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ORIGIN AND PREDICTION OF DITRIGONAL DISTORTIONS IN MICAS

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ABSTRACT

Two of the most important parameters characterizing the ditrigonal distortion of mica structures are the tetrahedral rotation angle α and the difference Δ between outer and inner interlayer cation-oxygen distances. Equations are derived to predict α and Δ from chemical composition and ionic radii. Theoretical calculations based on the rotation of ideal tetrahedra predict a linear relation, $\Delta(\text{Å}) = .047\alpha°$, which is accurately confirmed by experiment. Utilizing data from ten well-refined mica structures, a multiple regression equation for α is derived which demonstrates that α is primarily controlled by the tetrahedral-octahedral layer misfit, rather than the interlayer cation. This equation yields good results for all α values, whereas previously-derived formulae fail at small angles.

INTRODUCTION

Within the last few years several mica structures have been refined: lithium fluormica (Takeda and Donnay, 1966), fluorophlogopite (McCauley *et al.*, 1967), phengite (Güven, 1968), fluor-polylithionite (Takeda *et al.*, 1967), and $BaLiMg_2AlSi_3O_{10}F_2$ (McCauley and Newnham 1969). These refinements provide new structural data for micas with small ditrigonal distortions, data which are useful in testing structure-composition relations for this important mineral family (McCauley and Newnham, 1968).

Two parameters often used to characterize mica structures are the tetrahedral rotation angle α and the difference between the mean outer and inner interlayer cation-oxygen distances. The tetrahedral layer for an ideal hexagonal arrangement ($\alpha = 0°$) and for an ideally distorted one ($\alpha = \pm 20°$) are shown in Figure 1. The interlayer cation fits into the center of the ring of tetrahedra, between two adjacent tetrahedral sheets. Figure 1b shows how alternate tetrahedra rotate clockwise and counterclockwise through an angle α, thereby bringing six oxygen ions closer to the interlayer cation while taking the other six further away. The net result of this so-called ditrigonal distortion is that the coordination of the interlayer cation depends on the magnitude of α. The difference Δ between the outer and inner distances is a measure of the coordination of the interlayer cation.

The structures of the octahedral and tetrahedral sheets of mica have been summarized and analyzed by Bailey (1966) and Bailey *et al.*, (1967).

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Recently Franzini (1969) has also analyzed mica structures with special emphasis on the interlayer cation region. Not included in Franzini's analysis, however, were some new structural refinements which are very important with regard to full understanding of the variation of mica structures with chemical composition. Table 1 lists pertinent structural data for the interlayer sheet of accurately refined trioctahedral and dioctahedral micas. Also listed in this table are similar data for pyrophyllite, talc, α-$BaAl_2Si_2O_8$, and hexagonal $CaAl_2Si_2O_8$; the last two are compositionally feldspars but have structures that can be described as mica layers without an octahedral sheet—a 2:0 layer structure. The absence of an octahedral sheet in these compounds means that the magnitude of tetrahedral rotation must be controlled by the size of the interlayer cation and the lateral dimensions of the undistorted tetrahedral sheet.

