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Some Monoclinic Amphiboles and Relation of Their Physical Properties to Chemical Composition and Crystal Structure*

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ABSTRACT.—The amphibole mineral group has been difficult to classify due to complexities introduced by the large number of ions that can substitute, either partially or completely, in the five structural sites. Each site has definite size, valence, and coordination number requirements. By assigning a code number to each possible ion in each possible site, every possible combination of ion and position can be used to give a unique classification scheme relating structural position to chemical composition. A species of hornblende chosen from Dana's System of Mineralogy (1892) is used to illustrate this classification system.

Ten amphibole minerals obtained from supply houses were chemically analysed and physical properties—i.e. index of refraction, 2V angle, C∧Z, pleochroism, DTA, and X-ray — were observed to determine if the classification system would be applicable and to try correlation of chemical composition and physical properties. Fe^{2+} And Fe^{3+} give the mineral a higher refractive index, a smaller 2V angle, darker pleochroic colors and a more nearly black color in hand samples. Presence of fluoride ions, as seen in sample 6, seems to increase the C∧Z. Neither the number of Si^{4+} replaced in the tetrahedral sites nor the number of alkali ions present in position "A" show any observable effect upon optical properties. An expected cell size increase with increasing substitution of Al^{3+} for Si^{4+} in tetrahedral sites was not observed in X-ray patterns; however, there is a decrease in cell size with an increase of trivalent ions in octahedral sites. A decrease of Ca^{2+} in cubic sites also tends to indicate a decrease in cell size. DTA shows that oxidation and hyrdation take place gradually all along the heating curve. Structure does not break down even at temperatures of 1100°C. A decrease in Ca^{2+} and an increase in Na^{+} and K^{+} lowers the temperature at which the endothermic reaction takes place.

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*A thesis submitted to the Faculty of the Department of Geology, Brigham Young University in partial fulfillment of the requirements for the degree Master of Science.

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INTRODUCTION

Combined amphibole and pyroxene mineral groups make up about 17%, by weight, of the earth's crust and are second only to feldspars in abundance. Amphibole minerals occur in many types of rocks. Hornblende species, for example, occur in great abundance in intermediate igneous rocks, in metamorphic schists and gneisses, and as a detrital mineral in some sedimentary rocks. Some amphibole variety forms in nearly all igneous rocks, in many metamorphic rocks and even as alteration products of other ferro-magnesium minerals.

Classification of the amphibole group is poorly organized and confused by indefinite mineral species. Wahlstrom (1947) commented that the nomenclature of the amphiboles is one of convenience and is not completely established. Kerr (1959) noted that the amphibole group is one of the most complex of all mineral groups, and many amphibole minerals cannot be placed within his list of species.

Amphibole minerals are hydrous silicates containing some combination of aluminum, magnesium, calcium, ferric iron, ferrous iron, sodium, and many other elements in minor amounts through ionic substitution. Amphiboles have a double chain crystal structure which gives them a bladed form and 56°, 124° cleavage angles. Within this structural framework are five different coordination positions to be occupied by 20 different ions. Complexity of the amphiboles is caused by random substitution of ions in similar coordination positions, and even some substitution in dissimilar positions by the same ions. For example, aluminum ions may substitute for silicon ions in tetrahedral coordination and may also substitute for magnesium ions in octahedral coordination.

The amphibole structure was first worked out by Warren (1929) using tremolite. In general the structural framework is formed by four oxygen ions arranged around one silicon ion in tetrahedral coordination. Silica tetrahedra share oxygen ions, alternating two and three per tetrahedra, forming double chains of infinite length parallel to the c-axis. The distance from one oxygen link to the next determines the "c" unit cell dimension. Groups of double chains are held together by various cations between the double chains in holes or "sites" of six fold and eight fold coordination formed by the oxygen framework. The problem of nomenclature, therefore, is one of relating structural sites to the occupying elements, and to the amount of substitution permitted.

Acknowledgments

The writer wishes to express his gratitude to Dr. Wm. Revell Phillips, major professor and advisor, for his supervision of this project; to the Geology faculty for their helpful criticisms; to the Geology Department for the use of laboratory facilities; to the Brigham Young University Research Division for funds which defrayed a large part of the expense of this research; and also to the Pennsylvania University Experiment Station which helped with expenses.

HISTORY OF AMPHIBOLE NOMENCLATURE

The term "amphibole" first appeared in literature in 1801 when Haüy used it to denote a mineral group containing hornblende, actinolite, and tremolite. A large number of other poorly defined species have been included in the amphibole group since that time.

Tschermak (1864) was one of the earliest workers to investigate the silicate structures. He introduced the concept of solid solution in minerals, especially in the plagioclase feldspars and other silicate structures. From a consideration of mineral chemistry he was able to give the ionic requirements for isomorphous compounds. Tschermak discovered that an increase in the iron content was observable in forms with a higher index of refraction, an observation many other researchers have noted since his time.

Allen and Clement (1908) experimented with the effect of heat on tremolite. When heated to 900°C. and held at this temperature for a period of time, tremolite lost most of its water, but, the mineral still retained its homogeneity and no sudden property changes took place. They thought that perhaps the water was dissolved water and tremolite was a solid solution phase. Later work showed that water was chemically combined and not a separate phase.

Ford (1914) made a detailed study of optical properties of amphiboles and concluded that the mean index of refraction was the best indicator of the chemical composition and therefore of the mineral species. He noticed that silicon, calcium, and magnsium ions had little effect on the refractive index.

Clarke (1914) proposed the concept of silicic acids to help explain composition of the various silicates, including the amphibole group. Acidic, basic and normal salts were introduced, and elaborate structural formulae were derived. Later work proved these hypothetical silicic acids could not be synthesized, nor could they be found in solutions of the minerals themselves. Berry and Mason (1959) state that X-ray investigations provided the means to disprove the silicic acid theory and made possible a classification based on structure.

Schaller (1916), from chemical considerations, worked out the correct formula for tremolite. He expressed it, in oxides of the elements, as 2CaO-

$5MgO\text{-}8SiO_2\text{-}H_2O$. Schaller suggested that the water probably occured as OH ions and was a definite part of the structure, and not dissolved water in tremolite.

Kuntz (1930) derived the correct formulae for actinolite, kupfferite and grunerite, analysed numerous amphibole minerals, measured their optical properties, and correlated this information by means of a series of graphs.

Position of each atom in the amphibole structure was worked out by Warren (1929) for tremolite by X-ray rotation photographs. Warren showed how the tremolite structure could be derived from diopside, a pyrozene variety, that tremolite, hornblende, grunerite, and kupfferite all had the same structure but with slightly different measurements, and that these differences were due to replacement by different elements.

Bragg (1930) and his students investigated many other silicate minerals by X-ray diffraction. Their work suggested a classification of silicates based upon the number, arrangement, and number of shared oxygen atoms (or corners) of silica tetrahedra in the structure. This sheme is the basis of present day silicate nomenclature.

Berman (1937) divided monoclinic amphiboles, on a structural and chemical basis, into three series; the cummingtonite series with the form $X_7Z_8O_{22}(OH)_2$, the tremolite-actinolite series with the form $W_2X_5Z_8O_{22}(OH)_2$, and the hornblende series with form $W_3(XY)_5Z_8O_{22}(OH,F)_2$. In each case W may equal Ca, Na, Li, and K. X may equal Mg, Fe^{2+}, Mn^{2+}. Y may equal Al, Fe^{3+}, and Ti^{4+}. Z equals Al and Si in tetrahedral coordination. Berman further subdivides the hornblende series into four species (Table 1).

TABLE 1
Hornblende species of Berman (1937)

Species	*Si:Al*	*X*	*Y*
hornblende-edenite	7:1	5	0
hastingsite	6:2	4	1
glaucophane	8:0	3	2
arfvedsonite	8:0	4	1

It should be noted that Berman separated the ions in the octahedral sites into their bivalent and trivalent components.

Hallimond (1943) recognized the importance of aluminum ions replacing silicon ions in tetrahedral sites and the introduction of alkali ions into a position that is usually vacant in the cummingtonite and tremolite-actinolite series. Hallimond observed that the number of silicon ions rarely drops below six, *i.e.* two Si^{4+} out of eight replaced by 2 Al^{3+} ions per one-half unit cell of 24 anions, and that calcium ions rarely rise above two ions per one-half unit cell. Hence, by starting with the simple tremolite formula, $Ca_2Mg_5Si_8O_{22}(OH)_2$, and using two types of substitutions ($2Na^+$ and $2Al^{3+}$ for $2Si^{4+}$, and $4Al^{3+}$ for $2Si^{4+}$ and $2Mg^{2+}$) he could graphically reproduce most of the common hornblende species on a partial triangular diagram. Winchell (1945) noted that the former substitution ($2Na^+$ and $2Al^{3+}$ for $2Si^{4+}$) was inconsistant with the amphibole structure, *i.e.* too much Na for the position available, but, that it could be replaced by two other substitutions as follows; Na^+ and Al^{3+} for Si^{4+}, and $2Al^{3+}$ for Mg^{2+} and Si^{4+}.

Although he stated that the composition of hornblende varies in so many ways that no ordinary diagram can be used to represent these variations, Winchell (1931, 1945) still attempted to correlate changes in chemical composition with measured physical properties of the mineral, generally on two dimensional diagrams. Hence, he was limited to the consideration of only two variables, or two combinations of variables, at one time. Winchell diagramed the change in molecular percentage of end members versus various optical properties. He used Hallimond's partial triangle as a base and added a vertical coordinate to show, in addition to the variations in Hallimond's variables, the effects of decreasing the number of Al^{3+} ions in tetrahedral coordination and the substitution of Fe^{2+} for Mg^{2+} ions on the optical properties of hornblende. Sundius (1946) questioned the usefulness and accuracy of this diagram and Rabbitt (1948) suggested that showing changes in molecular percentage of end members is not appropriate because end members are seldom found in nature and mixing on a molecular basis doesn't occur.

Sundius (1946) stated the literature complicates and confuses the relationships in the hornblende group and that from a consideration of structural requirements, plus results of many chemical analyses, all hornblende species found in nature can be derived from the tremolite formula by a very small number of substitutions. The chief "type forming" kinds of substitutions he found were; (1) introduction of alkali ions plus the various methods by which the alkali ions substitute for other ions, usually Ca, and, (2) exchange of Si^{4+} and Mg^{2+} for $2Al^{3+}$. If a substitution is carried out to completion Sundius calls the new formula an "end member" formula. If a substitution proceeds only part way in nature, although theoretically it could proceed further, Sundius calls the formula a "standard type" formula. Sundius (1946) classified the hornblendes by means of these substitutions (Text-fig.1).

Since Mg^{2+} and Fe^{2+} are almost completely exchangeable, both formulae names are given. All other hornblendes can be derived from these standard formulae by various substitutions. Sundius noted the introduction of Al^{3+} ions into the tetrahedral site tends to increase the refractive index and decrease the 2V angle of the mineral.

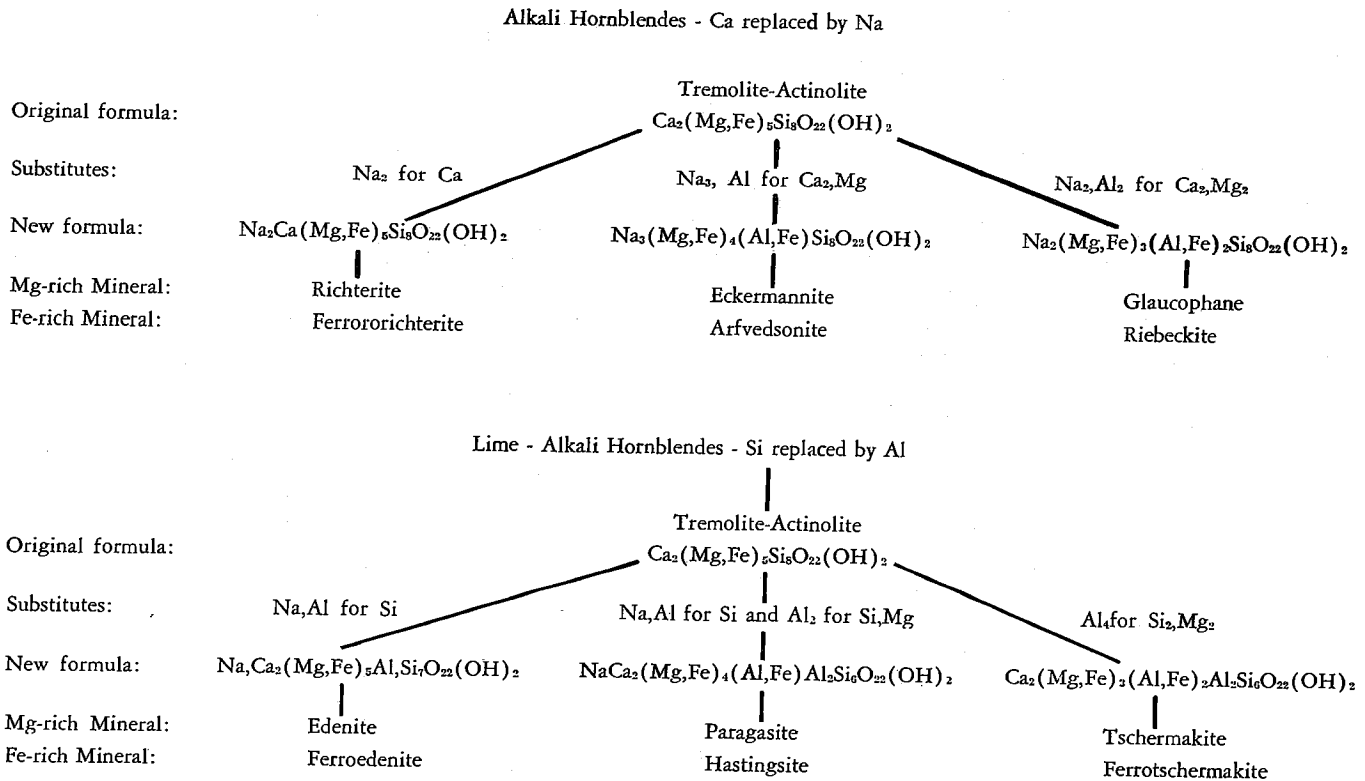
However complete this hornblende classification seems to be, it should be noted that minor elements, such as manganese, titanium, and fluorine, are not considered and these ions sometimes greatly influenced changes in physical properties. Also, as has been suggested, not only the ions involved but even their position in the structure affects physical properties of a mineral. Thus if it is known which elements occupy all possible structural sites, the amphibole species can be completely described.

