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A REVISED COMPUTER PROGRAM FOR AMPHIBOLE CLASSIFICATION

KENNETH L. CURRIE[1]

Geological Survey of Canada, 601 Booth Street, Ottawa Ontario K1A 0E8

Publication of the International Mineralogical Commission's revised scheme of amphibole nomenclature (Leake *et al.* 1997) makes obsolete older computer programs designed to process analytical data and supply the formal name of an amphibole. This letter announces that one such widely distributed program (Currie 1991) has been updated, and is available either as a listing by e-mail, or on a user-supplied diskette. The program is particularly useful for results of electron-microprobe analyses, following the "minimum ferric iron" criterion outlined by Schumacher (1997) for assignment of ferrous and ferric iron. However, the program can also be used for compositions in which the proportion of ferric iron is determined directly, as well as for site assignments in the case of structural formulae derived from other programs.

Recently discovered amphiboles, such as cannilloite and ungarettiite, require Ca in the *A* site, and conversion of some MnO from the electron-microprobe data to Mn_2O_3, respectively, neither of which can be accommodated by the rules outlined by Schumacher (1997). The program therefore makes a more complete site-assignment [to *T*, *A*, *M*4, *M*2 and a combined *M*13 (*M*1 + *M*3) site] than required by the IMA scheme, using the method of Mäder & Berman (1992) to assign Mg and Fe to sites by assuming constant distribution-coefficients for Fe and Mg among the possible sites [$(Mg/Fe)_{M2}*(Fe/Mg)_{M4} = 35.96$, and $(Mg/Fe)_{M2}*(Fe/Mg)_{M13} = 3.33$; *cf.* Makino & Tomita (1989), Bancroft *et al.* (1967)]. This procedure has the further advantage that the mol fraction of any compositionally possible amphibole end-member can be easily calculated by multiplying together the appropriate site-occupancies. The calculation of mol fractions of IMA end-member amphiboles, a feature of the original program (Currie 1991), has therefore been deleted from the revised program, particularly since these mol fractions have changed, and may change further, as a result of IMA decisions. An example of the results given by the revised program is given in Table 1.

TABLE 1. OUTPUT OF PROGRAM CLASAMPH

Pargasite (Deer *et al.* 1966, p. 152, Table 15, anal. 8)

Oxide*		Cell**		Site occupancy**	
SiO_2	48.100	Si	6.690	Si*T*	6.690
TiO_2	0.100	Ti	0.010	Al*T*	1.310
Al_2O_3	11.050	Al	1.811	Al*M*2	0.501
Fe_2O_3	0.670	Fe^{3+}	0.070	Ti*M*2	0.010
FeO	1.650	Fe^{2+}	0.192	Fe^{3+}*M*2	0.070
MgO	20.600	Mg	4.271	Fe^{2+}*M*2	0.113
CaO	12.500	Ca	1.863	Mg*M*2	1.306
Na_2O	2.540	Na	0.685	Fe^{2+}*M*13	0.076
K_2O	1.240	K	0.220	Mg*M*13	2.924
H_2O	0.710	H	0.659	Fe^{2+}*M*4	0.003
F	1.900	F	0.836	Mg*M*4	0.041
Total	101.060	Ions	15.812	Ca*M*4	1.863
				Na*M*4	0.093
				K*A*	0.220
				Na*A*	0.592

The amphibole is fluorian edenite

* Composition quoted in wt.%. ** In atoms per formula unit.

The program was tested on a group of analytical data-sets rated as superior by Hawthorne (1983) and by Deer *et al.* (1966). A surprising number of these (complete) data-sets failed one or more of the criteria listed by Schumacher (1997) as prerequisites for the satisfactory naming of an amphibole. A number of Fe-Mg-Mn-Li amphibole data-sets contained <15 ions in the unit cell, the lowest number being 14.895, whereas several sodic–calcic and sodic amphiboles had contents of (Ca + Na + K) > 3. Whereas the causes of these departures from acceptable results remain speculative, the most probable causes appear to be slight alteration in the first case, and erroneous analytical results for Na in the second. The computer program will not classify such compositions. Of the analyzed amphiboles that were classified, almost 20% received a different name under the 1997 scheme than they did under the 1978 scheme (Leake 1978). Changes were particularly common among calcic amphiboles, where a number are classified as edenite rather than hornblende or pargasite (Table 1), and among sodic–calcic amphiboles, where the number classified as winchite more than doubled.

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[1] *E-mail address*: kcurrie@NRCan.gc.ca

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