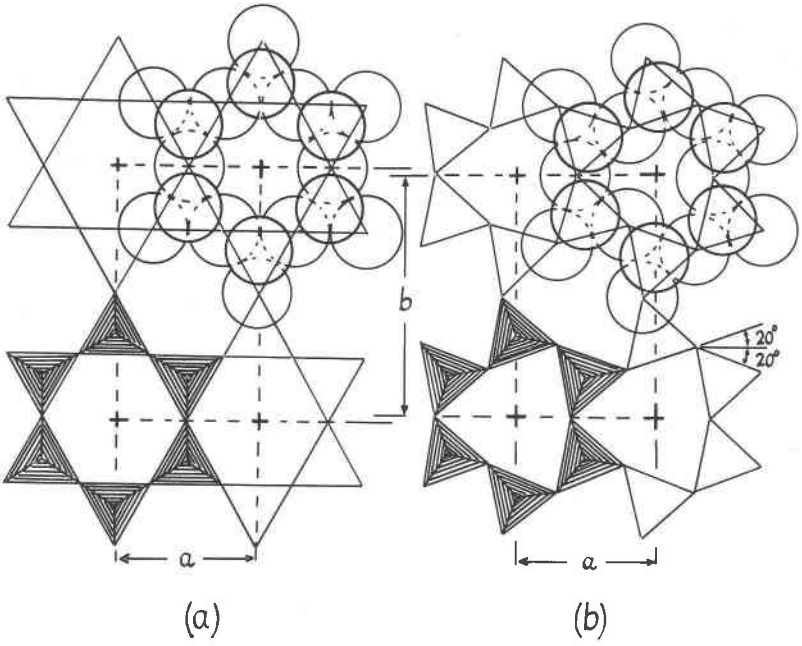

FIG. 1. Tetrahedral networks projected on (001). Large circles are oxygens. (after Brindley in Bailey *et al.*, (1967)). a. Ideal hexagonal arrangement. b. Ideal ditrigonal arrangement obtained by rotating the tetrahedra by $\alpha = \pm 20°$.

Our analysis of these distortions in mica proceeds in two stages. First a relation between Δ and α is established, and then a statistical equation is derived which relates α to ionic radii. The two equations provide some insight regarding the cause of the distortions, and can also be used to predict α and Δ in other micas.

RELATION BETWEEN α AND Δ

It is interesting to compare the ditrigonal distortion of the tetrahedral sheet with the difference (Δ) between the mean outer and inner interlayer cation (I-O) octahedral distances. A plot of Δ against α is shown in Figure 2. All the data (with the possible exception of celadonite) lie on a straight line through the origin, suggesting that Δ is a linear function of α. Notice that the data for α-$BaAl_2Si_2O_8$ and hexagonal $CaAl_2Si_2O_8$ also fall on the line. This relationship between α and Δ may be utilized to predict the interlayer structure of micas if an accurate estimate of α can be obtained. For this purpose a best fit line was calculated for the data of the 13 micas.

$$\Delta = K_{\text{obs}}\alpha \tag{1}$$

where $K_{\text{obs}} = 0.047$ Å/degree.

An approach used by Donnay *et al.*, (1964) is extended here to obtain a theoretical relation between α and Δ. Briefly, their model is an idealized one in which the basal faces of the tetrahedra are equilateral triangles parallel to (001). The triangles remain regular during the ditrigonal distortion, as in Figure 1b. From these assumptions it follows that $b = a\sqrt{3}$ for all α, and after some trigonometric manipulation,

$$\Delta = \left[\frac{4}{3}x^2 \sin^2 (60° + \alpha°) + y^2\right]^{\frac{1}{2}} - \left[\frac{4}{3}x^2 \sin^2 (60° - \alpha°) + y^2\right]^{\frac{1}{2}} \tag{2}$$

This relation between the ditrigonal parameters Δ and α involve x, the tetrahedral O-O distance, and y, one-half the interlayer thickness. Choosing typical values $x = 2.64$ Å and $y = 1.50$ Å, several values of $\Delta(\alpha)$ were calculated from (2) and plotted in Figure 2, in good agreement with the experimental points.

For small α, Eq. (2) reduces to

$$\Delta = \left(\frac{360}{\pi\sqrt{3}}\right)\left(\frac{x^2}{\sqrt{x^2 + y^2}}\right)(\alpha°) = K_{\text{calc}}\alpha° \tag{3}$$

The slope K_{calc} depends primarily on the tetrahedral layer through x and is insensitive to the interlayer distance, $2y$. Experimental values for y listed in Table 1 range from 1.4 Å in calcium micas to 1.8 Å in hydroxy-