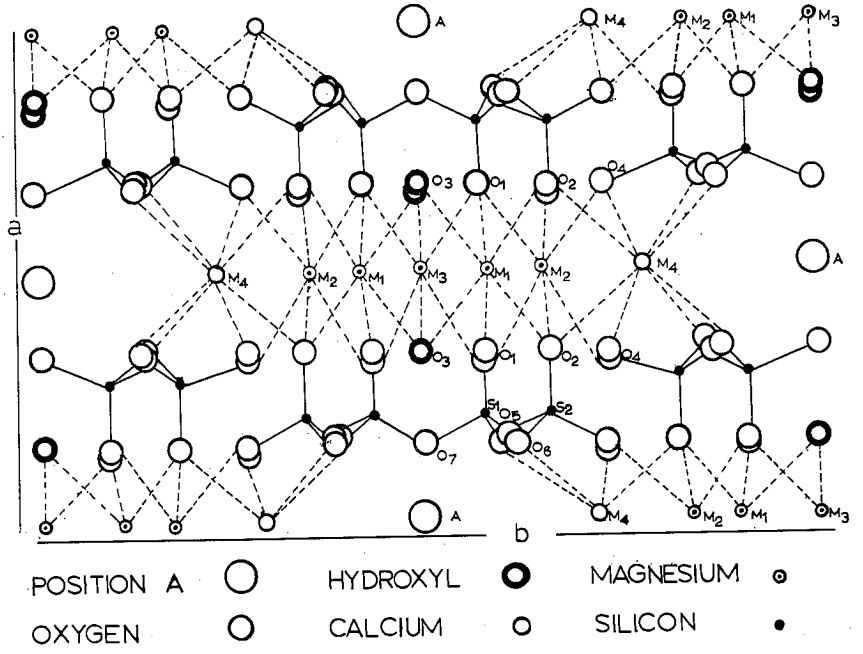
AMPHIBOLE STRUCTURE

Amphibole structure as determined by Warren (1930) is reproduced in text-figure 2 for reference purposes. The following discussion pertains to this diagram. Some oxygen ions should be superimposed but have been offset to indicate the third dimension. The view is perpendicular to the 001 plane, *i.e.* parallel to the c-axis.

There are 48 anions in the unit cell, however, one-half of the cell is the mirror image of the other half, thus, a working unit of 24 anions is convenient. In a one-half unit cell of 24 anions, 22 of these anions are normally oxygen ions surrounding the silicon ions in a tetrahedral arrangement. These

TEXT-FIGURE 1. —A classification for hornblendes as proposed by Sundius (1946).





TEXT-FIGURE 2. —Structure of monoclinic amphiboles.

oxygen ions form the framework of the amphibole minerals. The other two anions, O_3 in diagram, are normally OH^- ions although F^- or Cl^- ions sometimes substitute. The OH^- ions are bonded only to cations between the chains, not to the tetrahedra.

A one-half unit cell contains eight tetrahedral sites of four fold coordination within the chains, labeled S in figure 2. The four oxygen anions form a cavity that will accommodate a cation of ionic radius 0.316 Å without distortion of the structure, but, may also accept a cation with ionic radius as large as 0.580 Å before the structure will be distorted enough to shift to higher coordination. For a symmetrical distribution of charges throughout the structure, a cation in this position should have a valence of +4 although cations with +3 charge many times substitute in this position.

There are five octahedral sites of six fold coordination between the double chains, labeled $M_{1,2,3}$ in figure 2. The cavity formed by the anions exactly accommodates a cation of ionic radius 0.580 Å but will accept a cation with an ionic radius as large as 1.02 Å. The cation should have a valence of +2 for symmetrical distribution of charges throughout the structure, although cations with +3 charge or +1 charge are often substituted.

There are two cubic sites of eight fold coordination, per 24 anions, located between the chains and noted as M_4 in figure 2. This position requires a cation with a minimum ionic radius of 1.02 Å and a maximum radius of 1.40 Å. A charge of +2 is needed for a symmetrical balance of charges, but, many times cations with a +1 charge fill this position.

There is one position, per 24 anions, labeled A in the diagram, normally unoccupied in the actinolite-tremolite and cummingtonite series, but usually occupied, to some extent, in the hornblende series, that requires a cation with an ionic radius larger than 1.02 Å and a charge of +1.

Factors Influencing Ions and Positions

For purposes of reference during the following discussion a table of the possible cations occuring in amphibole minerals, listing their valence, ionic radius, radius ratio compared with oxygen, and their observed coordination numbers, is given below in table 2. Values were taken from Berry and Mason 1959, the Rankama and Sahama (1950). Stability ranges of the radius ratios for the various coordination numbers are also given. The smaller figure of this range is the size of the cavity with the anions "touching." The larger figure is the maximum size of the cavity with anions "spread apart" by cations. If the anions are separated more, there will be room for another anion to enter the arrangement and thus raise the coordination number. The most stable position is somewhere between the two extremes.

TABLE 2

Ion size and stability range

Ion	*Valence*	*Ionic Radius (Å)*	*Rc:Ra**	*Coordination Number*
Si	4	0.42 Å	0.30	4,
Al	3	0.51	0.36	4,6
Cr	3	0.63	0.45	6
Fe	3	0.64	0.46	6
Mg	2	0.66	0.47	6
Ti	4	0.68	0.49	6
Li	1	0.68	0.49	6
Ni	2	0.69	0.50	6
Mn	3	0.70	0.50	6
Fe	2	0.74	0.53	6
Zn	2	0.74	0.53	6
Mn	2	0.80	0.57	6
Na	1	0.97	0.69	6,8
Ca	2	0.99	0.71	6,8
K	1	1.33	0.95	8,12
Ba	2	1.34	0.96	8,12
O	-2	1.40		
OH	-1	1.40		
F	-1	1.36		
Cl	-1	1.81		

Stability Ranges for Radius Ratios
0.000 - 0.225 for 2-fold coordination
0.225 - 0.414 for 4-fold, tetrahedral coordination
0.414 - 0.732 for 6-fold, octahedral coordination
0.732 - 1.000 for 8-fold, cubic coordination
1.000 and larger for 12-fold coordination

*Ra is the radius of an O_2^- ion.

Many chemical analyses of amphiboles have been published and position in the structure which the various elements occupy has been determined, but, limits for the various substitutions, except for Al and perhaps Si, are not known. Various factors such as the ion's radius, its electronegativity, its co-

ordination number, its valence, and its availability at the time of the mineral's formation will have an effect on the limits of substitution and position occupied.

Tetrahedral Sites

The eight tetradedral sites, in a half unit cell of 24 anions, are all similar and may all be filled by Si^{4+} as in tremolite. Silicon ions fit well in this position and never exceed more than eight ions per half unit cell. It is assumed that all Si^{4+} are in tetrahedral sites because of their small radius and 4+ charge. Furthermore it is assumed that all tetrahedral sites are filled by some ion because the high negative charge would have the strongest attraction of any position in the structure for a cation. An empty position within the chain framework would cause a more unstable structure than an empty position between the chains.

Although the radius of Al^{3+} is larger and its valence smaller than Si^{4+}, it may substitute for Si^{4+} in the hornblende series. Its smaller charge can be balanced either by the introduction of a trivalent ion into the octahedral sites, or the introduction of a monovalent ion into a vacant position A (Text-figure2).

Occasionally there is not enough Si^{4+} plus Al^{3+} present to completely fill the tetrahedral sites and in such instances Fe^{3+} may be present in tetrahedral coordination. Although Fe^{3+} is large the structure seems to permit a certain amount of strain and usually the amount of Fe^{3+} needed to fill the remaining sites is small.

The only variation occurring in the tetrahedral sites is the amount of Si^{4+} replaced. Therefore, a number "Y" shall be used to indicate the number of tetrahedral sites, per 24 anions, not filled by a Si^{4+} ion, or the number filled by Al^{3+}. This notation has been used before in silicate structures, Phillips (1954 *ms.*). Sundius and Hallimond recognized the implications of an Al^{3+} ion replacing Si^{4+} in the amphibole structure. Sundius (1946) set the limit for Y at 2.27 which was the highest amount of Al^{3+} replacing Si^{4+} in hornblende. Hallimond (1943) gives an analysis for basaltic hornblende in which 2.44 Si^{4+} ions have been replaced by Al^{3+} and Fe^{3+}. Thus Y may vary from 0 to at least 2.44 although those greater than 2.00 will not be common.

Octahedral Sites

The five octahedral sites are not all similar but may all be filled by Mg^{2+} as in the case of tremolite. Positions of these octahedral sites in the structure are shown in text-figure 2 as Mg^{2+}. The slight difference in the octahedral sites is due to the fact that M_2 is bonded to six oxygen ions while M_3 and M_1 are bonded to one OH^- and five oxygen ions. Thus the M_2 position has a slightly lower electro-negativity than M_3 and M_1, and because Mg^{2+} has a slightly lower electro-negativity than Fe^{2+}, Mg^{2+} will be favored for this position (Ghose, 1962).

Bivalent ions reported in the octahedral sites are Mg^{2+}, Fe^{2+}, Mn^{2+}, Ni^{2+}, Zn^{2+} and Ca^{2+}. They all fall within the proper range of radius ratios although they occur near the upper limit. Mg^{2+} and Fe^{2+} usually fill this position and are usually considered completely replaceable, but, pure Fe^{2+} end members are seldom found in nature while pure Mg^{2+} end members are common. Tremolite often contains only Mg^{2+} in octahedral sites and actinolite rarely exceeds a ratio of 4 Fe^{2+}: 1 Mg^{2+}. Mn^{2+} is reported in many analyses but usually in small amounts. Zn^{2+} and Ni^{2+} are seldom reported in a chemical analysis of an amphibole. Ca^{2+} usually fills the eight-fold positions but may

substitute in the octahedral site if there is a vacancy and if cubic sites are filled.

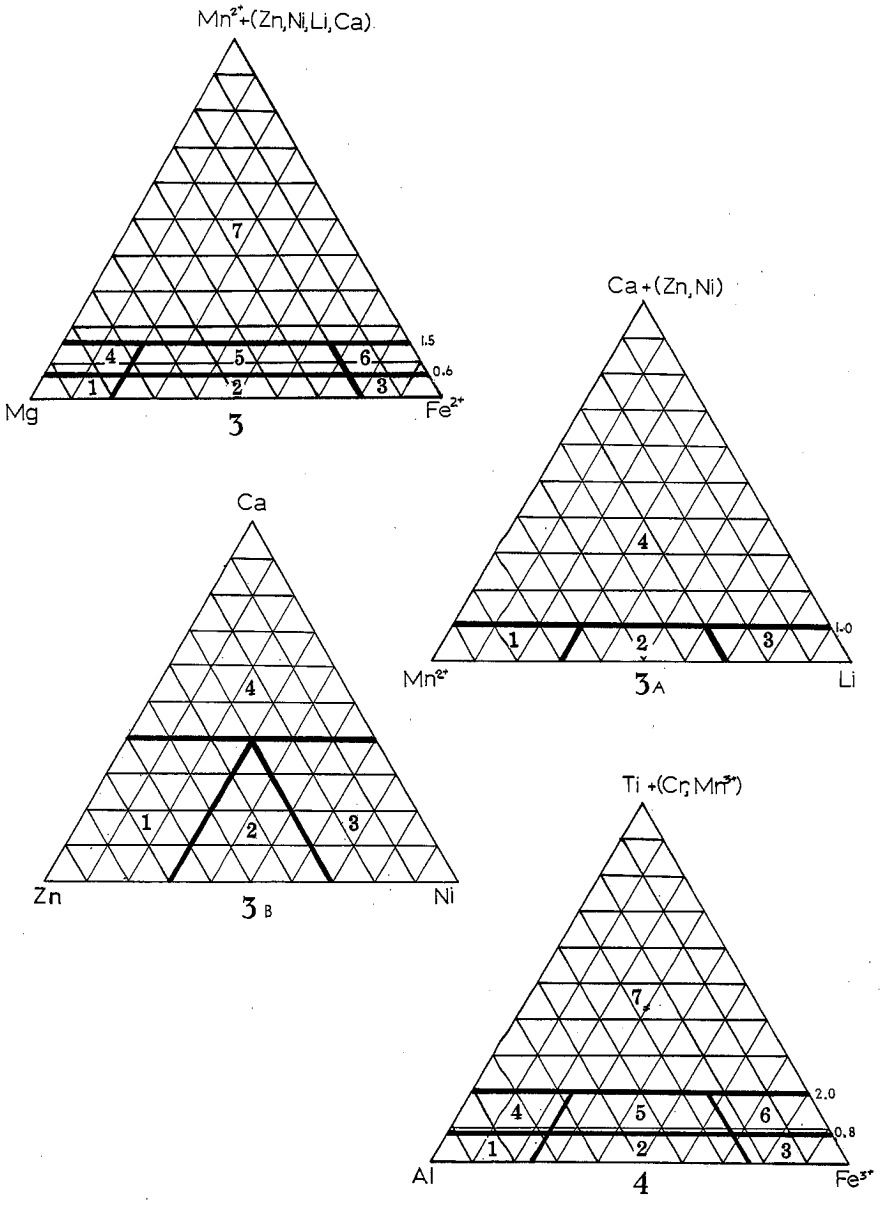
When Y=O the octahedral sites are usually filled by bivalent ions but as Y gets larger trivalent ions are introduced. Trivalent ions reported in octahedral positions are Al^{3+}. Fe^{3+}, Cr^{3+}, Mn^{3+} as are also tetravalent Ti^{4+}, and monovalent Li^{+}. These ions all are in the lower range of radius ratios for octahedral coordination. Al^{3+} and Fe^{3+} are the common trivalent ions found in this position, Ti^{4+} is often reported in small amounts, Cr^{3+} and Mn^{3+} are seldom reported, and Li^{+} is common but only occasionally present in relatively large amounts. Sundius (1946) gives an analysis, with Y=O, in which two trivalent ions in octahedral sites were balanced by $\frac{1}{2}$ ion of Li^{+} in octahedral position plus $1\frac{1}{2}$ ions of Na^{+} in cubic coordination.

