDENTIFICATION

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AMPHIBOLE GROUP : Fe-Mg-Mn

The Analysed Mineral is

	<u>MINERAL NAME</u>	: Gedrite
<u>OR</u>	<u>MINERAL NAME</u>	: Magnésio-Cumingtonite

Fig. 7a. A list of the result of site analysis in the equation form of a Fe-Mg-Mn amphibole mineral.

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-----
IN SITE T2  TOTAL CATIONS= 4  CHEM. FORM IS
T2=4.0000Si
-----
IN SITE T1  TOTAL CATIONS= 4  CHEM. FORM IS
T1=2.4130Si+1.5870Al
-----
IN SITE M2  TOTAL CATIONS= 2  CHEM. FORM IS
M2=0.2024Ti+0.4483Al+0.3083Fe3+0.4025Fe2+0.6385Mg
-----
IN SITE M13 TOTAL CATIONS= 3  CHEM. FORM IS
M13=1.1599Fe2+1.8401Mg+0.0000Ca
-----
IN SITE M4  TOTAL CATIONS= 2  CHEM. FORM IS
M4=1.8407Ca+0.1593Na
-----
IN SITE A1  TOTAL CATIONS= .584995  CHEM. FORM IS
A1=0.3828Na+0.2022K
-----

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D- MINERAL IDENTIFICATION

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AMPHIBOLE GROUP : Calcic

The Analysed Mineral is

	<u>MINERAL NAME</u>	: Ferroan-Pargasitic-Hornblend
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Fig. 7b. A list of the result of site analysis of a Calcic amphibole minerals in the equation form.

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برنامج شامل بلغة البيسك لحساب الكاتيونات وتصنيف الأمفيبولات

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كلية علوم الأرض - جامعة الملك عبد العزيز
جدة - المملكة العربية السعودية

المستخلص . يمثل هذا البحث برنامجاً شاملاً للحاسوب يُزود المستخدم بمعلومات عن الأمفيبولات المحللة كيميائياً . ولقد كتب هذا البرنامج بلغة البيسك بأسلوب المخاطبة ، حتى يمكن تشغيله بسهولة باستخدام معظم أنواع الحاسوب الشخصي المتوفرة في المعامل الكيميائية . والإدخال المطلوب هو النتائج الأولية للتحليل المعدنية في صورة أكاسيد أو العناصر المستقاة من المعامل الكيميائية التقليدية والمجهزة آلياً . ويقوم هذا البرنامج بتحقيق تسلسل في المهام التي تضم : التحويل من الأوكسيد إلى الكاتيون ، حساب الحديدوز/ حديدك (إذا كان مطلوباً) ، واقتراح مواقع الكاتيونات في البلورات المختلفة والتعرف على مجموعة الأمفيبول والمعدن . ويبلغ عدد العناصر التي يكشف عنها هذا البرنامج أربعة وعشرون ، وهي تغطي كل العناصر الداخلة في معادن الأمفيبولات المعروفة في المنشورات العلمية . ويتميز هذا البرنامج بتعدد المهام ، كما أن عدد العناصر التي يشملها هذا البرنامج أكثر من أي برنامج نُشر من قبل . وإلى جانب ذلك يتيح هذا البرنامج للمستخدم فرصاً كبيرة للخيارات مع شرح لكل منها بالجداول والرسوم البيانية لمساعدته في الاختيار المناسب . ويحتوي المخرج من هذا البرنامج عدداً من الجداول والرسوم البيانية التي تسمح بتتبع مختلف العمليات ، وكذلك دقة الحسابات ، وصنع القرار أثناء تشغيل البرنامج ، إضافة إلى تكوين صور مطبوعة قياسية نفي بغرض النشر .