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CLINOAMPHIBOLE REGRESSION STUDIES.
I. REGRESSIONS OF OPTICAL PROPERTIES AND DENSITY ON COMPOSITION

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ABSTRACT

Linear regression coefficients for five physical properties (refractive indices n_x, n_y, n_z; extinction angle Z/c; and density G) on 24 variables of chemical composition $(K,Na,Ca)_w(K,Na,Ca,Mn,Fe^{2+},Mg)_2(Ca,Mn,Fe^{2+},Mg,Ti,\ Fe^{3+},Al)_5(Ti,Fe^{3+},Al,Si)_8O_{22}(O,OH,F,H_2O)_2$ have been calculated by least-squares methods from data on about 400 analyses selected from the literature. These regressions yield high values for their coefficients of determination R^2 and variance ratio F, showing that they do empirically account for most of the variance.

Direct application of the present equations leads to preliminary predictions of the properties of a few interesting compositions in the clinoamphibole system, as follows: For tremolite $CaMg_5Si_8O_{22}(OH)_2$, $n_x=1.6005\pm.0012$, $n_y=1.6146\pm.0015$, $n_z=1.6266\pm.0017$, $Z/c=16.3°\pm1.7°$, $G=2.974\pm.014$. For tschermakite $Ca_2Mg_3Al_2Si_6Al_2O_{22}(OH)_2$ the same properties are 1.6259, 1.6362, 1.6460, 0.7°, and 3.068. For pargasite $NaCa_2Mg_4AlSi_6Al_2O_{22}(OH)_2$, they are 1.6253, 1.6319, 1.6408, 14.0°, 3.086. For hastingsite $NaCa_2Fe^{2+}{}_4Fe^{3+}Si_6Al_2O_{22}(OH)_2$, they are 1.7033, 1.7181, 1.7113, 30.1°, and 3.496. For glaucophane $Na_2Mg_3Al_2Si_8O_{22}(OH)_2$ they are 1.6083, 1.6064 [sic]. 1.6086, 35.1°, 3.042. The value of "n_z" is here the lowest index predicted for sections ‖010, and "n_y" is the predicted value for light vibrating parallel to the symmetry axis *b*. For cummingtonite $FeMg_4Fe^{2+}Si_8O_{22}(OH)_2$ they are 1.6349, 1.6500, 1.6689, 13.5° and 3.239.

Special tests are being made to determine whether non-linear regressions may be required for some of the chemical variables, especially for the regression of extinction angle on composition. Full tables of regression coefficients, predicted values for end-members, and residual errors of prediction for nearly 800 analyzed specimens have been prepared.

Indirect uses for such regressions include the discussion of order-disorder problems, temperature of formation, etc.

INTRODUCTION

Methods for computing regression coefficients have been well known among statisticians for many years; within the last few years the development of high-speed automatic computing machinery has made it possible for the first time to carry out such computations on a fairly large scale. Hey (1956) used the method to study the properties of a limited number of anthophyllites. Hori (1954), Henriques (1958a, b, c), Winchell and Tilling (1960), and Winchell (1961) applied it to clinopyroxenes. Henriques (1958d) used both first- and second-degree terms, for which there is theoretical, and in some cases practical justification. Similar studies have also been reported on garnet and other mineral groups.

Regression studies are in a sense no more than the analytical (algebraic) extension of the graphical methods that are familiar to all mineralogists. Regressions, however, remove the most serious limitation of charts, namely the necessity of picturing them on two-dimensional paper. After a third dimension is shown on the paper by means of isopleths (contour lines), it is difficult to consider any further dimensions in a meaningful way. A surprisingly rare device is to use many charts, as in the solution of a five-variable problem involving unknown quantities of thickness, birefringence, composition, and two variables of orientation in random sections of plagioclase twins (Nieuwenkamp, 1948; Laffitte, 1950).

For every advance in techniques there is a price to be paid; in the present case this is the price of substituting equations for the more familiar charts. We note the form, structure, and derivation of such equations in the next section, then consider their application to clinoamphiboles, and finally report the regression coefficients and some preliminary conclusions. Detailed discussion of applications will be reserved for a later report.

LEAST SQUARES METHOD, REGRESSION EQUATIONS

The least-squares method (Acton, 1959; Davies, 1958; Fisher, 1958; Williams, 1959) seeks to reduce to a minimum the overall discrepancy between a set of data that presumably contains errors of measurement, and an equation that describes a relationship between two or more of the variables. This "discrepancy" is defined as the sum of the squares of the residuals, or differences between equation and observation. These residuals are commonly assumed to be distributed about zero (their mean) according to the familiar *normal curve of error*, This assumption turns out to be fairly accurate in most cases involving physical measurements; its accuracy affects the

validity of certain statistical estimates, but it seems relatively unimportant with respect to the regression coefficients themselves.

Regression theory (Acton, 1959; Davies, 1958; Fisher, 1958; Williams, 1959). In the absence of any information about the independent, or controlling variable x, its mean value $\bar{x}$ is taken as the most probable value, and the corresponding value of the dependent variable y is its mean value, $\bar{y}$. Any deviation of x from its own mean $\bar{x}$ may be due partly to a "random error of measurement," and partly to a real or valid deviation from $\bar{x}$. For a given value x', the part due to error of measurement should have no effect upon the estimated value y', but the part due to real deviation of x' from $\bar{x}$ should cause a proportional difference between y' and $\bar{y}$. Where there are several independent variables x_1, x_2, x_3, $\cdots$, x_i, $\cdots$, each one of these is assumed to contribute a portion, or component, of the deviation of y' from $\bar{y}$, that is proportional to its own deviation from its own mean. Thus we have

$$y - \bar{y} = b_1(x_1 - \bar{x}_1) + b_2(x_2 - \bar{x}_2) + \cdots + b_i(x_i - \bar{x}_i) + \cdots$$

where the quantities b_1, b_2, $\cdots$, b_i, are the *regression coefficients* of y on the corresponding x_i. An alternative form of the same equation can be obtained by removing the parentheses and collecting the constant terms ($b_0 = \bar{y} + b_1\bar{x}_1 + b_2\bar{x}_2 + \cdots$), and rewriting as follows:

$$y = b_0 + b_1x_1 + b_2x_2 + \cdots + b_ix_i + \cdots + b_Ix_I \quad (1')$$

If we introduce a constant quantity $x_0 = 1$ the notation can be made more compact as follows:

$$y = \sum_{i=0}^{I} b_ix_i \quad (1)$$

The regression formula (1) may be made to represent not just one y, but a series of different dependent variables y_1, y_2, $\cdots$ (y_p with $p = 1, 2, \cdots$) such as refractive indices n_x, n_z, extinction angle Z/c, density G, lattice constants a, b, c, etc., by introducing another subscript p so as to represent all the different regression equations at once as follows:

$$y_p = \sum_{i=0}^{I} b_{ip}x_i \quad (2)$$

The standard error, s, of an estimated quantity, z, is a commonly used measure of the uncertainty, or precision, with which z can be estimated. It is closely analogous to the standard deviation of a population about its mean, and is formally represented by a very similar equation. In the better methods for obtaining the regression coefficients b_{ip}, their respective standard errors s_{ip} are made readily available. The standard error of regression may also be obtained; it is symbolized by s_p, and calculated from equation (3):

$$s_p^2 = \sum_{n=1}^{N} (y_{pn} - y'_{pn})^2/(N - I - 1) \quad (3)$$

where n designates the nth observation out of a total of N, and y and y' are the observed and regression-predicted values, respectively, of the dependent variable, and I, as in equations (1) and (2), is the number of computed regression coefficients.