Trivalent ions are necessary in the octahedral positions either to balance charges of trivalent ions in tetrahedral positions or monovalent ions in cubic positions. In some analyses more trivalent ions are present in octahedral sites than are needed to balance trivalent ions in tetrahedral sites and monovalent ions in cubic sites. In such cases one octahedral site must be left vacant for every two excess trivalent ions. Chemical analyses usually show an excess of ions available for octahedral sites rather than vacancies. The reason for this condition has not been determined. There actually may be an excess of ions present. Hallimond (1943) notes that an error of only one percent in the calculation of the percentage of H_2O can change the number of cations in the octahedral sites by 0.3 cations. A small change in the percentage of H_2O has a greater effect upon cations in octahedral positions than elsewhere. A chemical analysis with less than two OH^{-} ions usually shows more than five cations in octahedral sites while an analysis with more than two OH^{-} anions usually shows less than five cations in octahedral sites. Most chemical analyses show less than two OH^{-} anions.

The relationship between bivalent ions and trivalent ions in octahedral sites becomes very complex in the hornblende series. Thus, in considering the important variations in the octahedral sites, it is more convenient to consider trivalent and bivalent ions separately. The number "P" will be used to indicate the number of octahedral sites, out of 5 available sites, not filled by bivalent ions *i.e.* the number filled by trivalent ions. From reported chemical analyses of amphiboles it may be observed that P can vary from 0.000 in species such as tremolite, where all octahedral sites are filled with bivalent ions, to 3.45 in gastaldite where 3.45 out of five bivalent ions are replaced by trivalent ions (Sundius, 1946).

Number of bivalent ions in octahedral sites can be recalculated to 100% and position of the relative percentage of any combination of bivalent ions shown as a point on the triangular diagram in text-figure 3. The particular number of the subdivision into which some combination of bivalent ions falls will be called the "R^{2+}" number. If the R^{2+} is seven, Mn^{2+}, Zn^{2+}, Ni^{2+}, Ca^{2+} and Li^{+} are calculated to 100% and referred to the triangular diagram in text-figure 3a, to obtain an "$R^{2+}a$" number. If the $R^{2+}a$ number is four, Ca^{2+}, Zn^{2+} and Ni^{2+} are recalculated to 100% and referred to the triangular diagram in figure 3b for "$R^{2+}b$".

The trivalent ions are treated in a similar manner. Trivalent ions are calculated to 100% and represented as a point on the triangular diagram in



TEXT-FIGURE 3. —Triangular coordinate diagram used to find the "R^{+2}" number by plotting relative percentages of bivalent ions in octahedral coordinate positions.
TEXT-FIGURE 3a.—Triangular coordinate diagram used to find the "$R^{+2}a$" number.
TEXT-FIGURE 3b.—Triangular coordinate diagram used to find the "$R^{+2}b$" number.
TEXT-FIGURE 4. —Triangular coordinate diagram used to find the "R^{+3}" number by plotting relative percentages of trivalent ions in octahedral coordinate positions.

text-figure 4 to obtain an "R^{3+}" number. When no trivalent ions exist in octahedral position, R^{3+} equals zero. To completely define the octahedral position three variables are needed; the "P" number, the "$R^{2+}ab$" number, and the "R^{3+}" number.

Triangular coordinate diagrams are used so that three variables may be considered simultaneously, and only ions are considered, since the change involved is one of ionic substitution, not changes in end member molecules.

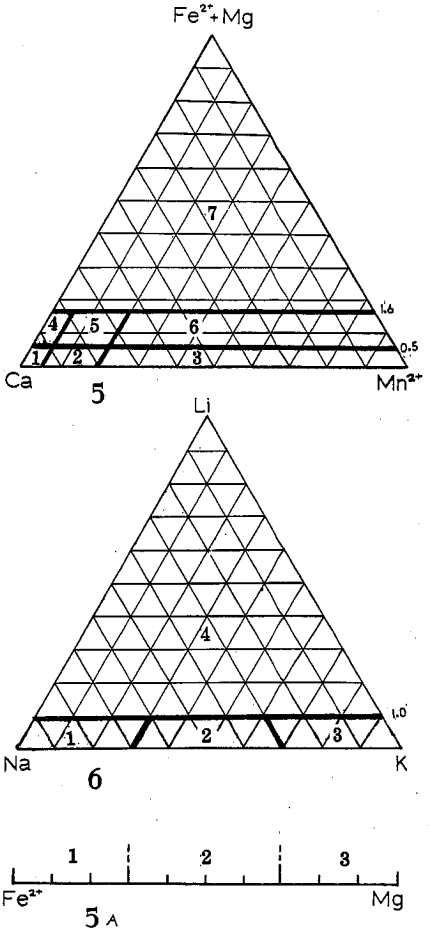
Cubic Sites

Cubic sites may contain the bivalent ions Ca^{2+}, Mn^{2+}, Fe^{2+}, Mg^{2+} and monovalent ions Na^{+}, K^{+} and Li^{+}. Ca^{2+} has an appropriate size and charge for this position and normally occurs here, sometimes completely filling this position in the tremolite-actinolite series. Although in minor amounts, Mn^{2+} usually appears in chemical analyses and may be found in either octahedral or cubic sites. Fe^{2+}, and especially Mg^{2+}, are small for cubic coordination, see table 1. However, in the cummingtonite series Warren (1930) gives a chemical analysis in which Mg^{2+} and Fe^{2+} fills all octahedral sites plus 90% of the cubic sites. Warren (1930) states, "it turns out that the eight oxygen atoms about Ca are so arranged that on replacement of Ca by Mg six of the oxygens can move closer and form a nearly regular octahedron about the Mg atom. Moreover the remaining two oxygens are each bound to two silicons and so have their valence bonds already fully satisfied." The shift effects the structure so little that almost identical X-ray patterns result. Ghose (1962) determined that the M_4 position (cubic site) in cummingtonite has a stronger affinity for Fe^{2+} than Mg^{2+} because of Fe^{2+}'s stronger electronegativity. Ghose also suggests that the M_4-O_4 bond (Text-fig. 2) is covalent. The M_4-O_4 bond is important in amphiboles because it controls the β angle which makes the mineral monoclinic or orthorhombic (Whittaker, 1960).

The monovalent ions Na^{+} and K^{+} also occur in 8-fold coordination and can substitute for Ca^{2+}, if there are excess trivalent ions in octahedral coordination, or excess alkali ions may fill the A position and require substitution of a monovalent ion for Ca^{2+} in cubic coordination to maintain charge balance. Li^{+} is much smaller than K^{+} or Na^{+} and will usually occur in a six-fold coordination like Mg^{2+}.

In considering various ions in cubic sites it is convenient to consider monovalent and bivalent ions separately. "T" will be used to indicate the number of cubic sites not filled by bivalent ions. Tremolite-actinolite have all cubic sites filled by Ca^{2+} and hence T=O. A chemical analysis of eckermannite given by Sundius (1946) has 1.95 ions of Na^{+} replacing Ca^{2+} in 8-fold coordination. Thus T must vary from 0 to at least 1.95.

The bivalent ions are calculated at 100% and plotted on the triangular diagram shown in figure 5. The number representing the relative percentage of bivalent ions will be called the "Q^{2+}" number. If this position falls in subdivision seven, the composition is referred to figure 5a for the "Q^{2+}" number. The same system is used for the monovalent ions and their relative percentage is plotted on the triangular diagram in text-figure 6 to obtain the "Q^{1+}" number. In many analyses there will be no monovalent ions in the 8-fold position in which case Q^{1+} equals zero. Three variables, T, $Q^{2+}a$, and Q^{1+} are necessary to completely define the cubic position.



TEXT-FIGURE 5. —Triangular coordinate diagram used to find the "Q^{+2}" number by plotting the relative percentages of bivalent ions in the cubic coordination position.
TEXT-FIGURE 5a.—Diagram used to find the "$Q^{+2}a$" number.
TEXT-FIGURE 6. —Triangular coordinate diagram used to find the "Q^{+1}" number by plotting the relative percentages of monovalent ions in the cubic coordinate position.

Position A*

Another possible position for an ion is the position at A (Text-fig. 2) which is usually vacant in the cummingtonite and tremolite-actinolite series but occupied in the hornblende series by Na^+, K^+, Ca^{2+} and sometimes Ba^{2+}. Warren (1930) stated, concerning position A,

> "in this position a small atom such as Mg^{2+} would have only two oxygen neighbors and these two oxygens are already bound to two silicons each and have their electrostatic valence bonds already satisfied. The position of AA' (position A in figure 2 of present paper) was

*As used by Bragg (1930) and Warren (1930).

therefore considered to be highly improbable for a small atom such as Mg^{2+}—A larger atom such as Na^{+} if situated at position AA' would have six oxygen neighbors—in normal amphiboles each of the six oxygens has its electrostatic valence bonds fully satisfied—in hornblendes with high aluminum content, where a large fraction of Si in the chains is replaced by Al this is no longer the case. In these circumstances the position AA' becomes a very probable one."

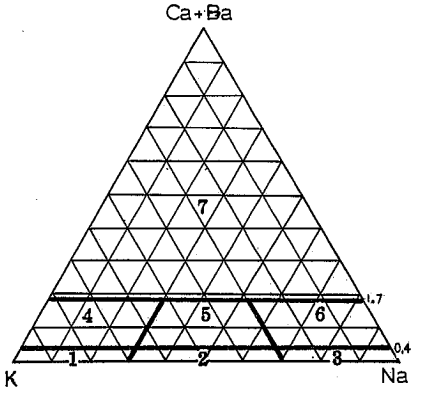
Na^{+} and K^{+} are large ions with small charges that can occupy this position. Ca^{2+} may occasionally occur here but only in very small amounts, possibly due to its higher charge. Ba^{2+} is very seldom reported in chemical analyses but when present it must occupy this position due to its large ionic radius.

"S" will be used to indicate the fraction of A sites filled. This position may be completely empty, as in tremolite, or completely filled, as in glaucophane. Thus S can vary from O to 1 in a 24 anion unit. Any combination of ions in this site can be indicated on the triangular diagram in text-figure 7 and represented by a "V" number.

OH Ions

One other possible variable in amphibole minerals concerns the OH^{-} ions. As shown in text-figure 2, two OH^{-} ions and 22 O^{2-} ions normally form the 24 anion unit. OH^{-} ions may be replaced by F^{-} or Cl^{-}. F^{-} has the same valence and about the same ionic radius as OH^{-}, and both OH^{-} and F^{-} ions are about the same size as O^{2-} ions. Cl^{-} has a large ionic radius and is rarely reported in amphibole analyses, and then only in very small amounts. Thus the only variable needed to define this position is an "H" number to indicate the number of OH^{-} ions not replaced by F^{-} ions.

The number of OH^{-} ions reported in chemical analyses varies widely, usually showing less than two OH^{-} per one-half unit cell but occasionally more than two. It has been suggested by Rabbitt (1948) and Hallimond (1943) that the chemical analysis procedures for H_2O are very inaccurate and there would be exactly two OH^{-} ions if determined accurately. Another possible explanation is loss of H^{-} ions with oxidation of FeO to Fe_2O_3 (basaltic hornblende) generally contain less water as seen in chemical analyses given by



TEXT-FIGURE 7.—Triangular coordinate diagram used to find the "V" number by plotting relative percentages of ions in the "A" position.

Hallimond (1943) and Winchell (1945). Hallimond (1943) suggested that some amphiboles do not contain two OH^- ions. Engel and Engel (1962) concludes that K^+ is able to replace H^+ in charge but not position, and thus is able to balance charges.

Suggested Order of Recording Variables

Variables should be arranged in a definite order for purpose of clarity and uniformity when describing an amphibole species. The following order is suggested; Y number, P number R^{3+} number, R^{2+}ab number, T number, Q^{2+}a number, Q^{1+} number, S number, V number, and H number. Although this is not the order of most importance in a classification scheme, it is a logical arrangement of the structural variables based upon increasing size of ions and coordination number.

CALCULATING NUMBER OF CATIONS

The first step in classification of an amphibole from chemical analyses is calculation of the number of cations of each type in an average half unit cell. A method used for the amphiboles is as follows:

1. Determine the relative number of oxide molecules present by dividing the weight percentages of each oxide by its molecular weight.
2. Obtain the relative number of oxygen ions each oxide contributes by multiplying the number of oxygen ions in the oxide with its relative number of oxide molecules (this does not apply to F^- or Cl^-).
3. Recalculate to half unit cell basis (24 anions) by dividing total number of oxygen ions into 24, thereby obtaining a ratio by which each oxide molecule is multiplied to obtain the number of cations per half unit cell. If the oxide contains more than one cation (i.e. Al_2O_3) multiply ratio by number of cations in oxide.

ASSIGNING IONS TO STRUCTURAL POSITION

When assigning ions to positions in the amphibole structure, all Si^{4+} ions are assigned to tetrahedral coordination and enough Al^{3+} ions are added to give the tetrahedral sites eight cations. If there is not enough Al^{3+} to make up the deficiency Fe^{3+} is added. The remaining Al^{3+}, Fe^{3+}, and any Cr^{3+}, Mn^{3+}, Ti^{4+} are assigned to octahedral coordination. Because of the charge on Ti^{4+}, the number of cations it contributes in filling octahedral sites should be doubled to maintain proper charge to site relationship. If there are more trivalent ions in octahedral position than necessary to balance electrostatic charges in the tetrahedral sites, when Ca^{2+} fills all cubic sites, then one vacant position should be allowed for each two trivalent ions. All Fe^{2+}, Mg^{2+}, Mn^{2+}, Ni^{2+}, Zn^{2+} and Li^+ are assigned to the octahedral sites if positions are available.