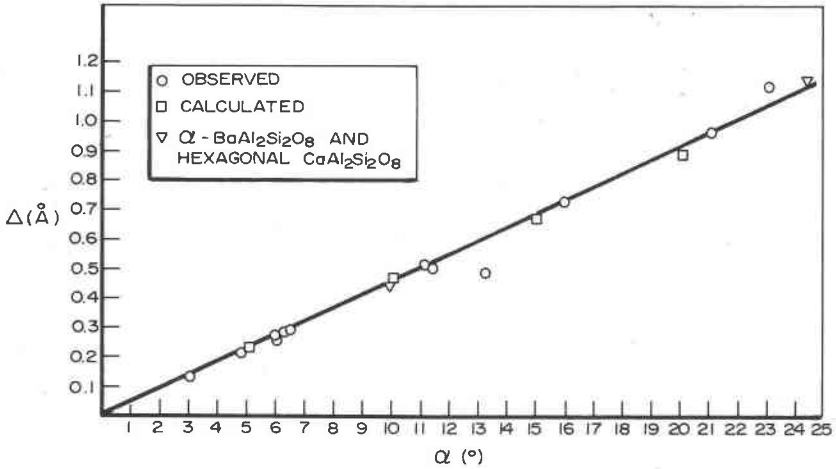

FIG. 2. Plot of the difference (Δ) between the outer and inner interlayer octahedral distances against the tetrahedral rotation angle α.

phlogopite. When substituted in equation (3) these y values hardly affect K_{calc}, changing it from 0.047 to 0.044 Å/degree, so that K_{calc} and K_{obs} are almost identical.

The preceding analysis suggests that Δ can be explained assuming regularity of tetrahedra throughout rotation. The nature of the interlayer cation, basal plane corrugation, and other deviations from the idealized model have little affect on the relation between Δ and α.

CAUSES OF DITRIGONAL DISTORTION

From the data listed in Table 1 one might conclude that tetrahedral rotation is primarily attributable to the interlayer cation; micas with smaller interlayer cations have large rotations. This is unambiguously exhibited in α-$BaAl_2Si_2O_8$ and hexagonal $CaAl_2Si_2O_8$ where α is 9.9° and 24.3° respectively. However, in micas with large interlayer cations α is considerably more variable, ranging from 3° to 13° in potassium micas. Moreover, comparing paragonite and muscovite, which are chemically alike except for the interlayer cation, α is only four degrees larger for the sodium mica. It is therefore apparent that other factors are important as well.

An analysis of dioctahedral and trioctahedral mica data led Takéuchi (1964) to conclude that the distortions in mica are primarily controlled by the octahedral sheet, while according to Franzini (1969), mica structures are primarily controlled by the interlayer cation. Neither presented