Student's ratio, t, is defined as the ratio of any number to its own standard error. For example,

$$t_{ip} = b_{ip}/s_{ip} \quad (4)$$

This ratio provides a means for estimating the probability that the number (here, b_{ip}) differs significantly from zero. Most textbooks of statistics give at least abbreviated tables of the distribution of t, which show values of t for given values of Φ (number of degrees of freedom) and P (probability, or confidence level, that a chance distribution would give equally high t). In the present study, many analyses have been used, giving Φ larger than 60: the t-distribution tables show that for such cases, the chance that a random "accident" would give equally great or greater value of t is about 0.3 (30%) if $t = 1$, 0.05 if $t = 2$, 0.01 if $t = 2.66$, and 0.005 if $t = 3$.

Hey (1956) adopted the value $t_{ip} = 1$ as the cutoff point for deciding that a regression coefficient b_{ip} differs significantly from zero. This is a compromise between the usual statistical choice $t = 2$ or 2.5 on the one hand, and the proposition that in the regression of physical properties on chemical composition every chemical component is expected to have an effect on the physical property.

Computation of the regression coefficients follows methods that are widely known and well described, and need not be reviewed here. A matrix of the sums of squares and products of all the variables is formed. This matrix is solved by inversion to obtain the matrix of variances and covariances of the x's and y's, augmented with one or more column-vectors containing the regression coefficients. The covariance matrix can be used to find standard errors of the regression coefficients, the standard error of the regression as a whole, and the standard error of a calculated value y' of the dependent variable y for any particular set of values of the independent variables x_i.

Availability of full data. A few copies of the matrices used in this study have been prepared, and may be

had while the supply lasts. A full listing of data, matrices, and residuals will be made available in a separate publication.

The Composition and Properties of Clinoamphibole

General statement. Clinoamphiboles have a well-known crystal structure with 48 atoms of oxygen plus fluorine, hydroxyl, etc., per unit cell. Half of this cell is a convenient unit for chemical calculations. Accordingly the chemical analyses u_i (Table 1) were recast as atoms per 24 (O, OH, H_2O, F, Cl) using an IBM 650 computer. The details of the program input and output, and the program itself, can be made available as long as the supply of copies lasts.

With 24 (O, etc.) per formula, there is space for 16 cations, but these are located in at least four crystallographically distinct types of formula-positions, one of which may be partly or wholly vacant. The formula of clinoamphibole is accordingly as follows:

$$A_w\ B_2\ C_5\ D_8\ O_{22}\ E_2, \qquad (5)$$

where E represents OH, F, Cl, and either O or H_2O depending upon the amount of H to be accommodated; A, B, C, and D represent cations in crystallographically distinct positions; and $0 \leqq w \leqq 1$.

Recasting procedure. A preliminary note (Winchell, 1962) described our program written for the IBM 650 computer for recasting amphibole analyses in terms of formula (5) above. Table 1 shows the method of calculation for an ordinary analysis. The chemical analysis in weights per cent (u_i) is first recast as number of atoms v_i of each component per 24,000 (O, F, Cl). The resulting quantities v_i are next distributed into the several positions of the chemical formula (5), the number w_1 of smallest atoms (Si) in position D first, then successively larger atoms (Al, Fe^{3+}, Ti for w_2, w_3, w_4), stopping when the 8000 spaces of position D are filled. A remainder of Si over this limit is made impossible by an automatic branch to two alternative programs which reduce Si to 8000 by (1) assuming free silica [quartz?] present as impurity in the analyzed sample and by (2) assuming that H_2O was missed in the analysis, and correcting the values of v_i accordingly. Any remainder of Al, Fe^{3+}, or Ti is assigned immediately to position C.

Position C is filled in a similar manner using

Table 1. Recasting Analysis 187

Hornblende from Stark, N. H. (Sandell and Goldich, 1943) recast as atoms (v_i) per 24,000 (O, F, Cl)					Distribution of atoms v_i to positions in formula $(A_wB_2C_5D_8O_{22}E_2)_{1000}$ in 25 variables w_i and selection x_i for regression									
	Oxide M_pO_q	Wt. % by anal. u_i	Mol. wt. m_i	Oxygen equiv. $\frac{10{,}000\ q \cdot u}{s \cdot m}$	Atoms $v_i = \frac{24{,}000\ p \cdot u}{s \cdot m}$	Position D[c]		Position C[c]		Position B[c]		Position A[c]		Position E[d]	
						Symb.	Amt.	Symb.	Amt.	Symb.	Amt.	Symb.	Amt.	Symb.	Amt.
1	SiO_2	45.63	60.09	15,187	Si 7341	w_1	7341								
2	Al_2O_3	2.52	101.96	741	Al 478	$w_2 = x_1$	478								
3	Fe_2O_3	7.47	159.70	1,403	Fe^{3+} 905	$w_3 = X_2$[e]	181	$w_5 = X_3$	0						
4	TiO_2	2.88	79.90	721	Ti 348	w_4	0	$w_6 = x_4$	724						
5	MgO	0.76	40.32	188	Mg 182			$w_7 = x_5$	348						
6	FeO	27.17	71.85	3,781	Fe^{2+} 3655			w_8	182	$w_{12} = x_9$	0				
7	MnO	1.02	70.94	144	Mn 139			$w_9 = x_6$	3655	$w_{13} = x_{10}$	0				
8	CaO	5.56	56.08	991	Ca 958			$w_{10} = x_8$	91	$w_{14} = X_{11}$	48				
9	Na_2O	4.19	61.994	676	Na 1307			$w_{11} = x_7$	0	w_{15}	958	$w_{18} = x_{14}$	0		
10	K_2O	1.09	94.20	116	K 223					$w_{16} = x_{13}$	994	$w_{19} = x_{15}$	313		
11	H_2O^+	1.24	18.016	688	H 1331					$w_{17} = x_{12}$	0	$w_{20} = x_{16}$	223		
12	F[a]	0.73	18.999	192	F 371									$F = w_{21} = X_{17}$	371
13	Cl[a]	0.00	35.457	0	Cl 0									$Cl = w_{22} = x_{18}$	0
	Rem.	0.00[b]												$H_2O = w_{23}$	0
														$OH = w_{24}$	1331
														$O = w_{25}$	298
14	Sum	100.26		S = 24,828	$v_{14} = \Sigma_1^{10} v_i$ = 15,536		8000		5000	[f] $w_{26} = 5536$			536	(E) = 2000	

[a] For F and Cl, "p" = 1, "q" = 0.5.
[b] H_2O^- = 0.00.
[c] Not more than one line may contain non-zero w-values in two adjacent columns for positions A, B, C, and D; also $w_3 \cdot w_5 = w_4 \cdot w_6 = w_9 \cdot w_{12} = w_{10} \cdot w_{13} = \cdots = 0$.
[d] At least one of the pair w_{23}, w_{25} must be zero, hence $w_{23} \cdot w_{25} = 0$.
[e] $x_2 = w_3 + w_4$.
[f] $w_{26} = 3000 + \Sigma(B) + \Sigma(A)$.

available Al (w_5), Fe^{3+} (w_6), Ti (w_7), then Mg (w_8), Fe^{2+} (w_9), Mn (w_{10}), Ca (w_{11}), in order, as necessary to make the total 5000 atoms in D. Residues from Mg, Fe^{2+}, Mn, Ca, and in addition Na and K, are assigned to position B as w_{12} to w_{17}, respectively, following the same procedure again until 2000 atoms have been assigned there. Excess Ca, Na, and K are finally assigned to position A as w_{18} to w_{20}, and a check sum equal to 3000+atoms in A+atoms in B is reported out for comparison with the total metals reported previously as v_{14}, which should be exactly 10,000 larger.