All Ca^{2+} is assigned to cubic coordination. If there is too much Ca^{2+} for cubic sites it may be assigned to octahedral sites if there is a vacancy. If no vacancy is present in octahedral sites then Ca^{2+} is assigned to position A. If there are too many ions for the octahedral sites, and there usually are, then Mn^{2+}, Li^+, Fe^{2+}, and Mg^{2+}, in order given, are assigned to the cubic sites if there are sites available. If not all cubic sites are filled by Ca^{2+} then enough Na^+ or K^+, in order listed, is assigned to the cubic sites to balance excess trivalent charges in octahedral coordination. The balance of Na^+ and K^+ is assigned

to position A. There may be an excess of bivalent ions in octahedral positions due perhaps to inaccurate analyses or oxidation.

To provide an example, the following chemical analysis of hornblende, (Table 3) was taken from Dana (1892) and will be classified according to the method given above.

TABLE 3
Analysis of Hornblende

Oxide	*Chem. anal. wt. %*		*Recalculated to 100 %*	*Molecular weight*	*Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	40.02	X.99473 =	39.809 ÷	60.06 =	0.6628 X 2	1.3256
Al_2O_3	15.55	"	15.468	101.94	0.1517 X 3	0.4551
Fe_2O_3	3.44	"	3.422	159.68	0.0214 X 3	0.0642
FeO	8.60	"	8.555	71.84	0.1191	0.1191
MgO	14.37	"	14.294	40.32	0.3545	0.3545
MnO	0.00	"	0.00	70.93	0.00	0.00
CaO	12.21	"	12.146	56.08	0.2166	0.2166
Na_2O	2.40	"	2.387	61.99	0.0385	0.0385
K_2O	2.13	"	2.118	94.19	0.0225	0.0225
H_2O	1.81	"	1.8004	18.02	0.0999	0.0999
Total	100.53					2.6960

$\frac{24}{2.696}$ = 8.902 = ratio needed to determine half unit cell

Cations	*Relative No. of oxide molecules*			*Ions per 24 anions*		
Si^{4+}	0.6628	X 8.902		5.80		8.00
Al^{3+}	0.1517	"	X 2	2.70	2.20	
Fe^{3+}	0.0214	"	X 2	0.38	.50	
Mg^{2+}	0.3545	"		3.15		5.01
Fe^{2+}	0.1191	"		1.06	.98	
Ca^{2+}	0.2166	"		1.927	.08	2.007
Na^{+}	0.0385	"	X 2	0.68		
K^{+}	0.0225	"	X 2	0.40		1.08
OH^{-}	0.0999	"	X 2	1.78		1.78

Calculation of Amphibole Number for above composition

Y = number of ions of Si^{4+} replaced by Al^{3+} = 8.00 - 5.80	= 2.20
P = number of octahedral sites not filled by bivalent ions = .50 + .38	= 0.88
R^{3+} = relative percentages of trivalent ions in octahedral coordination; number obtained from figure 4	= 2
$R^{2+}ab$ = relative percentages of bivalent ions in octahedral coordination; numbers obtained from figures 3, 3a, 3b.	= 2
T = number of cubic positions not filled with a bivalent ion	= 0
$Q^{2+}a$ = relative percentages of bivalent ions in cubic coordination; number obtained from figures 5 & 5a.	= 1
Q^{1+} = relative percentages of monovalent ions in cubic coordination; number obtained from figure 6.	= 0
S = total number of ions in position A	= 1
V = relative percentage of ions in position A; number obtained from figure 7.	= 2
H = number of H ions not replaced by F^{-}; the number is 2 because no H ions have been replaced	= 2

This species number will be found in table 2 and is assigned the name Girnarite.

PROPOSED SPECIES NAMES BASED UPON RANGES OF CRYSTAL CHEMICAL COMPOSITIONS

Although a number, as shown above and based on crystal chemical considerations, is able to describe an amphibole more completely than a name, it is customary to give names to minerals. Therefore, a variety name is assigned to many possible species numbers (Table 4). Many amphibole names in current use are associated with definite chemical and physical properties and it is essential to retain these associations. Care has been taken to assign names in agreement with original variety definitions. In some instances it has been necessary to broaden the orginal compositional range of the name, in other cases it has been necessary to considerably restrict the range to prevent extensive overlap. If several names included the same chemical composition the earliest name was retained. Names and formulae as given in Dana (1892), Hey (1955) and others were used and where necessary to expand the ranges beyond the original formulae, the extended ranges are given in parentheses in table 4. Names which had no composition given for them, such as Juddite which was described only as having a high manganese content, were assigned to appropriate divisions. Not all possible divisions were assigned names because it is not certain they exist in nature.

Nomenclature of amphiboles in the past has been based essentially upon the Y number, R^{+2}ab number, T number, Q^{+2}a number and the S number. Vague limits had been set for certain species and these limits were used whenever possible in this classification. The P, R^{+3}, Q^{+1}, and V numbers had been given no limits in original descriptions, consequently, it was necessary to assign rather large ranges to them. If an analysis shows more than one F^- ion per 24 anions the prefix "fluor" is added to the species name.

It will be noted that the name hornblende has not been used as a variety name in table 4. This name has been used in the past to cover a wide range of chemical compositions. Winchell (1942) has used hornblende to include all monoclinic amphiboles except the grunerite series and Sundius (1946) uses hornblende in about the same way. Usually any dark colored amphibole is called hornblende until it can be identified more specifically. The writer would retain the name hornblende for these particular usages.

COLLECTION AND ISOLATION OF SAMPLES

For purposes of checking the value of the proposed classification method and to gain experience in laboratory techniques, thirty samples of various amphibole minerals were obtained from several mineral supply houses in the United States. Ten specimens (Table 5) were chosen from this group for complete chemical analysis and determination of optical, X-ray powder diffraction and DTA properties. Numbers rather than the names were used to denote the specimens.

The mineral specimens were associated with many different rock types and various techniques were used to effect the isolation of the minerals. A binocular microscope, tweezers and a sharp steel point were used to separate large crystals or large pure masses from enclosing rock whenever possible. Next, the mineral was ground to 60 mesh in a mortar. A heavy liquid separation (Tetrabromoethene, sp. gr.=2.965) was used on most mineral samples. The amphiboles were just heavy enough to sink and most impurities floated to the top. Tetrabromoethene was removed from the mineral by rinsing several time

TABLE 4

Proposed amphibole variety names and corresponding species numbers

Variety	Y	P	R^{+3}	$R^{+2}ab$	T	$Q^{+2}a$	Q^{+1}	S	V
Grunerite	0-0.6	0-0.5	0,(1,2,3)	300	0-0.3	71	0,(1,2,3)	0-0.5	0,(1,2,3)
Cummingtonite	0-0.6	0-0.5	0,(1,2,3)	200	0-0.3	71	0,(1,2,3)	0-0.5	0,(1,2,3)
Kupfferite	0-0.6	0-0.5	0,(1-6)	100	0-0.3	72-73	0,(1,2,3)	0-0.5	0,(1,2,3)
Dannemorite	0-0.6	0-0.5	0,(1,2,3)	400,(500,600,710)	0-0.3	71,(40,60)	0,(1,2,3)	0-0.5	0,(1,2,3)
Tremolite	0-0.6	0-0.5	0,(1,2,3)	100	0-0.3	10	0,(1)	0-0.5	0,(1,2,3)
Tirodite	0-0-6	0-0.5	0,(1,2,3)	100	0-0.3	60,(30)	0,(1)	0-0.5	0,(1,2,3)
Soda-tremolite	0-0.6	0-0.5	0,(1,2,3)	100,(200)	0.3-1	10	1,(0)	0.5-1	3,(1,2)
Byssolite	0-0.6	0-0.5	0,1,2,3	(100,200,300)	(0-1)	(10)	(1,0)	(0-1)	(4,5,6,7)
Actinolite	0-0.6	0-0.5	0,(1,2,3)	200	0-0.3	10	0,(1)	0-0.5	0,(1,2,3)
Ferro-tremolite	0-0.6	0-0.5	0,(2,3)	300	0-0.3	10	0,(1)	0-0.5	0,(1,2,3)
Ferro-richterite	0-0.6	0-0.5	0,(2,3)	300,(600,710)	0.3-1	10,(20,40,50)	1,(2)	0.5-1	3,(1,2)
Richterite	0-0.6	0-0.5	0,(1,2,3)	400,(100)	0.3-1	10,(20-60)	1,(2,3)	0.5-1	2,(1,3)
Soda-richterite	0-0.6	0-0.5	0,(1,2,3)	710,(500)	0.3-1	10,(20-60)	1	0.5-1	3,(1,2)
Abkhazite	0-0.6	0-0.5	0,(1,2,3)	744	0-0.3	10	0,(1)	0-0.5	0,(1,2,3)
Waldheimite	0.0-6	0-0.5	0,(1,2,3)	744	1.0-2	0,(10)	1	0.5-1	3,(2)
Eckerite	0-0.6	0.5-1	3,(1,2)	400,(744)	0.3-1	10,(0)	1	0-0.5	0,(1,2,3)
Eckermannite	0-0.6	0.5-1	1,3,(2)	100,(200,400,730)	1.0-2	0,(10,40,71)	1	0-1	3,(0,1,2)
Mangan-tremolite	0-0.6	0-1	0,(1,2,3)	400,(100)	0-0.3	10,(20,40,50)	0,(1)	0-0.3	0,(1,2,3)
Mangan-actinolite	0-0.6	0-1	0,(1,2,3)	500,(200)	0-0.3	10,(20,40,50)	0,(1)	0-0.3	0,(1,2,3)
Grammatite	0-0.6	0-1	(4,5,6,7)	(100,200,300)	(0-1)	(0,10,20,40)	(0,1)	(0-1)	(0,1,2,3)
Torendrikite	0-0.6	1-1.5	3,(1,2)	200,(100)	1.0-2	10	1	0-0.5	0,(3)
Arfvedsonite	0-0.6	1-1.5	3,(2,5,6)	300,(200)	1.0-2	0,(10)	1	0.5-1	3,(1,2)
Holmquistite	0-0.6	1.5-2	1,(2,3)	200,(100,300)	1.0-2	0,(10)	4,(3,2)	0-0.5	0,(1,2,3)
Glaucophane	0-0.6	1.5-2	1,(2)	200	1.0-2	0,(10)	1	0-0.5	0,(3)
Juddite	0-0.6	1.5-2	2,(1,3)	400,(500,600,710)	1.0-2	10-60	1	0-0.5	0,(3)
Crossite	0-0.6	1.5-2	2,(3)	100	1.0-2	0,(10)	1	0-0.5	0,(3)
Riebeckite	0-0.6	1.5-2	3,(1,2,6)	300	1.0-2	0,(10-30)	1	0-0.5	0,(2,3,1)

TABLE 4 (Cont'd.)

Ferri-tremolite	0-0.6	1.5-2	3,(2)	3oo,(2oo)	0-0.3	1o	0,(1)	0-0.5	0,(1,2,3)
Carinthine	0.6-1	0-1	1,(2)	1oo	0.3-1	1o	1	0.3-1	3
Catophorite	0.6-1	0-1	2,(1,3)	2oo	0.3-1	1o	1	0.5-1	2,(1,3)
Phillipstadite	0.6-1	0-1	3,(1,2)	2oo,(3oo)	0-0.3	1o,(4o,2o,7)	0,(1)	0-0.5	0,(1,3,2)
Anophorite	0.6-1	0-1	7,(4-6)	2oo,(1oo,3oo)	0-1	0,(1o,2o,4o)	1,(0)	0-1	3,(0,1,2)
Ferro-edenite	0.6-1	1.5-2	3,(1,2)	3oo	0-0.3	1o	0,(1)	0.5-1	3,(1,2)
Glaucopargasite	1-1.4	0.5-1	1,(2,3)	2oo,(1oo)	0-1	1o	1,(0)	0.5-1	3,(1,2)
Edenite	1.4-2	0-0.5	1,(2,3)	1oo,(2oo)	0-0.3	1o	0,(1)	0.5-1	3,(6-7)
Tibergite	1.4-2	0-0.5	0,(2,3)	1oo,(2oo,4oo,5oo)	0.3-1	1o	1	0.5-1	3,(1,2)
Pargasite	1.4-2	0.5-1	1,(2,3)	1oo,(2oo,3oo)	0-0.3	1o,(4o,5o)	0,(1)	0.5-1	3,(2,5,6)
Dashkesanite	1.4-2	0.5-1	3,(1,2)	2oo,(1oo,3oo)	0,3-1	1o,(4o)	0,(1)	0-0.5	2,(1,3)
Soretite	1.4-2	1-1.5	3,(1,2)	2oo,(1oo)	0-0.3	1o,(4o)	0,(1)	0.5-1	3,(1,2)
Kaersutite	1-2	0-1	7,6,5,4	2oo,(1oo)	0-1	1o,(4o,2o)	1,(0)	0-1	2,(3,5,6,7)
Magnesio-hastingsite	1-2	1.0-2	2,(1,3)	2oo,(1oo)	0-1	1o	1,(2,3)	0-1	2,(1,3)
Noralite	1-2	1.0-2	1,(2)	3oo	0-0.3	1o	0,(1)	0-1	0,(3)
Linosite	1-2	1-2	7,6,5,4	2oo,(1oo,3oo)	0-1	1o,(4o,2o)	1,(0)	0-1	2,(1,3)
Tschermakite	1.4-2	1.5-2	1,(2,3)	1oo,(2oo)	0-0.3	1o	0,(1)	0-0.5	0,(2,3)
Barkevikite	1.4-2	1.5-2	2,(1,3)	2oo,(1oo)	0-0.3	1o	0,(1)	0.5-1	3,(1-2)
Hudsonite	1.4-2	1.5-2	2,(3)	3oo,(2oo)	0-0.3	1o,(4o)	0,(1)	0.5-1	2,(1,3)
Ferro-tschermakite	1.4-2	1.5-2	3,(2)	3oo,(2oo)	0-0.3	1o	0,(1)	0-0.5	0,(3)
Taramite	1.4-2	1.5-2	3,(2)	3oo,(2oo)	0.3-1	1o	1,(0)	0.5-1	2,(1,3)
Bergamaskite	2-2.4	1-1.5	2,(3)	3oo	0.3-1	1o	1	0.5-1	2,(1,3)
Basaltic Hornblende	2-2.4	1.5-2	2,(1,3)	1oo,(2oo)	0.3-1	1o	1,(0)	0.5-1	2,(1,3)
Ferro-hastingsite	2-2.4	1.5-2	3,(1,2)	3oo	0.3-1	1o	1,(0,2,3)	0.5-1	2,(1,3)
Girnarite	1.4-2.4	0.5-1.5	1,2,3	2oo,(1oo,3oo)	0-1	1o,(4o,2o)	0,(1,2,3,4)	0-1	2,(1,3)
Hastingsite	2-2.4	0-2	7,6,5,4	2oo,(1oo,3oo)	0-1	1o,(4o,2o)	0,(1,2,3)	0-1	2,(1,3)
Gastaldite	1.4-2.4	2-3.5	1,(2,3)	2oo,(1oo,3oo)	0-1	7r,(o,1o,4o)	1,(0)	0-0.5	3,(1,2)
Bababudanite	2-2.4	2-2.5	3,(2,1)	2oo,(1oo,3oo)	1.0-2	0,(1o,4o)	1,(0)	0.5-1	3,(1,2)

