Computers & Geosciences Vol. 13, No. 1, pp. 89–91, 1987
Printed in Great Britain.

0098-3004/87 $3.00 + 0.00

SHORT NOTE

PXC: AN APL PROGRAM FOR CALCULATING PYROXENE STRUCTURAL FORMULAE AND END MEMBERS

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(*Received* 24 *March* 1986; *accepted* 29 *May* 1986)

INTRODUCTION

Pyroxene compositions are important tools for studies of chemical differentiation and P–T paths of magmas. Analyses of pyroxenes are performed usually using electron-microprobe techniques that measure iron only in the ferrous state, and so many petrologists recalculate pyroxene formulae to derive Fe^{3+} by charge balancing (see Cawthorn and Collerson, 1974 for more discussion of the method). A measurement or estimate of the Fe^{3+} content of pyroxene also is useful in calculating some pyroxene end-member molecules. In addition, older analyses of pyroxenes from the literature may require recalculation of formulate from their oxide weight percents. This short program gives a table of pyroxene formula and end-member calculations using an interactive microcomputer system.

DESCRIPTION OF THE PROGRAM

The program or function asks for a label followed by an analysis of the pyroxene. The required order of 12 oxides is SiO_2, Al_2O_3, TiO_2, Cr_2O_3, Fe_2O_3, FeO, MnO, NiO, MgO, CaO, Na_2O, and K_2O. Enter a zero where no value is known. It is convenient to have the analyses stored as arrays of the values assigned to a label. APL makes it easy to store many such arrays as lines of a matrix in a data "workspace", which can be called into various program workspaces as needed. For more information, refer to one of the excellent guides such as by Pakin (1973), Gilman and Rose (1976), or IBM's manual included with their APL package.

The format of the program for calculating cation percentages per 6 oxygens generally follows Yoder and Tilley (1962). The output also gives the structural sites of the cations (per total of four) with lower-case letters in the last "cations/4 cations" column. To allow any extra precision needed for results in that last column, the number of digits printed needs to be assigned by the user beforehand . . . default 10 (generally, 5 is sufficient).

The "end-member" molecules are calculated in the sequence suggested by Kushiro (1962), as modified by Cawthorn and Collerson (1974). Jadeite (JD) is calculated before acmite (AC), followed by Ca-ferrit-schermak's molecule (CFTs), Ca-Ti-tschermak's molecule (CTTS), and Ca-tschermak's molecule (CATS). Ca not used in the tschermak's molecules is assigned to wollastonite (WO), Mg + Ni is calculated as enstatite (EN), and Fe^{2+} + Mn is calculated as ferrosilite (FS). Several schemes of end-member calculations are in use by mineralogists, and this should be kept in mind before making comparisons of calculated pyroxene molecules from the literature.

The computer used for this work is an IBM PC equipped with a monochrome graphics board and a math coprocessor chip. The APL interpreter software also is by IBM. Users of other APL systems may need to modify the program slightly. An increasing number of APL geology programs are being written or may be adapted for microcomputer systems (for examples, see McHone, 1977, and Glazner, 1984). In addition, mainframe systems will run these programs easily with minor changes of command functions.

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