All F and Cl is first assigned to position E, which is then completed with either OH+O, or $OH+H_2O$, to use up the H and bring total E to 2000. Warning cards are punched if there is a deficiency of atoms for assignment to position D or C, or if there is too much H to be accommodated in position E.

Table 1 shows the 25 quantities w_i available for study as a result of this recasting and assignment procedure.

Independent chemical variables x_i. The sum of all the atoms in position B must be exactly 2; in position C it is 5; in position D it is 8; in position E it is 2. Moreover, the condition of valency balance must be satisfied, making a linear interdependence among the variables v_i and hence among the w_i. Thus by the distribution procedure, some of the 25 chemical variables w_i are really dependent upon others. However, no linear dependence between variables can be tolerated in the matrix-algebraic procedure for solution of the simultaneous equations developed for the regression coefficients. It is therefore necessary to eliminate arbitrarily at least one of the chemical variables in each formula-position, and one more because of the valency balance.

There are several ways to remove these chemical dependences. A convenient and practical choice is to consider Si(D), Mg(C), Ca(B), and O, OH, H_2O in (E) as dependent upon all the other chemical variables. The remaining 19 include Ti in D, which is so rarely non-zero that it has been added to Fe^{3+} in D- and Cl in E, which is so rarely known that it has been ignored (equivalent to assuming it has no effect upon the physical properties). The final 17 independent variables are designated by x_i ($i=1$ to 17) in table 1. These are linearly independent; in particular, if all 17 are set arbitrarily equal to zero, the composition represented is that of the amphibole component $Ca_2Mg_5Si_8O_{22}(OH)_2$, called tremolite. By this choice of independent variables we assure that the constant term b_{0p} in each of the regression equations will represent the properties of an interesting and significant component of clinoamphibole.

Inhomogeneous chemical data. Some analyses are better than others. Particularly, only about 43% of the otherwise satisfactory analyses include determinations of the fluorine content. These 173 analyses seemed too valuable not to use for computing regressions on fluorine, but the whole set of 408, including these and the otherwise good ones, seem to offer equally good opportunity for important information. Accordingly, the regression computations were made on both groups, resulting in equations for physical properties y_p, numbered with $p=1$ to 4 for all 408 analyses, ignoring fluorine determinations, and with $p=6$ to 9 for 173 with fluorine data. The equation for y_p with $p=5$ is based upon a third group containing 249 analyses for which density data are available.

Physical variables, y_p. The indicatrix axis Z is always perpendicular to the crystallographic axis b in clinoamphiboles. There is thus no ambiguity in reference to Z, to the associated refractive index n_z, or to the extinction angle Z/c. (These symbols are compatible with and printable by, standard computing machinery, and are therefore adopted here.)

A second indicatrix axis is always perpendicular to Z and to the crystallographic axis b. In nearly all clinoamphiboles it is X, the vibration direction of the lowest principal refractive index; and for regression purposes it is so designated even though in rare cases (as crossite) it might more conventionally be called Y. The third indicatrix axis is always parallel to the crystallographic axis b, and for the regressions here described this is uniformly designated Y. A similar convention was used successfully in a previous regression study (Winchell, 1961).

Homogeneity of physical variables. A regression computation can be carried out separately for each dependent variable, y, but if several such variables depend upon the same set of independent variables (x_i), then it is much more economical to treat all of the y's and x's together. The formation of the augmented moments matrix, consisting of the squares and the products of all the variables, summed over all the observations (analyses in the present case) is time-consuming, and therefore costly, and should be done in such a manner that no data from a single analysis need be handled more than once individually. Selection of analyses actually used in the computa-

tion of regression coefficients was first made on the basis of chemical considerations as outlined below, and secondly on the basis of homogeneity of physical data and chemical data.

Homogenization of data. It is convenient to subdivide the data into five groups, numbered zero to four. Group 0 contains just under half of the analyses, and embraces all that have been rejected for any reason, as outlined below. Group 1 contains 46 acceptable analyses that include determinations of fluorine but not of density. Group 2 includes 113 with neither density nor fluorine data. Group 3 has 127 with both density and fluorine determinations. Group 4 comprises 122 analyses that have density but not fluorine determinations. Groups 1 to 4 include a total of 408 specimens, out of approximately 700 that were available.

The original list of available analyses is essentially unselective. It includes all that were used by A. N. Winchell (1945; 1938; 1932; etc.) in preparing several studies of amphiboles, plus many that have been gathered from the literature subsequently. No truly thorough search of the literature was attempted, although all available lists and bibliographical sources, especially *Mineralogical Abstracts*, volumes 1 to 14, were checked carefully. Dr. Bernard Leake of the University of Bristol, England, has kindly called my attention to a number of errors in these and has contributed a number of references for my use, but not in time for most of them to be included in the regressions. His contribution swelled my list of analyses to more than 850 before the cutoff time for using them in the residuals studies summarized here. (Dr. Leake's magnificently documented list of analyses of the calciferous clinoamphiboles has just become available to me in manuscript form, and swells my total list of clinoamphibole analyses with physical data, to well over 1000. The details of the total list will be published separately.) Several hundred more clinoamphibole analyses, for which no physical data have been published, are omitted from both Dr. Leake's and my lists, and a few score very old ones have been deleted.

Analyses of group 0 that were rejected for chemical and other reasons may be classified as follows into categories that are not mutually exclusive:

0.0 Rejections for essentially chemical reasons.

Class	Number	
0.01	59	cases with v_{14} (Sum of v's from 1 to 10) <14.900.
0.02	110	cases with $v_{14}>16.099$
0.03	24	cases with $v_1>8.000$ (shifted automatically into alternate programs 1 and 2 to make $v_1=8.000$; these were not used in regressions, but were considered among the data for calculations of residuals
0.04	10	cases with <7.900 atoms for position D (w_i with $i=1$–4)
0.05	19	cases with <4.900 atoms for position C (w_i with $i=5$–11)
0.06	13	cases with too much H (v_{11}) to be accommodated in position E, even as H_2O replacing the normal OH.

Remaining:

586 cases considered chemically acceptable.