Table 1. Interlayer Sheet Structure Data for Micas and Related Structures

Composition	Interlayer Thickness (2y)	α	Outer I-O	Inner I-O	Δ	Reference
a. TRIOCTAHEDRAL MICAS						
1M-Talc $Mg_3Si_4O_{10}(OH)_2$	2.70Å	3.4°	-	-	-	Rayner (per. com.)
1M-Fluor-polylithionite $KAlLi_2Si_4O_{10}F_2$	?	3.0°	3.133Å	2.998Å	0.135Å	Takeda et al., 1967
1M-Barium mica $BaLiMg_2AlSi_3O_{10}F_2$	3.17Å	4.73°	3.192Å	2.975Å	0.217Å	McCauley & Newnham, 1969
1M-Fluorophlogopite $KMg_3AlSi_3O_{10}F_2$	3.36Å	5.88°	3.273Å	3.006Å	0.267Å	McCauley et al., 1967
1M-Hydroxyphlogopite $KMg_3AlSi_3O_{10}(OH)_2$	3.61Å	5.9°	3.33Å	3.07Å	0.26Å	Zvyagin & Mischchenko, 1962
1M-Lithium fluormica $K(Mg,Li)_3(Si,Al)_4O_{10}F_2$	3.33Å	6.2°	3.278Å	2.995Å	0.283Å	Takeda & Donnay, 1966
1M-Ferri-annite $KFe_3^{2+}Fe^{3+}Si_3O_{10}(OH)_2$	3.39Å	6.4°	3.347Å	3.054Å	0.293Å	Donnay et al., 1964a
1M-Ferriphlogopite $KMg_3FeSi_3O_{10}(OH)_2$	3.48Å	11.03°	3.458Å	2.942Å	0.516Å	Steinfink, 1962
1M-Xanthophyllite $CaMg_2AlSiAl_3O_{10}(OH)_2$	2.82Å	23.0°	3.53Å	2.41Å	1.12Å	Takéuchi & Sadanaga, 1966
b. DIOCTAHEDRAL MICAS						
$2M_1$-Pyrophyllite $Al_2Si_4O_{10}(OH)_2$	2.73	~10.5°	-	-	-	Rayner & Brown, 1964
$2M_1$-Phengite $K(Al,Mg)_2(Si,Al)_4O_{10}(OH)_2$	3.36Å	6.03°	3.237Å	2.970Å	0.267Å	Güven, 1968
$2M_1$-Muscovite $KAl_2Si_3AlO_{10}(OH)_2$	3.39Å	11.37°	3.362Å	2.855Å	0.507Å	Güven, 1968
1M-Celadonite $K(Mg,Fe)_2(Al,Si)_4O_{10}(OH)_2$	3.35Å	13.2°	3.28Å	2.79Å	0.49Å	Zvyagin, 1957
$2M_1$-Paragonite $NaAl_2Si_3AlO_{10}(OH)_2$	3.08Å	15.9°	3.371Å	2.641Å	0.730Å	Burnham & Radoslovich, 1964
$2M_1$-Margarite $CaAl_2Si_2Al_2O_{10}(OH)_2$	2.86Å	21.0°	3.43Å	2.46Å	0.97Å	Takéuchi, 1964
c. OTHERS						
α-$BaAl_2Si_2O_8$	3.26Å	9.93°	3.34Å	2.89Å	0.45Å	Takéuchi, 1958
Hexagonal $CaAl_2Si_2O_8$	2.94Å	24.28°	3.53Å	2.39Å	1.14Å	Takéuchi & Donnay, 1959

quantitative arguments, so that the primary cause of the ditrigonal distortion of the tetrahedral sheet remains open to question.

The tetrahedral-octahedral sheet misfit and the size of the interlayer cation are two likely causes of ditrigonal distortion. The relative importance of these two factors in determining the alternate rotation of tetrahedra may be obtained by statistical analysis.

First, the degree of association or co-relation between α and misfit and α and interlayer cation is obtained by calculating the linear correlation, or the coefficient of determination. For example, a perfect linear correlation would have a correlation coefficient of 1.0; a correlation coefficient of zero indicates no linear relationship. The square of the correlation coefficient (coefficient of determination) indicates the proportion of the total sum of squares of deviations in the dependent variable (*e.g.*, α) that is attributable to the independent variable (*e.g.*, misfit). Multiple regression analysis can then be used to ascertain the magnitude of the coefficients relating misfit and interlayer cation to the ditrigonal distortion. To avoid circular reasoning, the parameters expressing tetrahedral-octahedral misfit and the interlayer cation effects should be independent of the mica structure analysis data, including measured cell dimensions as well as atomic coordinates. The most difficult part of the analysis is finding the best parameters to describe quantitatively the way in which misfit and the interlayer cation affect α.

To characterize the interlayer cation, we have chosen a field strength parameter given by the ratio of valence to ionic size. Ionic radii were obtained by subtracting the O^{2-} radius (1.32 Å) from bond lengths listed in Vol. III of the International Tables (1962) for X-ray Crystallography: Ba-O 2.76, K-O 2.83, Na-O 2.44, Ca-O 2.40 Å. The assertion that α is inversely proportional to the radius of the interlayer cation requires little justification. Not only is it obvious from the examples in Table 1, but trigonometric calculations based on the idealized model of rotating regular tetrahedra also predict $\alpha \sim 1/r$. It is less obvious that α is directly proportional to valence, for experimental evidence is scanty and inconclusive. Only one Na mica and one Ba mica have been refined, making it difficult to compare micas with interlayer cations of similar size but different valence, *i.e.*, Na with Ca and Ba with K. The α value for paragonite is smaller than those of the Ca micas but the barium and potassium micas differ little in α. Theoretically it seems reasonable that highly charged interlayer cations would promote distortion in adjacent layers.