with ethyl alcohol. Samples which contained carbonate impurities were washed for two minutes in dilute (1:5) cold hydrochloric acid. One sample was intermixed with magnetite which was removed by a small magnet. Another sample was separated from its host rock with the aid of a magnetic separator. A petrographic microscope was used to determine what impurities remained in the isolated samples and the percentage of each present. Ten grams of each sample, if available, were sent to the Mineral Constitution Laboratory at Pennsylvania State University for a chemical analysis. Enough of each sample was retained so that the physical properties of the mineral could be determined.

TABLE 5
Sample localities, preparation, and impurities

No.	*Locality*	*Methods used to isolate mineral*	*Amount and type of impurities remaining*
1	Fowler, N.Y.	Heavy liquid HCl acid	0.3% actinolite, zircon, and hornblende inclusions in tremolite
2	Chester, Vermont	Heavy liquid	0.1% tremolite
6	Nomingo mines North Bancroft, Ontario, Canada	Heavy liquid HCl acid	1% zircon
7	Verona, Ontario, Canada	Heavy Liquid	thin film, unidentified
8	Calumet mines, Chaffee County, Colorado	Heavy liquid magnet	0.2% actinolite
10	Old Colony Quarry Quincy, Norfolk County, Mass.	Heavy liquid	3% feldspar 1% quartz
13	Kragero, Norway	Heavy liquid	less than 0.1% tremolite and actinolite
18	Keystone, South Dakota	Heavy liquid	0.5% talc
19	Clay County, North Carolina	Heavy liquid	0.3% inclusions of actinolite tremolite and hornblende(?)
20	Murray Bay, Quebec, Canada		less than 1% hematite(?)

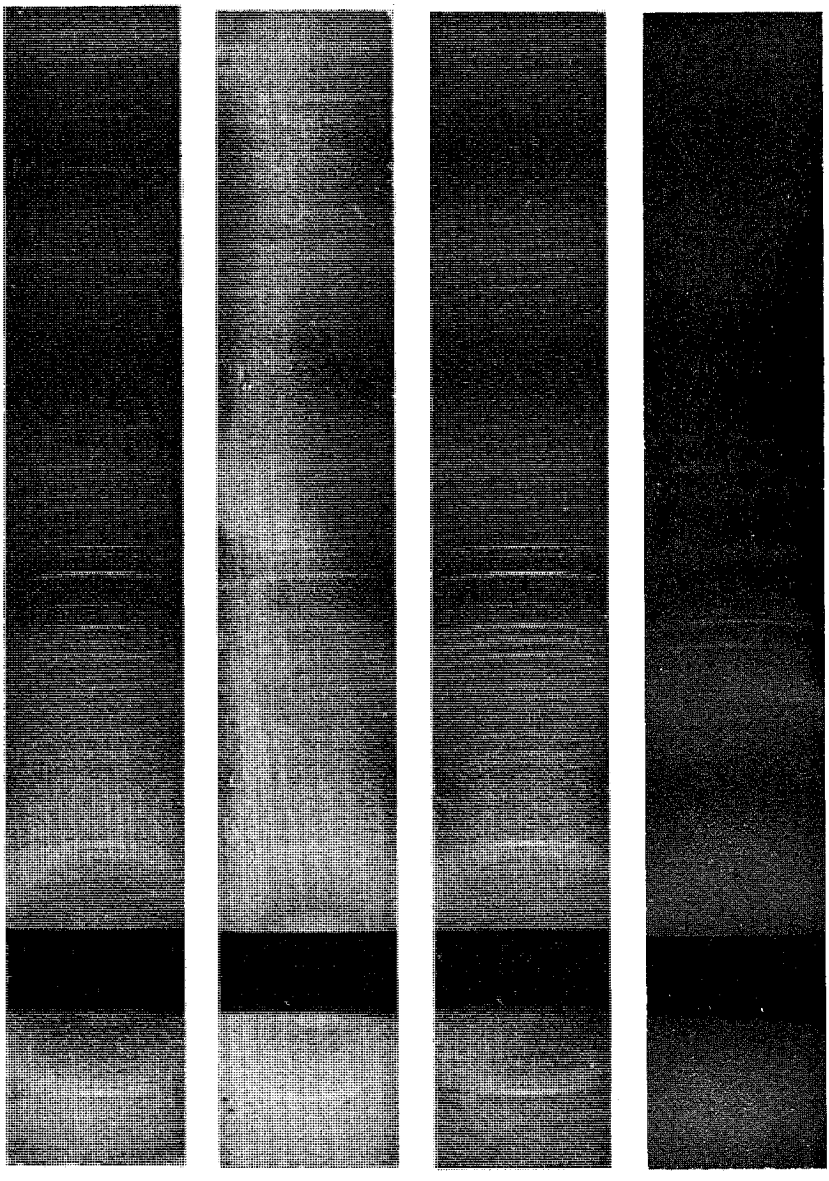
PHYSICAL PROPERTIES

Optical Properties

Optical properties of each sample were measured with a petrographic microscope and a four-axis universal stage. Index of refraction for α, β, and γ was determined, pleochroic colors described, the 2V angle and $C \wedge Z$ were measured.

Mineral fragments, 100 mesh or smaller, were sprinkled on a moistened gelatin-coated slide which held the fragments securely in many orientations, allowing one to choose a suitably oriented fragment with which to work. Fragments which gave an optic axis centered interference figure were used in finding and measuring the index of the β ray. Pleochroic colors were also noted. Several fragments were measured and an average value calculated in each case. Fragments which had the highest birefringence and showed flash interference figures were used to measure α and γ. The index of the γ ray (negative mineral) could be measured with the cleavage of the fragments essentially parallel to the north-south direction of the microscope and α could be measured with

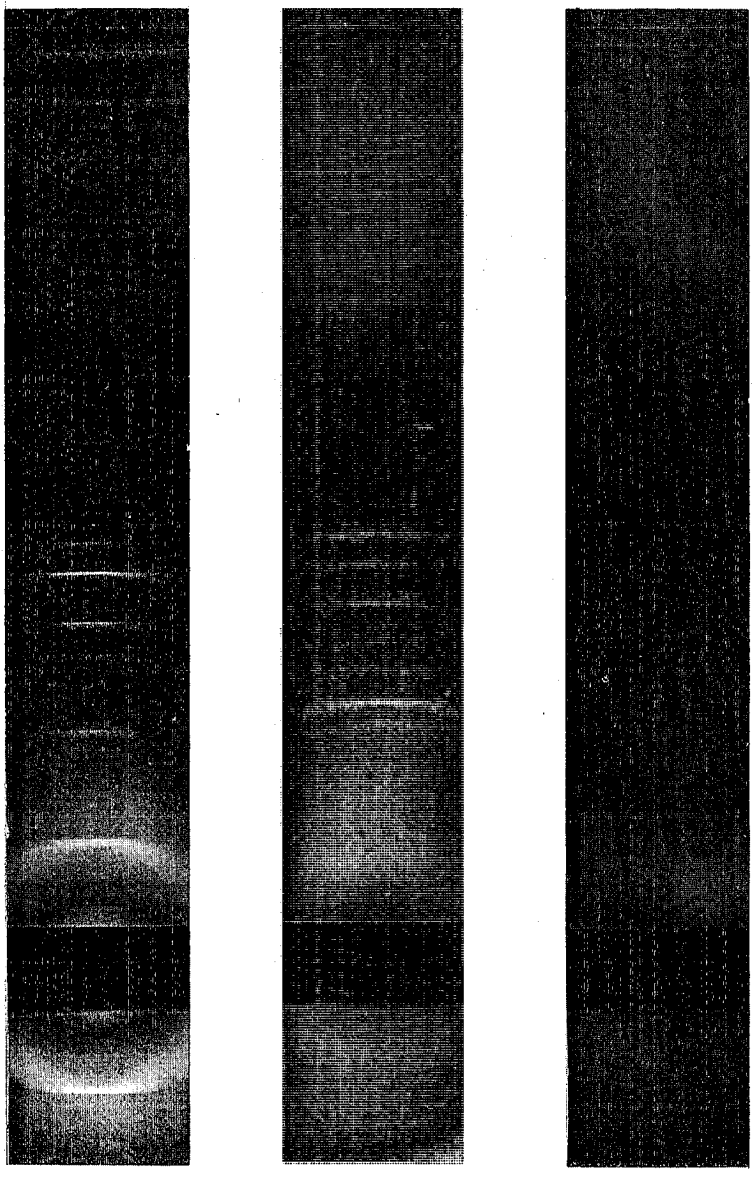
PLATE 1 — HAROLD KAUFMANN



EXPLANATION OF PLATE 1

X-RAY POWDER PATTERNS OF SAMPLE 10

FIG. 1. Pattern of sample taken at 25° C.
FIG. 2. Pattern of same sample taken after heating to 800° C.
FIG. 3. Pattern of same sample taken after heating to 950° C.
Pattern of same sample taken after heating to 1100° C.



1 2 3

EXPLANATION OF PLATE 2

X-RAY POWDER PATTERNS OF SAMPLE 18

FIG. 1. Pattern of sample taken at 25° C.
FIG. 2. Pattern of same sample taken after heating to 950° C.
FIG. 3. Pattern of same sample taken after heating to 1100° C.

the fragment in an east-west position. The pleochroic colors were noted in these position.

Indices of refraction were measured by index oils using standard techniques. The mineral was bracketed with a higher and lower index oil and an average value determined. White light and central illumination were used. When cleavages, dark color, or fine-grained size made the becke line indistinct oblique illumination was used to make the fragment more conspicuous. Indices of refraction of the oils were measured with an Abbe refractometer, using a sodium vapor light source. The upper limit of the refractometer was 1.70. Oils with a higher index are recorded as labelled on the container, followed by a question mark in table 6. These values are probably too high since checked values of oils less than 1.70 were slightly too high.

The 2V angle was easily measured on sectioned fragments mounted in balsam with the 110 cleavage almost perpendicular to the slide. The 2V angles were plotted on a stereographic net and angles calculated from the net. Samples number 7 and 10 were so highly colored that they were almost opaque and the values given are only approximations. Angles from several fragments were measured and an average value determined. The angle between the acute bisectrix and the cleavage normal (C∧Z in all except sample 10) could be measured easily because of the prominent 110 cleavage in amphibole minerals. A universal stage was used for measurements.

The indices of refraction measurements are the least satisfactory of the optical measurements because the deep colors, strong absorption, dispersion, cleavages and fine-grained size make the becke line very difficult to observe. The results may be no better than ±.005 for the most intensely colored of the specimens. Table 6 summarizes observed optical values.

TABLE 6

Observed optical properties

Sample No.	*Indices*	*Birefringence*	*Pleochroism*	*2V angle*	*C Z*
1.	α = 1.598		light yellow		
	β = 1.625		very light pink		
	γ = 1.627	.029	colorless to light pink	84° (—)	—15°
2.	α = 1.621		very pale green to pink		
	β = 1.651		pale green		
	γ = 1.657	.036	medium blue-green	86° (—)	—15°
6.	α = 1.621		light yellow-green		
	β = 1.628		pale yellow-green to colorless		
	γ = 1.643	.022	pale green	86° (+)	—22°
7.	α = 1.654		very dark green		
	β = 1.701 ?		medium brown-green		
	γ = 1.720 ?	.066 ?	dark green	74° (—)	—16°
8.	α = 1.609		pale reddish-brown		
	β = 1.632		colorless to pale yellow		
	γ = 1.634	.025	light yellow-brown	88° (—)	—15°
10.	α = 1.693		medium blue-green		
	β = 1.696		dark blue-green		C∧Z
	γ = 1.730 ?	.037 ?	dark blue-green	40° ? (+)	+27 ?
13.	α = 1.629		light yellow-green		
	β = 1.650		pale green		C∧Z
	γ = 1.654	.025	medium green	88° (+ & —)	—17°

TABLE 6 (CONT.)

18.	α = 1.636		light blue-green		
	β = 1.649		pale green		
	γ = 1.662	.026	medium blue-green	86° (—)	—14°
19.	α = 1.626		pale yellow-blue		
	β = 1.643		colorless to pale yellow		
	γ = 1.671	.045	colorless to pale yellow-blue	84° (+)	—16°
20.	α = 1.621		very light yellow		
	β = 1.640		colorless		
	γ = 1.704 ?	.083 ?	pale pink	78° (+)	—4°

Fe^{2+} and Fe^{3+} seem to cause the greatest change in optical properties. This effect may be observed in a comparison of samples 1, 2, 7, and 10. Increasing Fe^{2+} and Fe^{3+}, with decreasing Mg^{2+} cause the mineral to have a blacker hand sample color, darker pleochroic colors, more opacity, higher index of refraction and smaller 2V angle. Sample 6 has a high percentage of F^- which may account for the large $C \wedge Z$. The optical properties of sample 20 are quite different from those of sample 1 although both show very similar chemical analysis. This difference must be due to the fiberous habit of sample 20. Neither the number of atoms of Si^{4+} replaced in the tetrahedral position nor the number of alkali atoms present in position "A" seem to show any observable effect upon optical properties.