In an antilogous manner the chemically acceptable cases were classified on the basis of availability (+) and absence (−) of certain physical measurements, as follows:

0.1 Classification of 586 chemically acceptable cases.

Class	Number	n_x	n_y	n_z	Z/c	G
0.11	24	−	−	−	−	−
0.12	83	(other combination)				
0.13	7	+	−	+	−	+
0.14	9	+	−	+	+	−
0.15	16	+	−	+	+	+
0.16	28	+	+	+	−	−
0.17	11	+	+	+	−	+
0.18	159	+	+	+	+	−
0.19	249	+	+	+	+	+

To accomplish the final homogenization of data in four groups, the 159 analyses in 0.18 were subdivided into two groups, Group 1 with, and Group 2 without fluorine determinations, and the 249 cases in 0.19 were similarly divided into two groups, Group 3 with, and Group 4 without fluorine determinations.

The four homogeneous groups of useful data thus defined were used to generate four augmented moments-matrices of order 24, each of which (except Group 3) contains some rows and columns based on partial data with missing items treated as zeroes.

Regressions for optics, ignoring fluorine. The sum of the four matrices, 1, 2, 3 and 4, is a matrix containing rows and columns that are dependent upon the amounts of fluorine and chlorine, which were assumed zero if not determined, and upon the values of G, also assumed zero if not determined. These three columns and rows were therefore dropped from the matrix, reducing it to order 21 with four instead of five dependent variables; the resulting basic moments-matrix, inverted and combined properly with the

four columns containing data on the dependent variables, yields the regression coefficients b_{ip} and their standard errors s_{ip} for four equations (p=1, 2, 3, 4) of the form (2):

$$\left.\begin{aligned}
&\text{for p = 1:}\quad n_x = y_1 = \sum_{i=0}^{16} b_{i1}x_i;\ \text{also}\ s_{i1}, t_{i1}, s_1\\
&\text{for p = 2:}\quad n_y = y_2 = \sum_{i=0}^{16} b_{i2}x_i;\ \text{also}\ s_{i2}, t_{i2}, s_2\\
&\text{for p = 3:}\quad n_z = y_3 = \sum_{i=0}^{16} b_{i3}x_i;\ \text{also}\ s_{i3}, t_{i3}, s_3\\
&\text{for p = 4:}\quad Z/c = y_4 = \sum_{i=0}^{16} b_{i4}x_i;\ \text{also}\ s_{i4}, t_{i4}, s_4
\end{aligned}\right\} \qquad (6)$$

where the regression coefficients are b_{ip}, their standard errors are s_{ip}, their t-ratios are t_{ip}, and the root-mean-square residual for the pth equation is s_p. These results are summarized in Table 2.

Regression for G, ignoring fluorine. The sum of matrices 3 and 4 contains nearly all the data that give information on the density G. Treating this sum-matrix in the same manner as the previous sum-matrix, but eliminating columns and rows corresponding to F, Cl, n_x, n_y, n_z, and Z/c, we obtain the following:

$$\text{for p = 5:}\quad G = y_5 = \sum_{i=0}^{16} b_{i5}x_i;\ \text{also}\ s_{i5}, t_{i5}, s_5 \qquad (7)$$

where the quantities are all as defined above; their values appear in Table 2.

Regressions allowing for fluorine. The sum of matrices 1 and 3 is a matrix that contains all the information about optical properties and fluorine as well as the other chemical variables. Eliminating rows and columns corresponding to Cl and to G, and solving as before, the four equations obtained are as follows:

$$\left.\begin{aligned}
&\text{for p = 6:}\quad n_x = y_6 = \sum_{i=0}^{17} b_{i6}x_i;\ \text{also}\ s_{i6}, t_{i6}, s_6\\
&\text{for p = 7:}\quad n_y = y_7 = \sum_{i=0}^{17} b_{i7}x_i;\ \text{also}\ s_{i7}, t_{i7}, s_7\\
&\text{for p = 8:}\quad n_z = y_8 = \sum_{i=0}^{17} b_{i8}x_i;\ \text{also}\ s_{i8}, t_{i8}, s_8\\
&\text{for p = 9:}\quad Z/c = y_9 = \sum_{i=0}^{17} b_{i9}x_i;\ \text{also}\ s_{i9}, t_{i9}, s_9
\end{aligned}\right\} \qquad (8)$$

The values of b_{ip}, t_{ip}, and s_p for these equations are in table 2.

Residuals. Residuals have been computed for about 750 cases of clinoamphiboles that have been analyzed and at least partially studied optically. These have been grouped and summarized by the classification groups 0–4 defined above, and the summaries are presented in Table 3, in which the boxes surrounded by single lines contain valid data, those surrounded by double lines summarize the data on which regression coefficients are directly based, and data not boxed represent invalid application of equations 6–9 to analyses that do not all contain fluorine determinations. The unboxed data should be ignored in most evaluations; they clearly show that it is not wise to use equations 6–9 for estimating physical properties of specimens on which no fluorine determination is available. The other groups tend to show that the analyses in group 0 (including the individual subgroups as well as the entire collection in group 0) contain more specimens that have large residual earrors of estimation of optical properties and density than the analyses in groups 1–4, taken individually or collectively.

Interesting compositions. The key to Table 4 presents a number of interesting hypothetical compositions, together with names that might be applied to them as "end-members" of the clinoamphibole system. The main section of this table presents the estimated optical properties and densities y′ together with respective standard errors $s(y'_p)$ estimated according to equation (9),

$$s(y'_p) = s_p\left\{\sum_i x_i^2 c_{iip} + 2\sum_i\sum_j x_i x_j c_{ijp}\right\}^{1/2} \qquad (9)$$

where symbols are as defined above, c_{ijp} is the component from column i, row j, (i>j) of the covariance matrix for equation p, and c_{iip} is the ith diagonal element of the same matrix. The standard errors are shown in Table 4 in the columns *preceding* the numbers to which they refer. The amount of fluorine is known in these cases, but regressions for y_p with p=1−4 give smaller estimated standard errors in some cases because certain regression coefficients are better known for p=1−4 than for regressions of y_p with p=6−9. The latter, however, are essential for cases where effects of fluorine are specifically studied.

Discussion

A full discussion of these results, and some further results and comparisons, will be presented elsewhere. As with clinopyroxenes (Winchell, 1961), so also with clinoamphiboles, the prospect arises of making significant comparisons that may lead to immediate tests for degree of order in the distribution of certain atoms. Should such tests succeed, there is a good

TABLE 2. REGRESSION COEFFICIENTS B(I,P) WITH CORRES. S(I,P) AND T(I,P)