The parameter used to measure misfit should be a good estimate of the unrestrained dimensions of the tetrahedral and octahedral sheets. Assuming regular octahedra and tetrahedra, ideal dimension of the two sheets were calculated for $\alpha = 0°$ from

$$b_t = \sqrt{3}a_t = 4\sqrt{2}D_t$$

$$b_o = \sqrt{3}a_o = 3\sqrt{2}D_o.$$

D_t and D_o are tetrahedral and octahedral bond lengths, again taken from Vol. III of the International Tables: Al^{VI}-O 1.91, Mg^{VI}-O 2.10, Li^{VI}-O 2.16, Fe^{2+VI}-O 2.14, Al^{IV}-O 1.79, Si^{IV}-O 1.61, Fe^{3+IV}-O 1.86 Å. The ratio b_t/b_o $(=a_t/a_o) = 4D_t/3D_o$ was tested as a quantitative measure of α by numerically evaluating b_t/b_o for the chemical compositions of the re-

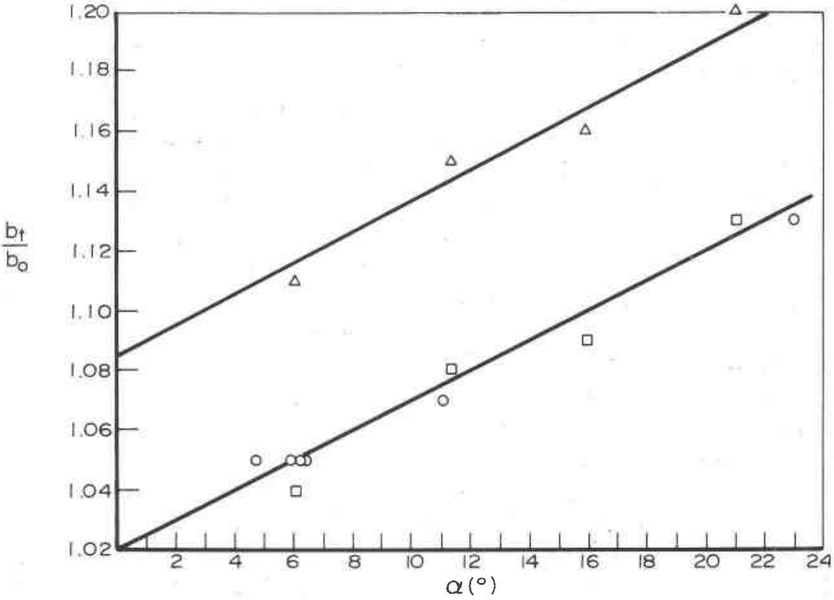

FIG. 3. Plot of tetrahedral-octahedral sheet misfit (b_t/b_o) against tetrahedral rotation angle α. Circles indicate trioctahedral micas, triangles are dioctahedral micas, and squares are empirically corrected dioctahedral mica data.

fined micas. Observed values of α are plotted against b_t/b_o values in Figure 3; all the micas in Table 1 are plotted except flour-polylithionite, hydroxyphlogopite, and celadonite. The structures of the latter two micas are not refined, and the complete structural details of the former have not been published. Note that two parallel straight lines can be drawn through the data points in Figure 3: one for dioctahedral micas and another for trioctahedral micas, with a discrepancy in intercept of 0.07. The difference is attributed to the b_o calculation for dioctahedral micas, which is in error by a larger constant amount than the trioctahedral b_o calculation because of the distortions associated with shared edges and octahedral vacancies. To test this explanation, oxygen-oxygen distances were calculated from the chemical compositions of the octahedral sheets and compared to the measured distances. Two sets of ratios,

$$\frac{\text{O-O (measured)}}{\text{O-O (calculated)}}$$

were observed. The dioctahedral micas exhibited values in the range $1.11 \pm .01$, while the trioctahedral micas yielded an average value of

1.03 ± .01. The difference 0.08 is consistent with the discrepancy between the b_t/b_o values for the two sets of data. In subsequent analyses, the b_t/b_o values were placed on the same scale by substracting 0.07 from the b_t/b_o values for dioctahedral micas.