X-Ray Photographs

X-ray diffraction powder photographs of each specimen were taken on a General Electric XRD-1 x-ray machine. The camera used had an eight centimeter radius and rotated the sample 360°. The mineral sample was ground in an agate mortar until fine enough to pass through a 325 mesh screen and then packed into a capillary tube with a diameter of 0.05 millimeters. Samples 1, 2 and 13, however, gave so much fluorescence that it was necessary to use a 0.02 millimeter diameter capillary tube to produce a usable photograph. Photographs were taken using iron radiation, with a $K\alpha_1$ wave length of 1.93597Å, and a manganese filter. Each photograph was exposed 2.75 hours at eleven milliampers and 30,000 volts. Spacing of each line on the film was measured by a vernier scale on a Flourline illuminated screen. Intensity of each line was estimated visually. Values are given in table 7. Repeated measurement showed the line spacing could be reproduced within 0.02 millimeters. The 002 line and 110 line were indexed by comparison to known powder patterns.

The expected increase in cell size with increase of Al^{3+} in the tetrahedral sites can not be observed in the x-ray powder patterns from these analysed samples; however, they seem to show a decrease in cell size with increase of trivalent ions in octahedral sites. A decrease in Ca^{2+} in cubic sites may also decrease cell size but the range of Ca^{2+} variation in these samples is insufficient for a good comparison. Any other relationships between chemical analysis and x-ray data are vague.

Another value of these x-ray powder photographs is to make available the patterns of several chemically analyzed amphiboles. Only six powder patterns of amphibole species could be found in the A.S.T.M. card file.

TABLE 7

X-ray powder patterns of Amphibole species

Line	*Sample No. 1*		*Sample No. 2*		*Sample No. 6*		*Sample No. 7*		*Sample No. 8*	
	d Å	I/I_0	*d Å*	I/I_0	*d Å*	I/I_0	*d Å*	I/I_0	*d Å*	I/I_0
1	1.5022	5	1.4333	25	1.5022	2	1.5097	1	1.4355	40
2	1.5103	5	1.4678	1	1.5122	2	1.5244	3	1.4997	5
3	1.5302	3	1.5009	3	1.5765	5	1.5401	1	1.5103	5
4	1.5751	8	1.5122	3	1.6159	1	1.5886	10	1.5289	1
5	1.6159	3	1.5276	3	1.6500	5	1.6235	1	1.5751	5
6	1.6476	10	1.5765	10	1.6843	1	1.6540	2	1.5966	1
7	1.6826	3	1.6182	1	1.8411	1	2.0209	1	1.6129	1
8	1.8622	3	1.6468	10	1.8654	1	2.0511	1	1.6484	5
9	1.8882	3	1.6851	1	1.8971	1	2.1679	20	1.6826	1
10	2.0118	5	1.7417	1	2.0183	3	2.2956	1	1.8600	1
11	2.0431	5	1.8622	1	2.0431	1	2.3468	20	1.8871	1
12	2.1588	15	1.8871	1	2.0458	1	†2.5531	50	2.0106	2
13	2.2734	3	2.0118	5	2.1588	10	2.6043	40	2.0391	1
14	2.2939	3	2.0405	3	2.2836	1	2.7184	100	2.1558	5
15	2.3182	3	2.1573	20	2.2991	1	2.8140	1	2.2718	1
16	2.3324	15	2.2904	1	2.3432	10	2.9493	5	2.3324	8
17	†2.5316	30	2.3112	1	2.3698	20	3.1257	80	†2.5252	50
18	2.5941	10	2.3289	15	†2.5337	40	3.2846	5	2.5862	10
19	2.7035	100	†2.5273	40	2.5930	20	3.3962	50	2.6962	100
20	2.9375	20	2.5685	80	2.7035	100	4.5366	1	2.7927	1
21	3.0992	80	2.5315	25	2.7410	1	4.9058	1	3.1058	100
22	3.2661	20	2.6624	30	2.8087	1	*8.3965	100	3.2588	10
23	3.3843	40	2.7060	100	2.9375	30			3.3725	40
24	3.8608	8	2.7980	1	3.1291	60			3.6684	20
25	4.5150	10	2.9316	40	3.3752	50			3.8713	5
26	4.8804	10	3.3725	60	3.8818	2			4.4864	5
27	5.0913	3	3.8608	5	4.5150	2			4.8720	5
28	5.3622	12	4.4935	5	4.8973	2			5.0549	2
29	*8.3713	60	4.8553	5	*8.4730	50			*8.3463	50
30	9.0501	30	5.0731	1	9.0796	8			0.0796	20
31			*8.2967	80						
32			8.4473	5						

* = 110 plane
† = 002 plane

Line	*Sample No. 10*		*Sample No. 13*		*Sample No. 18*		*Sample No. 19*		*Sample No. 20*	
	d Å	I/I_0	*d Å*	I/I_0	*d Å*	I/I_0	*d Å*	I/I_0	*d Å*	I/I_0
1	1.2893	30	1.4388	25	1.3595	25	1.4284	60	1.4361	60
2	1.3398	10	1.5028	10	1.3955	1	1.4466	2	1.4696	1
3	1.3733	8	1.5148	10	1.4306	35	1.4661	2	1.5022	1
4	1.4172	20	1.5342	1	1.4534	1	1.4941	2	1.5103	8
5	1.4608	1	1.5807	15	1.4677	1	1.5135	10	1.5329	1
6	1.4960	2	1.6174	1	1.5022	1	1.5475	2	1.5744	15
7	1.5097	5	1.6492	15	1.5148	5	1.5758	20	1.6159	1
8	1.5822	8	1.6868	1	1.5276	1	1.5996	10	1.6476	8
9	1.6047	8	1.7437	1	1.5793	30	1.6062	2	1.6843	2
10	1.6460	40	1.8654	1	1.6137	1	1.6243	2	1.8600	1

TABLE 7 (CONT.)

11	1.6893	1	1.8904	1	1.6445	25	1.6366	40	1.8882	1
12	1.7142	1	2.0170	10	1.7428	1	1.7373	5	2.0118	2
13	1.7186	1	2.0484	1	1.8611	1	1.7957	5	2.0405	1
14	1.7879	1	2.1603	30	2.0118	8	1.8547	5	2.1558	10
15	1.8516	1	2.2819	1	2.1528	15	1.8762	5	2.2768	1
16	2.0106	3	2.3360	20	2.2768	1	1.9866	2	2.2939	1
17	2.0578	2	2.5337	50	2.3324	10	1.9991	2	2.3324	10
18	2.1499	40	2.5930	40	†2.5316	40	2.0352	2	†2.5252	70
19	2.2435	2	2.7035	100	2.5795	15	2.0796	20	2.6816	5
20	2.2991	3	2.8033	5	2.6937	100	2.1410	35	2.6962	100
21	†2.5104	50	2.9375	40	3.1058	80	2.2734	2	2.8033	1
22	2.5729	3	3.1191	90	3.2478	2	2.3235	35	2.9258	20
23	2.6889	100	3.2661	40	3.3725	20	†2.5337	70	3.1091	80
24	2.9493	1	3.3882	50	3.6684	15	2.6864	100	3.2551	5
25	3.0570	70	3.8765	1	3.8871	1	2.7720	2	3.3607	40
26	3.2155	1	4.5150	3	4.5078	2	2.9142	30	3.8765	1
27	3.3607	20	4.9058	5	4.8973	2	3.0828	90	4.4794	3
28	3.8197	1	*8.3463	80	*8.4219	50	3.2370	25	4.8636	3
29	4.4030	25	9.0208	5	8.5771	3	3.3491	40	*8.5247	30
30	7.9655	90					3.8608	2	9.0796	3
31	*8.2967	80					4.4513	2		
32							4.8636	2		
33							*8.2234	50		
34							8.9629	8		

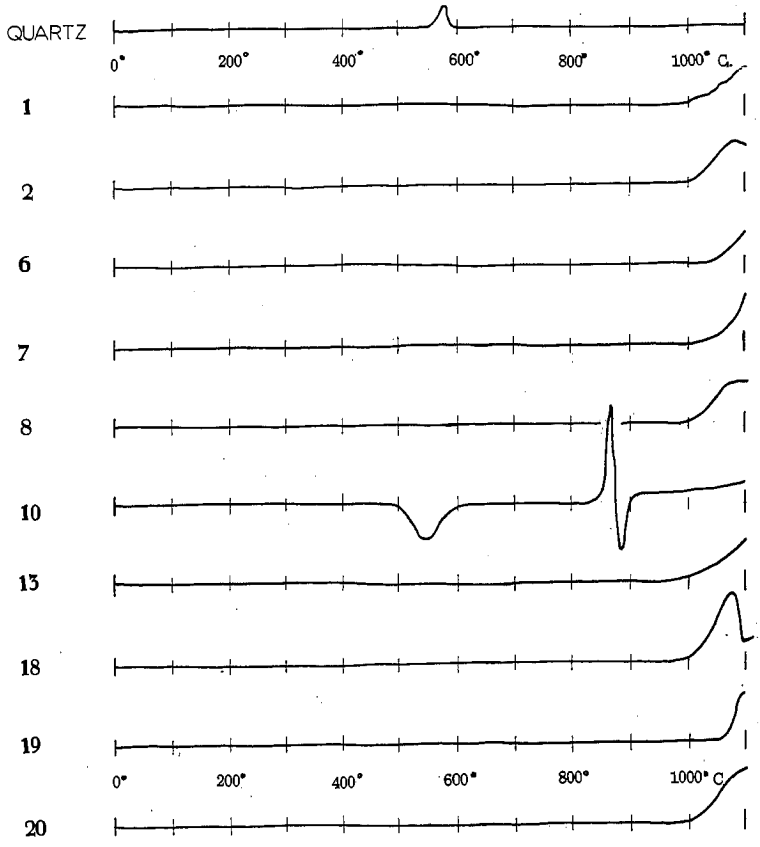
* = 110 plane
† = 002 plane

Differential Thermal Analyses

Equipment used consisted of a Hoskins electric furnace capable of producing temperatures up to 1100°C, controlled by a continuously variable autotransformer made by General Radio. A thermocouple recorded the temperature of the furnace through a Leeds and Northrup Micromax. A differential thermocouple, consisting of two chromel wires connected by an alumel wire, recorded the differential temperature between the mineral sample and pure Al_2O_3 through a six channel Minneapolis Honeywell recorder. The mineral sample was ground fine enough to pass through a 100 mesh screen, then packed tightly into a cavity, $\frac{1}{4}$ inch by $\frac{3}{4}$ inch, in the heating block. Quartz was simultaneously run for control and comparison. The variac was adjusted so that it required two hours to raise the temperature from 20° to 1100°C. Repeated heating of one sample indicated the position of the peak with respect to the temperature was reproducable within 10°C, but, amplitude of the peak was variable.

Only two of the ten samples, 10 and 18, show a complete endothermic reaction below 1100°C. Only sample 10 shows an exothermic reaction below 1100°C, a broad curve at 550°C and a sharp peak at 890°C. The other specimens have endothermic reactions above 1100°C (Text-fig. 8).

X-ray diffraction powder photographs of samples 10, and 18 were taken before and after the endothermic reactions. Several samples were analyzed for percent of FeO and Fe_2O_3 at various temperatures, to determine causes of endothermic reactions. Table 9 shows oxidation takes place gradually throughout the heating at least at the heating rate used in these tests.



TEXT-FIGURE 8. —Differential thermal curves of studied amphiboles.

TABLE 8

X-ray powder patterns of samples 10 and 18 at higher temperatures

Line	*Sample No. 18 at 950°C*		*Sample No. 18 at 1100°C*		*Sample No. 10 at 800°C*		*Sample No. 10 at 950°C*		*Sample No. 10 at 1100°C*	
	d Å	*I/I₀*	*d Å*	*I/I₀*	*d Å*	*I/I₀*	*d Å*	*I/I₀*	*d Å*	*I/I₀*
1	1.4268	30	1.4099	1	1.2799	20	1.4528	10	1.2603	10
2	1.5122	2	1.4637	1	1.3336	15	1.4826	10	1.3100	10
3	1.5772	20	1.6197	1	1.3647	2	1.6910	20	1.4540	40
4	1.6382	5	1.7400	1	1.4062	2	1.8349	10	1.4856	30
5	1.6859	1	2.0299	5	1.4899	2	2.2003	5	1.6935	50
6	1.8632	1	2.1263	10	1.5028	2	2.5104	55	1.8432	20
7	2.0055	1	2.2209	1	1.5556	2	2.6816	50	2.5104	30
8	2.1484	2	2.5295	30	1.5765	2	2.8913	5	2.6986	30
9	2.2751	2	2.9084	25	1.6382	10	2.9762	40		
10	2.2973	1	2.9884	80	2.1410	40	3.3260	5		

TABLE 8 (CONT.)

11	2.3289	10	3.1908	50	2.5038	25	3.6637	5
12	2.5316	80	3.7062	5	2.6913	100	4.0696	60
13	2.5862	40	4.0238	5	3.0538	50		
14	2.6365	2			3.3491	30		
15	2.6937	100			4.4305	5		
16	3.0861	70			8.1993	80		
17	3.2551	2						
18	3.3725	50						
19	3.8818	3						
20	4.0523	2						
21	4.5150	3						
22	4.8804	2						
23	8.3214	90						
24	9.1994	3						

TABLE 9

Percentages of FeO vs. Fe_2O_3 at selected temperatures to determine degree of oxidation

Sample	*Percent*	
No. 10	*FeO*	*Fe_2O_3*
@ 450°C	16.94	13.99
@ 630°C	7.17	25.47
@ 930°C	1.07	32.86
No. 18		
@ 700°C	8.22	2.34
@ 900°C	3.78	7.12
@ 1100°C	0.70	11.84

Plates 1 and 2 shows x-ray diffraction patterns before and after reaction. It can be seen that there has been a structural change but not a complete breakdown of the structure in sample 10 even though it was heated until fused, at a temperature less than 1100°C. Thus the reaction seems to be due essentially to structural change and not to oxidation of Fe^{2+} to Fe^{3+}.