P=1 Y(1) = N(X) R-SQ = .906 F = 236.9 V = 16 W = 391 S = .007958 MATRIX 5			P=2 Y(2) = N(Y) R-SQ = .877 F = 174.9 V = 16 W = 391 S = .009889 MATRIX 5			P=3 Y(3) = N(Z) R-SQ = .845 F = 133.0 V = 16 W = 391 S = .010979 MATRIX 5			
B	S	T	B	S	T	B	S	T	
1.60049	.00120	99.99	1.61460	.00149	99.99	1.62660	.00166	99.99	CONST
.00807	.00113	7.09	.00698	.00141	4.93	.00385	.00157	2.45	AL(D)
.00821	.00494	1.65	.00895	.00615	1.45	-.00017	.00682	.02	FE3(D)
.00463	.00156	2.96	.00331	.00194	1.70	.00583	.00215	2.70	AL(C)
.02583	.00132	19.49	.03267	.00164	19.84	.03308	.00182	18.10	FE3(C)
.03849	.00321	11.98	.04961	.00399	12.42	.05933	.00443	13.38	TI(C)
.01424	.00048	29.24	.01420	.00060	23.47	.01331	.00067	19.82	FE2(C)
.00535	.00383	1.39	.00733	.00476	1.53	.01345	.00528	2.54	MN(C)
.01815	.00454	3.99	.01909	.00564	3.38	.02178	.00626	3.47	CA(C)
-.00014	.00120	.12	.00049	.00149	.32	.00105	.00166	.63	MG(B)
.01010	.00124	8.09	.01055	.00155	6.80	.01451	.00172	8.42	FE2(B)
.01061	.00266	3.98	.01214	.00330	3.66	.00913	.00367	2.48	MN(B)
.01557	.01393	1.11	.01021	.01732	.58	.01356	.01922	.70	NA(B)
-.00073	.00154	.47	-.00735	.00192	3.82	-.01477	.00213	6.92	K(B)
.00024	.00311	.08	-.00656	.00387	1.69	-.01224	.00430	2.84	CA(A)
.00396	.00185	2.14	.00002	.00230	.01	.00056	.00255	.22	NA(A)
.00619	.00408	1.51	.00582	.00507	1.14	.00880	.00563	1.56	K(A)

P=4 Y(4) = Z/C R-SQ= .387 F= 15.4 V = 16 W = 391 S = 11.171 MTX 5			P=5 Y(5) = G R-SQ = .751 F = 43.7 V = 16 W = 232 S = .06918 MATRIX 6			P=6 Y(6) = N(X) R-SQ = .955 F = 193.6 V = 17 W = 155 S = .006378 MATRIX 7			
B	S	T	B	S	T	B	S	T	
16.28	1.69	9.61	2.9736	.0135	99.99	1.60226	.00151	99.99	CONST
2.53	1.59	1.58	.0437	.0126	3.46	.00981	.00175	4.60	AL(D)
-5.17	6.94	.74	.0139	.0520	.46	.01594	.00605	2.63	FE3(D)
-5.24	2.19	2.38	.0033	.0183	.17	.00661	.00258	25.55	AL(C)
-1.78	1.85	.95	.0727	.0150	4.83	.02863	.00175	16.28	FE3(C)
-14.95	4.51	3.31	.0354	.0343	1.03	.04077	.00420	9.70	TI(C)
3.16	.68	4.62	.0854	.0055	15.46	.01447	.00074	19.55	FE2(C)
-11.52	5.37	2.14	-.0198	.0375	.52	.02136	.01172	1.82	MN(C)
-.83	6.37	.13	.0297	.0422	.70	.02280	.00709	3.21	CA(C)
.37	1.69	.22	.1308	.0382	3.41	-.00066	.00103	.63	CA(C)
-2.99	1.75	1.70	.0899	.0146	6.13	.01009	.00197	5.10	FE2(B)
-7.83	3.73	2.09	.0833	.0289	2.87	-.00225	.00558	.40	MN(B)
-18.50	19.56	.94	-1.0546	.2236	4.71	-.00744	.03221	.23	NA(B)
14.66	2.17	6.75	.0306	.0168	1.82	-.00171	.00227	.75	K(B)
12.57	4.36	2.87	-.0000	.0327	.00	.00041	.00381	.10	CA(A)
8.07	2.59	3.10	.0205	.0212	.96	.00005	.0276	.02	NA(A)
14.60	5.72	2.54	.0159	.0465	.34	-.00291	.0513	.56	K(A)
						-.00567	.00158	3.58	F(E)

P=7 Y(7) = N(Y) R-SQ = .937 F = 135.6 V = 17 W = 155 S = .008582 MATRIX 7			P=8 Y(8) = N(Z) R-SQ = .909 F = 90.5 V = 17 W = 155 S = .010301 MATRIX 7			P=9 Y(9) = Z/C R-SQ = .428 F = 6.8 V = 17 W = 155 S = 9.342 MATRIX 7			
B	S	T	B	S	T	B	S	T	
1.61587	.00203	99.99	1.62693	.00244	99.99	15.21	2.21	6.87	CONST
.00407	.00235	1.73	.00185	.00282	.65	-.85	2.56	.33	AL(D)
.01156	.00815	1.41	.00936	.00978	.95	-15.28	8.87	1.72	FE3(D)
.00440	.00347	1.26	.00492	.00417	1.17	-.40	3.78	.10	AL(C)
.04388	.00236	18.55	.04500	.00283	15.85	-6.12	2.57	2.37	FE3(C)
.05899	.00565	10.43	.06949	.00678	10.23	-13.51	6.15	2.19	TI(C)
.01464	.00099	14.70	.01312	.00119	10.98	1.34	1.08	1.23	FE2(C)
.03955	.01576	2.50	.04361	.01892	2.30	23.90	17.16	1.39	MN(C)
.03075	.00954	3.22	.02900	.01145	2.53	-3.71	10.38	.35	CA(C)
-.00034	.00138	.25	.00006	.00166	.03	-.00	1.51	.00	MG(B)
.01123	.00265	4.22	.01665	.00319	5.21	-.41	2.89	.14	FE2(B)
-.00337	.00750	.44	-.00291	.00901	.32	-17.18	8.17	2.10	MN(B)
-.02386	.04334	.55	-.04194	.00367	.80	12.09	47.18	.25	NA(B)
-.01682	.00306	5.48	-.02267	.00367	6.16	18.67	3.33	5.59	K(B)
-.00824	.00513	1.60	-.01067	.00616	1.73	10.10	5.58	1.80	CA(A)
.00304	.00372	.81	.00572	.00446	1.28	6.55	4.05	1.61	NA(A)
-.00214	.00691	.31	-.00285	.00829	.34	8.40	7.52	1.11	K(A)
-.00609	.00212	2.86	-.00594	.00255	2.32	.15	2.31	.06	F(E)

prospect of being able to estimate the metamorphic grade of a rock by a consideration of the properties of its amphibole alone. Ghose (1962) predicts that ordering of Mg and Fe″ should be common in hornblendes, but aside from a few ultra-precise determinations of crystal structure his evidence is inductive from principles of chemical crystallography. No method can replace the refined analysis of crystal structure for ultimate decision on this point, but contributory evidence may be obtainable from other physical measurements. Such measurements must be corrected, however, for all the chemical components. Any residual difference can be examined for correlation with the temperature history of the specimen, as reflected in the order of its cations and/or its geologic setting. Clearly one way of making allowance for chemical components is through empirical regressions based on very many data, as herein presented.

An estimate of the composition of a clinoamphibole cannot be based upon a few measured physical properties alone when there are so many chemical variables. However, as with clinopyroxenes (Winchell, 1961), the geologist ordinarily has at least an approximate idea of the composition, and can calculate the properties of an arbitrary "first approximation." He can then compare these with the observed properties of a specimen in hand, and observe what adjustments in the trial composition will produce better agreement.

