American Mineralogist, Volume 75, pages 1426–1427, 1990

SOFTWARE NOTICE

PX: A program for pyroxene classification and calculation of end-members

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ABSTRACT

The use of pyroxene compositions in studies of igneous and metamorphic rocks usually requires their classification and calculation of end-members. The program PX constitutes a useful tool for such purposes: it performs the classification recently proposed by the International Mineralogical Association (IMA) and two widely accepted normalizations for determination of end-member components as well as other parameters for application in geothermometry.

INTRODUCTION

The Subcommittee on Pyroxenes (Commission on New Minerals and Mineral Names of the International Mineralogical Association) has recently approved the new classification and nomenclature for pyroxene minerals (Morimoto, 1988, 1989). The subcommittee has compiled and systematized the widely accepted methods of classifying pyroxenes and it simplified the nomenclature through the application of the "50% rule." However, despite the use of this classification system, the calculation of pyroxene end-members remains necessary for many studies (e.g., to estimate PT paths of magmas or metamorphic rocks).

Both classification and determination of end-member components involve tedious and time-consuming calculations. The program PX has been developed to avoid them.

DESCRIPTION OF THE PROGRAM

PX has been written with the TurboBasic compiler and operates on any PC-IBM computer or compatible. Although it has been conceived as an independent program, with few modifications it can be included in the Minfile package (Afifi and Essene, 1988).

The program requires a data file containing the pyroxene analyses expressed as oxide wt%. The following oxides are considered: SiO_2, TiO_2, ZrO_2, Al_2O_3, Fe_2O_3, Cr_2O_3, Sc_2O_3, FeO, MnO, MgO, CaO, ZnO, NiO, Na_2O, K_2O, Li_2O, and V_2O_5.

In the second step of the program structural formulae of the pyroxenes are calculated. Several calculation methods have been developed to achieve this (e.g., Dollase and Newman, 1984; Guiraud, 1986). However, the well-known scheme by Yoder and Tilley (1962) remains the most used. When this method is followed, the pyroxene formula unit is normalized to six O atoms. As the IMA proposes, if Fe_2O_3 is not available, the program recalculates the formula to four cations to estimate the Fe^{3+} by charge balance. For classification purposes cations are then allocated to their structural sites. According to the IMA suggestions, Si^{4+} and convenient amounts of Al^{3+} and Fe^{3+} are situated in tetrahedral sites. The remaining cations are considered as belonging to M1 or M2 sites.

The program then assigns each pyroxene to one of the four chemical groups defined in the Q-J diagram by Morimoto and Kitamura (1983): Ca-Mg-Fe pyroxenes (Quad), Na-Ca pyroxenes (Na-Ca), Na pyroxenes (Na) and other pyroxenes (Other). The Quad pyroxenes are classified in the En-Fs-Di-Hd quadrilateral, where the 50% rule has been applied to simplify the nomenclature. The Na-Ca and Na pyroxenes are plotted in the Quad-Jd-Ae triangle. There is no definitive classification for the pyroxenes in the Other group.

Several methods have been proposed for the calculation of pyroxene end-members. Most of them are sequential schemes that usually differ in the order of the calculation sequence. The sequential calculation obviously leads to an overestimation of the component calculated first. One attempt to solve this problem was made by Dietrich and Petrakakis (1986), who developed an algebraic method that allows the calculation of 11 linearly independent pyroxene components. However, Lindsley (1986) showed that some of those end-members have little chemical justification, as is evidenced by crystal-chemistry experiments.

For the reasons given above, the program includes two widely accepted norms (by Kushiro, 1962, and by Cawthorn and Collerson, 1974) with different calculation sequences that consider only the nine end-members that can be chemically justified at the moment.

When the normalization scheme proposed by Kushiro is used, the end-members are calculated in the following order: acmite (ACM), jadeite (JAD), Ca-Ti-Tschermak's molecule (CTA), Ca-Fe^{2+}-Tschermak's molecule (CFA), Tschermak's molecule (TSC), Ca-Fe^{3+}-Tschermak's molecule (CFS), wollastonite (WO), enstatite (EN), and ferrosilite (FS). The sequence is changed in the normalization scheme of Cawthorn and Collerson, where JAD is calculated before ACM and CFS before CTA, and CFA is not calculated. Such a sequence implies that the value obtained for JAD is a maximum, whereas it has a minimum value in Kushiro's normalization procedure. This parameter is used to estimate physical conditions of crystallization of magmas and metamorphic rocks, and as a consequence further interpretations or calculations from the pyroxene end-members are strongly dependent on the normalization procedure selected. For the same reason, programs that consider only one of these normalization schemes (e.g., McHone, 1987) appear to be very limited for petrological studies.

In addition to the IMA classification and the two normalization calculations, the program calculates the WO, EN, and FS parameters following the scheme by Lindsley and Andersen (1983). These components can be directly plotted on the graphical thermometer calibrated by Lindsley (1983).

The output shows the input data, structural formula, cations in M sites, IMA classification, and end-member components for each pyroxene analysis (see Appendix 1). The program also checks for errors in analyses. Copies of the program and further information are available from the author.

ACKNOWLEDGMENTS

This work is part of the investigation project PB87-0372 supported by the Dirección General de Investigación Científica y Técnica, Spain. I am thankful to R. Arenas (UCM), who greatly contributed to theoretical aspects of the program, and to D.H. Lindsley (SUNY–Stony Brook) for his constructive comments.

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MANUSCRIPT RECEIVED FEBRUARY 21, 1990
MANUSCRIPT ACCEPTED SEPTEMBER 13, 1990

Appendix 1. Program PX output example. Sample used is augite analysis from Deer et al. (1978), Vol.2A, Table 31, No.1.

SAMPLE: EXAMPLE / CPX

Program PX, by J.M.CEBRIA, 1990

I.M.A. CLASSIFICATION

Group: QUAD
Name: AUGITE

Q= 1.728 J= 0.134
Wo(%)= 35.553
En(%)= 54.317
Fs(%)= 10.130

A-Kushiro (1964)
B-Cawthorn & Collerson (1974)
C-Lindsley & Andersen (1983)

	wp(%)		str.for.	M
SIO2	52.430	SI	1.896	
TIO2	0.370	TI	0.010	0.010
AL2O3	4.160	AL	0.177	0.073
FE2O3	2.660	FE3+	0.072	0.072
CR2O3	1.060	CR	0.030	0.030
FEO	3.530	FE2+	0.107	0.107
MNO	0.120	MN	0.004	0.004
MGO	18.190	MG	0.980	0.980
CAO	16.560	CA	0.641	0.641
NIO	0.080	NI	0.002	0.002
NA2O	0.960	NA	0.067	0.067
K2O	0.070	K	0.003	0.003

	ACM	JAD	CTA	CFA	TSC	CFS	WO	EN	FS
(A)	7.121	0.000	1.016	3.249	6.314	0.000	27.109	49.615	5.576
(B)	0.000	7.121	1.016	0.000	4.378	5.185	27.109	49.615	5.576
(C)	---	---	---	---	---	---	30.611	62.574	6.814