Chemical analyses do not show exactly what determines the ease of the endothermic-exothermic reactions. Anaylses seem to indicate that low concentration of Ca^{2+} and high concentrations of Na^{+} and K^{+} may lower the temperature at which the reactions take place.

Works by Wittels (1952) and Korzhinskii (1961) indicate dehydration products of amphiboles may contain various mixtures of two or more of the following products depending upon the variety of the amphibole: magnetite, maghemite, olivine, plagioclase, glass, several varieties of pyroxene, cristobalite, hematite, and water.

Chemical Analyses

The ten amphibole samples were analyzed at the Pennsylvania Experiment Station by C.O. Ingamells (See Tables 10-18). It was hoped that chemical composition could be related to physical properties, but only Fe^{2+} and Fe^{3+}

seem to show any possible correlation in these ten samples. Ten samples may be too few to permit any visible trends.

As in most amphibole analysis, it can be seen that the number of OH^- ions is variable, sometimes more than two and sometimes less than two. Except for samples 7 and 20, there is an excess of positive ions when there are more than 2 OH^- ions and a deficiency of positive ions when there are less than 2 OH^- ions. Samples 13 and 6, which are very deficient in OH^- ions, were reported to probably contain Cl^- ions but were not analyzed for Cl^-.

BaO and SrO were reported not present in appreciable amounts. Sample 2 was reported to contain B_2O_3. This was probably an impurity and may explain the deficiency of ions in the octahedral and cubic sites. ZrO_2 was reported as present and included with the Al_2O_3. It was probably present as an impurity.

SUMMARY AND CONCLUSIONS

Ten amphibole samples were analyzed chemically and their sturctural composition calculated to determine how well they fit the classification developed in this paper. They correlated well as is shown by their name and number.

Optical, X-ray, and DTA properties of these ten samples were determined in an attempt to relate physical properties to chemical composition. Fe^{2+} and Fe^{3+} gave the mineral higher refractive index, smaller 2V angle, and darker pleochroic colors. Fluoride ions seem to increase C∧Z. Neither replacement of Si^{4+} in tetrahedral sites, nor introduction of alkali ions in position "A" have any effect upon optical properties. Substitution of Al^{3+} for Si^{4+} in tetrahedral coordination did not give a larger cell size as can be seen from the X-ray patterns, but, an increase of trivalent ions in octahedral sites and a decrease of Ca^{2+} in cubic sites cause the species to show a smaller cell size. DTA curves show oxidation and hydration take place gradually all along the heating curve. The structure does not break down, up to temperatures of 1100°C, but, there is a shift of X-ray lines. A decrease in the amount of Ca^{2+} present and an increase of Na^+ and K^+ lower the temperature at which the endothermic reaction takes place.

Only six powder patterns of amphibole species are in the ASTM card file. Now ten more powder patterns of chemically analyzed species are available. Also, X-ray patterns are included which show a shift in the structure as the mineral is heated. DTA curves are now available for analysed amphibole minerals showing an endothermic reaction due to structure change that, for most amphiboles, takes place above 1100°C. The relationship between valence, chemical composition, and structural position can now be clearly shown by use of the number system developed in this paper.

The current study indicated there is not enough correlation between chemical composition and physical properties to be useful in a definitive classification. If a larger number of samples were analyzed, however, some meaningful trends may appear which would be useful in defining the many variables now operating. Any future advances in a method to give reasonably good chemical analysis much more quickly and less expensively would be very helpful, even necessary, for the greatest usefulness of this classification. At the present time good chemical analyses cost about $125.00 per sample and require months for a complete analysis. If emission spectroscopy or X-ray fluorescence could give more quantitative results minerals could be analyzed much more rapidly and the proposed classification made more useful.

TABLE 10

Analytical data and structural composition of sample 1

Oxide	*Chem. anal. wt. %*	×	*Correction*		*Recalculated to 100%*	÷	*Molecular weight*	=	*Relative No. of oxide molecules*		*Oxygen ions*
SiO_2	58.60	X	1.0008	=	58.65	÷	60.06	=	.9752	X 2	1.9508
Al_2O_3	.52		"		0.52		101.94		.0051	X 3	.0153
Fe_2O_3							159.68				
TiO_2	.04		"		0.04		79.90		.0005	X 2	.0010
V_2O_5							181.90				
Cr_2O_3							152.02				
FeO	.22		"		0.22		71.84		.0031		.0031
NiO							74.71				
MnO	.50		"		0.52		70.93		.0073		.0073
MgO	24.66		"		24.68		40.32		.6121		.6121
Li_2O	.06		"		0.06		29.88		.0020		.0020
CaO	12.26		"		12.27		56.08		.2188		.2188
Na_2O	.73		"		0.70		61.99		.0113		.0113
K_2O	.16		"		0.16		94.19		.0017		.0017
H_2O^-	.01		"		0.01		18.02		.0006		.0006
H_2O^+	1.89		"		1.89		18.02		.1048		.1048
F	.42		"		0.42		19.00		.0221		.0221
P_2O_5	.01		"		0.01		141.95		.0001		.0001
	100.08										2.9510
O=F	.16				24	=	8.130	=	ratio needed for one-half unit cell		
					2.9510						
Total	99.92										

Cations	*Relative No. of oxide molecules*	*Ratio*			*Ions per 24 anions*		
Si^{4+}	.9754	X 8.13	X 1	=	7.93	]	
Al^{3+}	.0051	"	X 2		0.04	]	7.974
Ti^{4+}	.0005	"	X 1		0.004	=	
Mg^{2+}	.6121	"	X 1		4.98	]	4.98
Fe^{2+}	.0031	"	X 1		0.03	]	
Mn^{2+}	.0073	"	X 1		0.06	]	
Ca^{2+}	.2188	"	X 1		1.78	]	
						]	1.993
Li^{1+}	.0002	"	X 2		0.003	]	
Na^{1+}	.0113	"	X 2		0.09	]	
K^{1+}	.0017	"	X 2		0.03	]	
OH^-	.1048	"	X 2		1.70	]	
						]	1.88
F^-	.0221	"	X 1		0.18	]	

Composition Number = 0.044, 0, 0, 1oo, 0.12, 1o, 1, 0, 0, 1.82
Name - Tremolite

TABLE 11

Analytical data and structural composition of sample 2

Oxide	*Chem. anal. wt. %*	× *Correction*	*Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	55.60	X 1.0003 =	55.62	60.06	.9261 X 2	1.8522
Al_2O_3	2.41	"	2.41	101.94	.0236 X 3	.0708
Fe_2O_3	1.55	"	1.55	159.68	.0097 X 3	.0291
TiO_2				79.90		
V_2O_5	.02	"	0.02	181.90	.0001 X 5	.0005
Cr_2O_3	.27	"	0.27	152.02	.0017 X 3	.0051
FeO	4.81	"	4.81	71.84	.0670	.0670
NiO	.17	"	0.17	74.71	.0023	.0023
MnO	.32	"	0.32	70.93	.0045	.0045
MgO	20.31	"	20.32	40.32	.5040	.5040
Li_2O	.01	"	0.01	29.88	.0003	.0003
CaO	11.90	"	11.90	56.08	.2122	.2122
Na_2O	.55	"	0.55	61.99	.0089	.0089
K_2O	.07	"	0.07	94.19	.0008	.0008
H_2O^-				18.02		
H_2O^+	1.92	"	1.92	18.02	.1065	.1065
F^-	.11	"	0.11	19.00	.0058	.0058
P_2O_5				141.95		
	100.02					2.8700
O=F	.05					
Total	99.97					

$\frac{24}{2.8700} = 8.36$ ratio needed for one-half unit cell

Note: analyst reported some Zn_2^+ present

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.9261	X 8.36	X 1	7.74	0.26	8.00
Al^{3+}	.0236	"	X 2	0.395	0.13	
Fe^{3+}	.0097	"	X 2	0.13		4.96
Cr^{3+}	.0017	"	X 2	0.03		
Mg^{2}	.5040	"	X 1	4.21		
Fe^{2+}	.0670	"	X 1	0.56		
Mn^{2+}	.0045	"	X 1	0.04		
Ni^{2+}	.0023	"	X 1	0.02		
Li^{1+}	.0003	"	X 2	0.004		1.994
Ca^{2+}	.2122	"	X 1	1.77		
Na^{1+}	.0089	"	X 2	0.15		
K^{1+}	.0008	"	X 2	0.01		
OH^-	.1065	"	X 2	1.78		1.83
F^-	.0058	"	X 1	0.05		

Composition Number = 0.26, 0.16, 5, 1oo, 0.16, 1o, 1, 0, 0, 1.95
Name - Grammatite

TABLE 12

Analytical data and structural composition of sample 6

Oxide	*Chem. anal. wt. %*	× *Correction*	= *Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	53.23	× 1.0042	= 53.45	60.06	.8899 × 2	1.7798
Al_2O_3	3.62	"	3.64	101.94	.0357 × 3	.1071
Fe_2O_3	1.92	"	1.93	159.68	.0123 × 3	.0369
TiO_2	.15	"	0.15	79.90	.0019 × 2	.0038
V_2O_5				181.90		
Cr_2O_3				152.02		
FeO	2.59	"	2.60	71.84	.0362	.0362
NiO				74.71		
MnO	.20	"	0.20	70.93	.0028	.0028
MgO	21.17	"	21.26	40.32	.5273	.5273
Li_2O	.01	"	0.01	29.88	.0003	.0003
CaO	11.74	"	11.79	56.08	.2102	.2102
Na_2O	2.12	"	2.13	61.99	.0343	.0343
K_2O	.98	"	0.98	94.19	.0104	.0104
H_2O^-				18.02		
H_2O^+	.68	"	0.68	18.02	.0377	.0377
F	2.18	"	2.19	19.00	.1153	.1153
P_2O_5				141.95		
	100.59					2.9021
O=F	1.01					
Total	99.58					

$\frac{24}{2.9021} = 8.27$ ratio needed for one-half unit cell

Note: analyst reported some Cl^- present

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.8899	× 8.27	× 1	7.36		8.00
Al^{3+}	.0357	"	× 2	0.59	.05	
Fe^{3+}	.0123	"	× 2	0.20	.15	
Ti^{4+}	.0019	"	× 1	0.02		5.005
Mg^{2+}	.5273	"	× 1	4.36		
Fe^{2+}	.0362	"	× 1	0.30		
Mn^{2+}	.0028	"	× 1	0.02		
Li^{1+}	.0003	"	× 2	0.005		
Ca^{2+}	.2102	"	× 1	1.74	.13 1.61	2.00
Na^{1+}	.0343	"	× 2	0.57	.39 .18	.35
K^{1+}	.0104	"	× 2	0.17		
OH^-	.0377	"	× 2	0.62		1.57
F^+	.1153	"	× 1	0.95		

Composition Number = 0.64, 0.17, 6, 1oo, 0.39, 1o, 1, 0.35, 2, 1.05
Name - Anophorite

TABLE 13

Analytical data and structural composition of sample 7

Oxide	*Chem. anal. wt. %*	× *Correction*	= *Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	41.03	X 1.0008	41.06	60.06	.6836 X 2	1.3672
Al_2O_3	10.82	"	10.83	101.94	.1062 X 3	.3186
Fe_2O_3	7.53	"	7.54	159.68	.0472 X 3	.1416
TiO_2	.77	"	0.77	79.90	.0096 X 2	.0192
V_2O_5	.02	"	0.02	181.90	.0001 X 5	.0005
Cr_2O_3				152.02		
FeO	16.10	"	16.11	71.84	.2242	.2242
NiO						
MnO	.97	"	0.97	70.93	.0136	.0136
MgO	7.12	"	7.13	40.32	.1768	.1768
Li_2O	.03	"	0.03	29.88	.0010	.0010
CaO	10.04	"	10.05	56.08	.1792	.1792
Na_2O	1.49	"	1.45	61.99	.0234	.0234
K_2O	1.71	"	1.71	94.19	.0185	.0185
H_2O^-	.10	"	0.10	18.02	.0055	.0055
H_2O^+	1.83	"	1.83	18.02	.1015	.1015
F	.59	"	0.51	19.00	.0270	.0270
P_2O_5	.01	"	0.01	141.95	.0000	
	100.16					2.6138
O=F	.24					
Total	99.92					

$$\frac{24}{2.6138} = 9.18$$ ratio needed for one-half unit cell

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.6836	X 9.18	X 1	6.27	1.73	8.00
Al^{3+}	.1062	"	X 2	1.95	.22	
Fe^{3+}	.0472	"	X 2	0.87		5.00
Ti^{4+}	.0096	"	X 1	0.09		
Mg^{2+}	.1768	"	X 1	1.62		
Fe^{2+}	.2242	"	X 1	2.06		
Li^{1+}	.0010	"	X 2	0.002	.05	
Mn^{2+}	.0136	"	X 1	0.12	.07	2.00
Ca^{2+}	.1792	"	X 1	1.65	.28	
Na^{1+}	.0234	"	X 2	0.43	.15	.49
K^{1+}	.0185	"	X 2	0.34		
OH^-	.1015	"	X 1	1.86		2.11
F^-	.0270	"	X 1	0.25		

Composition Number = 1.73, 1.18, 3, 200, 0.28, 10, 1, 0.49, 1, 1.75
Name - Magnesio-hastingsite