Conclusion. Further Work in Progress

With several non-significant coefficients b_{ip} in each of the regressions here presented, it seems advisable to reconsider the variables x_i to be used, and possibly to assign arbitrary zero values to some b's. This and similar experiments are contemplated. A further investigation of the data that present large residual differences between observed and estimated

Table 3

	gp 1 (46 anals.)			gp 2 (113 anals.)			gp 3 (126 anals.)			gp 4 (123 anals.)		
EQ	Ē	s	N	Ē	s	N	Ē	s	N	Ē	s	N
1	−.00167	.00700	46	.00053	.00858	113	−.00104	.00746	126	.00120	.00759	123
2	−.00260	.01098	46	.00043	.00988	113	−.00090	.00955	126	.00150	.00903	123
3	−.00429	.01284	46	.00040	.01046	113	−.00085	.01093	126	.00210	.00984	123
4	2.08	8.69	46	−.47	10.84	113	1.25	10.09	126	−1.62	2.49	123
5	—	—		—	—		−.0056	.0436	126	.0057	.0841	123
6	−.00037	.00603	46	.00461	.01070	113	.00011	.00605	126	.00482	.01092	123
7	−.00118	.00820	46	.00363	.01317	113	.00035	.00806	126	.00574	.01448	123
8	−.00276	.00986	46	.00341	.01422	113	.00086	.00957	126	.00672	.01536	123
9	0.71	6.89	46	−.71	12.27	113	−0.23	9.48	126	−1.29	15.89	123
	gp 5=Σgps 1–4			gp 6=gp(3+4)			gp 7=gp(1+3)			gp 0 (280 anals.)		
1	−.00000	.00778	408	+.00007	.00752	249	−.00121	.00734	172	−.00063	.01148	158
2	−.00000	.00967	408	.00029	.00930	249	−.00135	.00995	172	−.000013	.01514	121
3	−.00000	.01072	408	.00061	.01041	249	−.00177	.01147	172	.00072	.01294	156
4	.00000	10.93	408	−.17	11.34	249	1.47	9.74	172	2.18	17.80	148
5	−.00000	.0668	249	−.00000	.0668	249	−.0056	.0436	126	−.0053	.0647	164
6	.00272	.00911	408	.00244	.00880	249	−.00001	.00605	172	.00241	.01153	158
7	.00271	.01178	408	.00301	.01168	249	−.00006	.00810	172	.00548	.01855	121
8	.00292	.01290	408	.00375	.01276	249	−.00010	.00965	172	.00552	.01779	156
9	−.57	12.29	408	−.75	13.05	249	0.02	8.86	172	1.81	20.07	148

Legend. Mean deviations Ē, root-mean-square deviations s, and number of observations N for equations 1 to 9, inclusive, applied to certain groups of clinoamphibole analyses defined in the text. Note. The boxed sections represent data to which the equations are properly applied; other sections involve data that have not been computed according to the assumptions implied. The double-lined boxes contain data for the observation-sets from which the regression coefficients were actually computed.

properties is also required. No doubt this procedure will identify a few errors, and it will probably also point out a number of suspect analyses or incorrect optical data.

Acknowledgments

I acknowledge with gratitude the support of the Higgins Trust Fund of Yale University, without which the extensive programming and calculations would have been quite impossible. Theresa Y. Park of the Yale Computer Center did most of the programming, and indeed all of the recasting of the analyses, as well as much of the actual operation of the IBM 650. The Computer Center cooperated generously with me in developing a new program for calculating residuals, which I used on an IBM 1620 machine that supersedes the 650.

Philip Goodell and a number of other students spent long hours with a desk computer doing the standard errors for Table 4.

Key to Table 4 *(On next page)*

NUMBER	NAME	NUMBER OF ATOMS W(I) (SEE TABLE 1)																			
	INDEX I OF W(I)	2		3		6		8		10		13		15		19		25			
			1		5		7		9		12		14		16		24		21		
9901	TREMOLITE	0	8	0	0	0	0	5	0	0	0	0	0	2	0	0	2	0	0		
9902	FLUORINE-TREMOLITE	0	8	0	0	0	0	5	0	0	0	0	0	2	0	0	0	0	2		
9903	FERROTREMOLITE	0	8	0	0	0	0	0	5	0	0	0	0	2	0	0	2	0	0		
9904	FLUORINE FERROTREMOLITE	0	8	0	0	0	0	0	5	0	0	0	0	2	0	0	0	0	2		
9905	OXYFERROTREMOLITE	0	8	0	0	2	0	0	3	0	0	0	0	2	0	0	0	2	0		
9906	TSCHERMAKITE	2	6	0	2	0	0	3	0	0	0	0	0	2	0	0	2	0	0		
9907	FERROTSCHERMAKITE	2	6	0	2	0	0	0	3	0	0	0	0	2	0	0	2	0	0		
9908	OXYFERROTSCHERMAKITE	2	6	0	2	2	0	0	1	0	0	0	0	2	0	0	0	2	0		
9909	FERROFERRITSCHERMAKITE	2	6	0	0	2	0	0	3	0	0	0	0	2	0	0	2	0	0		
9910	FLUORINE-TSCHERMAKITE	2	6	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	2		
9911	PARGASITE	2	6	0	1	0	0	4	0	0	0	0	0	2	0	1	2	0	0		
9912	FERROPARGASITE	2	6	0	1	0	0	0	4	0	0	0	0	2	0	1	2	0	0		
9913	FERRIPARGASITE	2	6	0	0	1	0	4	0	0	0	0	0	2	0	1	2	0	0		
9914	HASTINGSITE	2	6	0	0	1	0	0	4	0	0	0	0	2	0	1	2	0	0		
9915	OXYHASTINGSITE	2	6	0	0	3	0	0	2	0	0	0	0	2	0	1	0	2	0		
9916	EDENITE	1	7	0	0	0	0	5	0	0	0	0	0	2	0	1	2	0	0		
9917	FERROEDENITE	1	7	0	0	0	0	0	5	0	0	0	0	2	0	1	2	0	0		
9918	FLUORINE-EDENITE	1	7	0	0	0	0	5	0	0	0	0	0	2	0	1	0	0	2		
9919	FLUORINE-FERROEDENITE	1	7	0	0	0	0	0	5	0	0	0	0	2	0	1	0	0	2		
9920	OXYFERROEDENITE	1	7	0	0	2	0	0	3	0	0	0	0	2	0	1	0	2	0		
9921	RICHTERITE	0	8	0	0	0	0	5	0	0	0	0	0	1	1	1	2	0	0		
9922	FERRORICHTERITE	0	8	0	0	0	0	0	5	0	0	0	0	1	1	1	2	0	0		
9923	FLUORINE-RICHTERITE	0	8	0	0	0	0	5	0	0	0	0	0	1	1	1	0	0	2		
9924	FLUORINE-FERRORICHTERITE	0	8	0	0	0	0	0	5	0	0	0	0	1	1	1	0	0	2		
9925	OXYFERROFERRIRICHTERITE	0	8	0	0	2	0	0	3	0	0	0	0	1	1	1	0	2	0		
9926	GLAUCOPHANE	0	8	0	2	0	0	3	0	0	0	0	0	0	2	0	2	0	0		
9927	FERROGLAUCOPHANE	0	8	0	2	0	0	0	3	0	0	0	0	0	2	0	2	0	0		
9928	MAGNESIORIEBECKITE	0	8	0	0	2	0	3	0	0	0	0	0	0	2	0	2	0	0		
9929	RIEBECKITE	0	8	0	0	2	0	0	3	0	0	0	0	0	2	0	2	0	0		
9930	OXYRIEBECKITE	0	8	0	0	4	0	0	1	0	0	0	0	0	2	0	0	2	0		
9931	MAGNESIO-ALUMINOARFVEDSONITE	0	8	0	1	0	0	4	0	0	0	0	0	0	2	1	2	0	0		
9932	ALUMINO-ARFVEDSONITE	0	8	0	1	0	0	0	4	0	0	0	0	0	2	1	2	0	0		
9933	MAGNESIO-ARFVEDSONITE	0	8	0	0	1	0	4	0	0	0	0	0	0	2	1	2	0	0		
9934	ARFVEDSONITE	0	8	0	0	1	0	0	4	0	0	0	0	0	2	1	2	0	0		
9935	OXYARFVEDSONITE	0	8	0	0	3	0	0	2	0	0	0	0	0	2	1	0	2	0		
9936	FLUORINE-PARGASITEIL	2	6	0	1	0	0	4	0	0	0	0	0	2	0	1	0	0	2		
9937	FLUORINE-HASTINGSITE	2	6	0	0	1	0	0	4	0	0	0	0	2	0	1	0	0	2		
9938	FLUORINE-GLAUCOPHANE	0	8	0	2	0	0	3	0	0	0	0	0	0	2	0	0	0	2		
9939	FLUORINE-RIEBECKITE	0	8	0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	2		
9940	FLUORINE-ARFVEDSONITE	0	8	0	0	1	0	0	4	0	0	0	0	0	2	1	0	0	2		
9941	CROSSITE	0	8	0	1	1	0	1	2	0	0	0	0	0	2	0	2	0	0		
9942	CHIKLITE	0	8	0	0	2	0	1	0	2	0	0	0	0	2	0	2	0	0		
9943	BARKEVIKITE	2	6	0	0	1	1	1	2	0	0	0	0	2	0	1	2	0	0		
9944	KUPFFERITE	0	8	0	0	0	0	5	0	0	2	0	0	0	0	0	2	0	0		
9945	5 KUPFFERITE + 2 GRUNERITE	0	8	0	0	0	0	5	0	0	0	2	0	0	0	0	2	0	0		
9946	3 KUPFFERITE + 4 GRUNERITE	0	8	0	0	0	0	3	2	0	0	2	0	0	0	0	2	0	0		
9947	GRUNERITE	0	8	0	0	0	0	0	5	0	0	2	0	0	0	0	2	0	0		
9948	MANGANESE GRUNERITE	0	8	0	0	0	0	0	5	0	0	0	2	0	0	0	2	0	0		
9949	MANGANESE-CUMMINGTONITE	0	8	0	0	0	0	3	0	2	0	0	2	0	0	0	2	0	0		
9950	F-NA-CUMMINGTONIT (F-NA-RICHTERITE)	0	8	0	0	0	0	5	0	0	0	0	0	0	1	1	0	0	2		

