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 (Alfi and Essene, 1988).

The program requires a data file containing the pyroxene analyses expressed as oxide wt%.

The second step of the program involves the pyroxene compositions. The program includes a data file containing the pyroxene analyses expressed as oxide wt%. The following oxides are considered: SiO₂, TiO₂, ZrO₂, Al₂O₃, FeO, Fe₂O₃, Cr₂O₃, Sc₂O₃, FeO, MnO, MgO, CaO, ZnO, NiO, Na₂O, K₂O, Li₂O, and V₂O₅.

The output shows the input data, structural formula, cations and components for the pyroxene end-members, and the calculation of the components 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.

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REFERENCES CITED


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