TABLE 14

Analytical data and structural composition of sample 8

Oxide	*Chem. anal. wt. %*	× *Correction*	= *Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*		*Oxygen ions*
SiO_2	57.57	X 1.0020	57.68	60.06	.9605	X 2	1.9210
Al_2O_3	1.02	"	1.02	101.94	.0100	X 3	.0300
Fe_2O_3	.70	"	0.70	159.68	.0044	X 3	.0132
TiO_2	.08	"	0.08	79.90	.0010	X 2	.0020
V_2O_5							
Cr_2O_3							
FeO	2.79	"	2.80	71.84	.0389		.0389
NiO							
MnO	.14	"	0.14	70.93	.0020		.0020
MgO	22.59	"	22.64	40.32	.5615		.5615
Li_2O	.01	"	0.01	29.88	.0004		.0004
CaO	12.34	"	12.36	56.08	.2204		.2204
Na_2O	.18	"	0.18	61.99	.0029		.0029
K_2O	.13	"	0.13	94.19	.0014		.0014
H_2O^-	.04	"	0.04	18.02	.0022		.0022
H_2O^+	2.05	"	2.05	18.02	.1138		.1138
F	.23	"	0.23	19.00	.0126		.0126
P_2O_5	.01	"	0.01	141.95	.0000		
	99.88						2.9223
O=F	.08						
Total	99.80						

$\frac{24}{2.9223} = 8.21$ ratio needed for one-half unit cell

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.9605	X 8.21	X 1	7.89		
Al^{3+}	.0100	"	X 2	0.16	.11	8.00
Fe^{3+}	.0044	"	X 2	0.07	.05	
Ti^{4+}	.0010	"	X 1	0.01		
Mg^{2+}	.5615	"	X 1	4.61		5.00
Fe^{2+}	.0389	"	X 1	0.32	.25	
Li^{1+}	.0004	"	X 2	0.006	0.7	
Ca^{2+}	.2204	"	X 1	1.81		
Na^{1+}	.0029	"	X 2	0.05		1.956
K^{1+}	.0014	"	X 2	0.02		
OH^-	.1138	"	X 2	1.87		
F^-	.0126	"	X 1	0.10		1.97

Composition Number = 0.11, 0.13, 2, 1oo, 0.08, 1o, 1, 0, 0, 1.90
Name - Mangan-tremolite

TABLE 15

Analytical data and structural composition of sample 10

Oxide	*Chem. anal. wt. %*	× *Correction*	= *Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*		*Oxygen ions*
SiO_2	50.77	X 1.0008	50.81	60.06	.8459	X 2	1.6918
Al_2O_3	2.32	"	2.32	101.94	.0228	X 3	.0684
Fe_2O_3	14.35	"	14.36	159.68	.0899	X 3	.2697
TiO_2	1.41	"	1.41	79.90	.0177	X 2	.0354
V_2O_5							
Cr_2O_3							
FeO	20.16	"	20.18	71.84	.2809		.2809
NiO							
MnO	.47	"	0.47	70.93	.0066		.0066
MgO	.07	"	0.07	40.32	.0017		.0017
Li_2O	.27	"	0.27	29.88	.0090		.0090
CaO	1.02	"	1.02	56.08	.0183		.0183
Na_2O	5.95	"	5.95	61.99	.0960		.0960
K_2O	1.27	"	1.20	94.19	.0128		.0128
H_2O^-	.03	"	0.03	18.02	.0017		.0017
H_2O^+	1.59	"	1.59	18.02	.0882		.0882
F	.40	"	0.40	19.00	.0211		.0211
P_2O_5	.01	"	0.01	141.95	.0000		
	100.09						2.6015
O=F	.17						
Total	99.92						

$\frac{24}{2.6015} = 9.23$ ratio needed for one-half unit cell

Note: analyst reported some Zn_2^+ present

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.8495	X 9.23	X 1	7.84	.16	8.00
Al^{3+}	.0228	"	X 2	0.42	.26	
Fe^{3+}	.0899	"	X 2	1.66		
Ti^{4+}	.0177	"	X 1	0.16		5.00
Mg^{2+}	.0017	"	X 1	0.02		
Fe^{2+}	.2809	"	X 1	2.59	.15	
Li^{1+}	.0090	"	X 2	0.17	0.2	
Mn^{2+}	.0066	"	X 1	0.06		2.00
Ca^{2+}	.0182	"	X 1	0.17	1.75	
Na^{1+}	.0960	"	X 2	1.77	.02	
K^{1+}	.0128	"	X 2	0.24		0.26
OH^-	.0882	"	X 2	1.63		1.82
F^-	.0211	"	X 1	0.19		

Composition Number = 0.16, 2.23, 3, 300, 1.77, 30, 1, 0.26, 1, 1.81
Name - Riebeckite

TABLE 16

Analytical data and structural composition of sample 13

Oxide	*Chem. anal. wt. %*	× *Correction*	*Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	51.44	X 1.0041 =	51.65	60.06	.8597 X 2	1.7194
Al_2O_3	5.49	"	5.51	101.94	.0541 X 3	.1623
Fe_2O_3	2.84	"	2.85	159.68	.0178 X 3	.0534
TiO_2	.95	"	0.95	79.90	.0119 X 2	.0238
V_2O_5	.05	"	0.05	181.90	.0003 X 5	.0015
Cr_2O_3						
FeO	4.97	"	4.99	71.84	.0681	.0681
NiO						
MnO	.04	"	0.04	70.93	.0005	.0005
MgO	18.75	"	18.82	40.32	.4667	.4667
Li_2O	.02	"	0.02	29.88	.0007	.0007
CaO	10.80	"	10.84	56.08	.1933	.1933
Na_2O	2.14	"	2.15	61.99	.0347	.0347
K_2O	.29	"	0.29	94.19	.0031	.0031
H_2O^-	.01	"	0.01	18.02	.0004	.0004
H_2O^+	1.68	"	1.69	18.02	.0938	.0938
F	.20	"	0.20	19.00	.0105	.0105
P_2O_5	.01	"	0.01	141.95	.0000	
	99.67					2.8322
O=F	.08					
Total	99.59					

$$\frac{24}{2.8322} = 8.47 \text{ ratio needed for one-half unit cell}$$

Note: analyst reported some Cl^- present

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.8597	X 8.47	X 1	7.28	.72	8.00
Al^{3+}	.0541	"	X 2	0.92	.20	
Fe^{3+}	.0078	"	X 2	0.30		5.005
Ti^{4+}	.0119	"	X 1	0.10		
V^{5+}	.0003	"	X 2	0.005		
Mg^{2+}	.4667	"	X 1	3.95	.35	
Fe^{2}	.0681	"	X 1	0.58	.23	
Mn^{2+}	.0005	"	X 1	0.004		2.00
Li^{1+}	.0007	"	X 2	0.01		
Ca^{2+}	.1933	"	X 1	1.63	.13	
Na^{1+}	.0347	"	X 2	0.59	.46	.51
K^{1+}	.0031	"	X 2	0.05		
OH^-	.0938	"	X 2	1.59		1.68
F^-	.0105	"	X 1	0.09		

Composition Number = 0.72, 0.60, 5, 1oo, 0.14, 4o, 1, 0.51, 3, 1.91

Name - Anophorite

TABLE 17
Analytical data and structural composition of sample 18

Oxide	*Chem. anal. wt. %*	× *Correction*	= *Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	49.53	X 1.0027	49.66	60.06	.8268 X 2	1.6536
Al_2O_3	9.92	"	9.95	101.94	.0977 X 3	.2931
Fe_2O_3	1.10	"	1.10	159.68	.0069 X 3	.0207
TiO_2	.59	"	0.50	79.90	.0063 X 2	.0126
V_2O_5	.04	"	0.04	181.90	.0002 X 5	.0010
Cr_2O_3	.06	"	0.06	152.02	.0004 X 3	.0012
FeO	10.59	"	10.62	71.84	.1478	.1478
NiO	.02	"	0.02	74.71	.0003	.0003
MnO	.26	"	0.26	70.93	.0036	.0036
MgO	14.64	"	14.68	40.32	.3641	.3641
Li_2O	.01	"	0.01	29.88	.0003	.0003
CaO	9.75	"	9.78	56.08	.1744	.1744
Na_2O	1.01	"	1.01	61.99	.0163	.0163
K_2O	.17	"	0.17	94.19	.0018	.0018
H_2O^-						
H_2O^+	2.00	"	2.01	18.02	.1115	.1115
F	.01	"	0.01	19.00	.0005	.0005
P_2O_5	.03	"	0.03	141.95	.0002 X 5	.0010
	99.73					2.8038
O=F	.00					
Total	99.73					

$$\frac{24}{2.8038} = 8.56$$ ratio needed for one-half unit cell

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.8268	X 8.56	X 1	7.08	.92	8.00
Al^{3+}	.0977	"	X 2	1.67	.75	
Fe^{3+}	.0069	"	X 2	0.12		
Ti^{4+}	.0063	"	X 1	0.05		
V^{5+}	.0002	"	X 2	0.003		5.00
Cr^{3+}	.0004	"	X 2	0.006		
Mg^{2+}	.3641	"	X 1	3.12	.90	
Fe^{2+}	.1478	"	X 1	1.27	.37	
Ni^{2+}	.0003	"	X 1	0.003		
Mn^{2+}	.0036	"	X 1	0.03		2.00
Li^{1+}	.0003	"	X 2	0.005		
Ca^{2+}	.1744	"	X 1	1.49	.10	
Na^{1+}	.0163	"	X 2	0.28	.18	
K^{1+}	.0018	"	X 2	0.03		.21
OH^-	.1115	"	X 2	1.91		
F^-	.0004	"	X 1	0.004		1.91

Composition Number = 0.92, 0.92, 1, 2oo, 0.10, 7i, 1, 0.21, 3, 2
Name - Phillipstadite

TABLE 18

Analytical data and structural composition of sample 19

Oxide	*Chem. anal. wt. %*	× *Correction*	*Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	45.34	X 1.0011 =	45.39	60.06	.7557 X 2	1.5114
Al_2O_3	18.66	"	18.68	101.94	.1832 X 3	.5496
Fe_2O_3	.41	"	0.41	159.68	.0026 X 3	.0078
TiO_2	.02	"	0.02	79.70	.0003 X 2	.0006
V_2O_5						
Cr_2O_3	.22	"	0.22	152.02	.0014 X 3	.0042
FeO	3.14	"	3.14	71.84	.0437	.0437
NiO	.11	"	0.11	74.71	.0015	.0015
MnO	.06	"	0.06	70.93	.0008	.0008
MgO	16.36	"	16.38	40.32	.4062	.4062
Li_2O	.01	"	0.01	29.88	.0003	.0003
CaO	12.21	"	12.22	56.08	.2179	.2179
Na_2O	1.19	"	1.19	61.98	.0192	.0192
K_2O	.16	"	0.16	94.19	.0017	.0017
H_2O^-						
H_2O^+	1.99	"	1.99	18.02	.1104	.1104
F						
P_2O_5	.01	"	0.01	141.95	.0000	
	99.89					2.8733
O=F	.00					
Total	99.89					

$\frac{24}{2.8733} = 8.35$ ratio needed for one-half unit cell

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*		
Si^{4+}	.7557	X 8.35	X 1	6.31	1.69	8.00
Al^{3+}	.1832	"	X 2	3.06	1.37	
Fe^{3+}	.0026	"	X 2	0.04		5.006
Ti^{4+}	.0003	"	X 1	0.003		
Cr^{3+}	.0014	"	X 2	0.02		
Mg^{2+}	.4062	"	X 1	3.39	.18	
Fe^{2+}	.0437	"	X 1	0.36	.18	
Mn^{2+}	.0008	"	X 1	0.007		2.002
Li^{1+}	.0003	"	X 2	0.005		
Ni^{2+}	.0015	"	X 1	0.01		
Ca^{2+}	.2179	"	X 1	1.82	1.80	
Na^{1+}	.0192	"	X.2	0.32	.02	
K^{1+}	.0017	"	X 2	0.03		.37
OH^-	.1104	"	X 2	1.84		1.84

Composition Number = 1.69, 141, 1, 1oo, 0, 4o, 4, 0.37, 3, 2
Name - Girnarite

TABLE 19
Analytical data and structural composition of sample 20

Oxide	*Chem. anal. wt. %*	× *Correction*	*Recalculated to 100%*	÷ *Molecular weight*	= *Relative No. of oxide molecules*	*Oxygen ions*
SiO_2	59.92	× 1.0014	= 60.00	60.06	.9990 × 2	1.9980
Al_2O_3						
Fe_2O_3						
TiO_2						
V_2O_5						
Cr_2O_3						
FeO	.08	"	0.80	71.84	.0111	.0111
NiO						
MnO	.03	"	0.03	70.93	.0004	.0004
MgO	24.36	"	24.39	40.32	.6049	.6049
Li_2O	.01	"	0.01	29.88	.0003	.0003
CaO	13.38	"	13.40	56.08	.2389	.2389
Na_2O	.12	"	0.12	61.98	.0019	.0019
K_2O	.02	"	0.02	94.19	.0002	.0002
H_2O^-						
H_2O^+	2.19	"	2.19	18.02	.1210	.1210
F	.05	"	0.05	19.00	.0263	.0263
P_2O_5						
	99.88					3.0030
O=F	.02					
Total	99.86					

$$\frac{24}{3.0030} = 7.99$$ ratio needed for one-half unit cell

Cations	*Relative No. of oxide molecules*	*Ratio*		*Ions per 24 anions*	
Si^{4+}	.9990	× 7.99	× 1	7.98	7.98
Mg^{2+}	.6049	"	× 1	4.83	
Fe^{2+}	.0111	"	× 1	0.09	4.93
Mn^{2+}	.0004	"	× 1	0.003	
Li^{1+}	.0003	"	× 2	0.005	
Ca^{2+}	.2389	"	× 1	1.91	
Na^{1+}	.0019	"	× 2	0.03	1.94
K^{1+}	.0002	"	× 2	0.003	
OH^-	.1210	"	× 2	1.93	2.14
F^-	.0263	"	× 1	0.21	

Composition Number = 0, 0, 0, 1oo, 0.03, 1o, 1, 0, 0, 1.79
Name - Tremolite

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