TABLE 4. CALCULATED VALUES FOR INTERESTING COMPOSITIONS

Standard Errors S′(P) and Physical Properties Y′(P), Calculated from Regressions

	Y(1)=N(X)		Y(2)=N(Y)		Y(3)=N(Z)		Y(4)=Z/C		Y(5)=G		Y(6)=N(X)		Y(7)=N(Y)		Y(8)=N(Z)		Y(9)=Z/C	
N	S(X)	N(X)	S(Y)	N(Y)	S(Z)	N(Z)	S(/)	Z/C	S(G)	G	S(X)	N(X)	S(Y)	N(Y)	S(Z)	N(Z)	S(/)	Z/C
9901	.0012	1.6004	.0015	1.6146	.0017	1.6266	1.7	16.2	.014	2.973	.0015	1.6022	.0020	1.6158	.0024	1.6269	2.2	15.2
9902	.	1.6004	.	1.6146	.	1.6266	.	16.2	.	2.973	.0030	1.5909	.0040	1.6036	.0049	1.6150	4.4	15.5
9903	.0025	1.6717	.0031	1.6856	.0035	1.6931	3.5	32.1	.027	3.400	.0038	1.6746	.0051	1.6891	.0061	1.6925	5.5	21.9
9904	.	1.6717	.	1.6856	.	1.6931	.	32.1	.	3.400	.0049	1.6632	.0066	1.6769	.0080	1.6806	7.3	22.2
9905	.0030	1.6948	.0037	1.7225	.0051	1.7327	4.2	22.2	.034	3.375	.0041	1.7029	.0056	1.7475	.0067	1.7563	6.1	6.9
9906	.0023	1.6259	.0029	1.6352	.0032	1.6460	3.2	.7	.055	3.067	.0036	1.6351	.0049	1.6328	.0059	1.6405	5.3	14.3
9907	.0024	1.6686	.0030	1.6778	.0033	1.6859	3.4	10.2	.056	3.324	.0035	1.6785	.0047	1.6767	.0057	1.6798	5.1	18.3
9908	.0035	1.6918	.0043	1.7147	.0048	1.7254	4.9	.3	.063	3.298	.0051	1.7068	.0069	1.7352	.0083	1.7436	7.5	3.4
9909	.0024	1.7110	.0030	1.7365	.0033	1.7404	3.4	17.1	.031	3.462	.0036	1.7225	.0048	1.7557	.0058	1.7600	5.2	5.2
9910	.	1.6259	.	1.6352	.	1.6460	.	.7	.	3.067	.0052	1.6237	.0070	1.6206	.0084	1.6286	7.7	14.6
9911	.0020	1.6252	.0025	1.6319	.0028	1.6407	2.8	14.0	.040	3.084	.0023	1.6285	.0031	1.6314	.0037	1.6413	3.4	20.4
9912	.0027	1.6822	.0034	1.6887	.0038	1.6939	3.8	26.6	.044	3.426	.0037	1.6864	.0050	1.6900	.0060	1.6938	5.4	25.8
9913	.0023	1.6464	.0029	1.6612	.0032	1.6679	3.2	17.5	.026	3.154	.0032	1.6505	.0041	1.6709	.0051	1.6813	4.5	13.9
9914	.0027	1.7034	.0034	1.7180	.0038	1.7212	3.8	30.1	.029	3.496	.0042	1.7084	.0057	1.7295	.0068	1.7338	6.2	19.3
9915	.0034	1.7265	.0042	1.7550	.0047	1.7607	4.8	20.2	.061	3.470	.0050	1.7367	.0067	1.7880	.0081	1.7976	7.4	4.3
9916	.0017	1.6125	.0021	1.6216	.0023	1.6310	2.4	21.8	.021	3.037	.0028	1.6121	.0037	1.6230	.0045	1.6345	4.1	20.9
9917	.0020	1.6837	.0025	1.6926	.0028	1.6976	2.8	37.6	.034	3.465	.0048	1.6844	.0065	1.6962	.0078	1.7001	7.0	27.6
9918	.	1.6125	.	1.6216	.	1.6310	.	21.8	.	3.037	.0029	1.6007	.0040	1.6108	.0048	1.6226	4.3	21.2
9919	.	1.6837	.	1.6926	.	1.6976	.	37.6	.	3.465	.0052	1.6731	.0071	1.6840	.0085	1.6882	7.7	27.9
9920	.0029	1.7069	.0036	1.7295	.0040	1.7371	4.1	27.7	.033	3.440	.0045	1.7128	.0061	1.7546	.0073	1.7638	6.6	12.6
9921	.0021	1.6037	.0026	1.6072	.0029	1.6123	2.9	39.0	.029	3.024	.0031	1.6006	.0041	1.6021	.0050	1.6099	4.5	40.4
9922	.0032	1.6749	.0040	1.6782	.0044	1.6789	4.5	54.8	.036	3.452	.0019	1.6729	.0066	1.6753	.0079	1.6756	7.2	47.1
9923	.	1.6037	.	1.6072	.	1.6123	.	39.0	.	3.024	.0031	1.5892	.0042	1.5899	.0050	1.5980	4.5	40.7
9924	.	1.6749	.	1.6782	.	1.6789	.	54.8	.	3.452	.0053	1.6616	.0071	1.6631	.0086	1.6637	7.7	47.4
9925	.0028	1.6981	.0035	1.7152	.0039	1.7185	3.9	44.9	.030	3.426	.0043	1.7012	.0058	1.7338	.0069	1.7393	5.3	32.2
9926	.0030	1.6082	.0037	1.6065	.0042	1.6087	4.3	35.1	.037	3.041	.0054	1.6120	.0073	1.5910	.0087	1.5914	7.9	53.3
9927	.0032	1.6510	.0039	1.6491	.0043	1.6486	4.4	44.6	.038	3.297	.0051	1.6554	.0069	1.6349	.0083	1.6308	7.5	57.3
9928	.0025	1.6507	.0031	1.6652	.0034	1.6632	3.4	42.0	.029	3.180	.0038	1.6501	.0050	1.6700	.0061	1.6715	5.5	40.3
9929	.0025	1.6934	.0030	1.7078	.0034	1.7031	3.4	51.5	.028	3.436	.0036	1.6995	.0048	1.7139	.0058	1.7109	5.2	44.3
9930	.0040	1.7165	.0050	1.7448	.0055	1.7427	5.6	41.6	.047	3.411	.0054	1.7278	.0073	1.7724	.0088	1.7747	8.0	29.3
9931	.0033	1.6076	.0041	1.6032	.0045	1.6034	4.6	48.4	.032	3.058	.0055	1.6054	.0074	1.5896	.0089	1.5922	8.1	59.5
9932	.0037	1.6645	.0045	1.6600	.0050	1.6567	5.1	61.1	.037	3.400	.0041	1.6633	.0055	1.6482	.0066	1.6447	6.0	64.8
9933	.0031	1.6288	.0048	1.6325	.0042	1.6307	4.3	51.9	.028	3.128	.0038	1.6275	.0051	1.6291	.0062	1.6323	5.6	52.9
9934	.0035	1.6857	.0043	1.6894	.0048	1.6839	4.9	64.5	.033	3.470	.0046	1.6854	.0061	1.6877	.0074	1.6848	6.7	58.3
9935	.0036	1.7089	.0045	1.7263	.0050	1.7235	5.1	54.6	.036	3.444	.0048	1.7137	.0064	1.7462	.0077	1.7485	7.0	43.4
9936	.	1.6252	.	1.6319	.	1.6407	.	14.0	.	3.084	.0032	1.6172	.0042	1.6192	.0051	1.6294	4.6	20.7
9937	.	1.7034	.	1.7180	.	1.7212	.	30.1	.	3.496	.0048	1.6971	.0065	1.7173	.0078	1.7219	7.1	19.6
9938	.	1.6082	.	1.6065	.	1.6087	.	35.1	.	3.041	.0065	1.6007	.0087	1.5788	.0105	1.5795	9.5	53.6
9939	.	1.6934	.	1.7078	.	1.7031	.	51.5	.	3.436	.0048	1.6881	.0065	1.7017	.0077	1.6990	7.0	44.6
9940	.	1.6857	.	1.6894	.	1.6839	.	64.5	.	3.470	.0050	1.6740	.0067	1.6755	.0065	1.6729	7.3	58.6
9941	.0022	1.6579	.0027	1.6642	.0030	1.6626	3.0	44.9	.026	3.281	.0040	1.6630	.0054	1.6598	.0080	1.6577	5.9	49.5
9942	.0088	1.6869	.0109	1.7034	.0121	1.7068	12.4	40.3	.081	3.239	.0138	1.7016	.0186	1.7315	.0223	1.7296	20.2	32.8
9943	.0037	1.7134	.0045	1.7393	.0050	1.7539	5.1	8.8	.034	3.360	.0035	1.7202	.0048	1.7592	.0057	1.7771	5.2	3.1
9944	.0026	1.6001	.0033	1.6155	.0036	1.6287	3.6	17.0	.075	3.235	.0025	1.6009	.0034	1.6151	.0041	1.6270	3.7	15.2
9945	.0076	1.6207	.0094	1.6357	.0105	1.6556	10.7	10.3	.028	3.153	.0038	1.6224	.0052	1.6383	.0062	1.6602	5.6	14.3
9946	.0066	1.6491	.0082	1.6641	.0091	1.6822	9.3	16.6	.025	3.324	.0032	1.6513	.0043	1.6676	.0052	1.6864	4.7	17.0
9947	.0077	1.6919	.0095	1.7067	.0106	1.7222	10.8	26.1	.029	3.580	.0034	1.6948	.0046	1.7115	.0055	1.7258	5.0	21.0
9948	.0053	1.6929	.0066	1.7099	.0073	1.7114	7.5	16.4	.057	3.567	.0107	1.6701	.0144	1.6823	.0173	1.6867	15.8	12.4
9949	.0092	1.6580	.0115	1.6770	.0127	1.6884	13.0	-1.0	.085	3.199	.0162	1.6433	.0217	1.6706	.0261	1.6791	23.7	26.5
9950	.	1.6035	.	1.6077	.	1.6134	.	39.4	.	3.155	.0031	1.5885	.0042	1.5895	.0050	1.5981	4.5	40.7

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Discussion

B. Leake, (Bristol, England) Your regression equations should be capable of being modified to find out in any one amphibole in which position in the structure certain elements are really present. This would give some decisive new information to assist in the assignment of elements to particular lattice sites in the structure. Have you obtained any results along these lines yet?

Author's reply: These equations are indeed applicable to studies of the sort you mention. We may, for example, study the distribution of a pair of elements, both of which can reasonably enter the formula in either of two positions, by assuming two or more plausible distributions, computing the physical properties, and comparing the results with observed properties. Moreover, the estimated standard error for each computation will afford the means of deciding whether or not the differences so calculated are significant, and if so at what probability-level.

Allan Wilson (Brisbane, Australia) How can you be sure of the reliability of the fluorine determinations of the analyses which you have used, especially in view of the importance of fluorine in the amphibole structure?

Author's reply: Individual fluorine determinations are hard to carry out, especially by the methods used in many of the analyses here considered. That they are, on the average fairly valid when considered *en masse,* is indicated by the small, but consistent improvement in the standard deviations of observed and calculated y_p-values set forth in Table 3, group 7, equations 6–9 compared with equations 1–4, and also compared with group 5, equations 1–4. I have not investigated the statistical significance of these differences.