Theoretically, it is fairly obvious that b_t/b_o provides a measure of misfit, although it is less obvious why α should vary linearly with b_t/b_o, as shown in Figure 3. A relation between α and b_t/b_o can be derived from the idealized model of rotating regular tetrahedra. From Figure 1b, it can be shown that $b=2\sqrt{3}x \cos \alpha$ where x is the tetrahedral 0-0 distance. When $\alpha=0°$, $b=b_t$, as calculated previously, so that $b_t=2\sqrt{3}\,x$. If we assume that misfit causes α to differ from zero, and that the actual value of b must conform to the octahedral layer dimension b_o, then $b_o=b_t \cos \alpha$ or

$$\alpha° \cong \frac{360}{2\pi}\sqrt{2(b_t/b_o-1)}.$$

This theoretical expression predicts α values which are about twice the size of the observed values in Table 1. The probable reason for the discrepancy is the assumption that the tetrahedral layer conforms in size to the octahedral layer. *Both* will deform since all oxides have comparable stiffness coefficients. In any case, the theroetical expression $\alpha \sim \sqrt{(b_t/b_o-1)}$ is linear for the small ranges of b_t/b_o (1.04 to 1.12 for the trioctahedral micas), justifying the choice of b_t/b_o as a measure of the dependence of α on misfit.

STATISTICAL ANALYSIS

Separate statistical analyses were carried out on the trioctahedral and dioctahedral data. The two sets of data were combined in a third analysis by empirically subtracting 0.07 from b_t/b_o values of the dioctahedral

TABLE 2. Degree of Linear Correlation Between α and Misfit, and α and field Strength of Interlayer Cation for Trioctahedral and Dioctahedral Micas.

	r_m	r_f
Dioctahedral micas	96%	74%
Trioctahedral micas	99%	49%
Trioctahedral micas and corrected dioctahedral micas	97%	53%

r_m = degree of linear correlation between α and misfit

r_f = degree of linear correlation between α and field strength

TABLE 3. Results from Multiple Regression Analysis of the Effect of Misfit and Field Strength on Tetrahedral Rotation

	r'_m	r'_f	V_m
Dioctahedral micas	0.96	0.03	97%
Trioctahedral micas	1.11	-0.15	99%
Trioctahedral and corrected dioctahedral micas	1.08	-0.12	97%
Trioctahedral and corrected dioctahedral micas using measured T-O distances	0.98	0.01	99%

r'_m = standard regression coefficient for misfit

r'_f = standard regression coefficient for field strength

V_m = percentage of variance explainable by variation in misfit only.

micas. The results obtained for the degree of linear correlation between α and b_t/b_o, and α and field strength are listed in Table 2. In the table r_m and r_f represent the degree of correlation (coefficient of determination) between α and b_t/b_o and field strength, respectively. The statistical analysis clearly indicates that there is a much larger linear relationship between α and misfit than between α and the field strength of the interlayer cation. The dioctahedral mica results are less conclusive because data from only four micas were available.

Multiple regression analysis was then used to determine the equation relating α to misfit and field strength simultaneously. The results are recorded in Table 3, where r_m and r_f are standard regression coefficients. The coefficient r_m describes the average *relative* importance of the independent parameter b_t/b_o in the determination of α, while r_f similarly characterizes the interlayer cation field strength. *Vm* is the percentage of the variance in α which can be explained by the variation in misfit alone.

The standard regression coefficients in Table 3 reveal that the interlayer cation has an average contribution of about 10% to the amount of rotation. The primary control of the ditrigonal distortion, therefore, is the tetrahedral-octahedral sheet misfit. Apparently, the major function of the interlayer cation is to hold the layers together, without appreciably altering their structure. The validity of this conclusion depends on how well the field strength represents the effect of the interlayer cation.

The equation of the multiple regression plane through the trioctahedral and empirically corrected dioctahedral mica data is as follows:

$$\alpha(^\circ) = 218.0(b_t/b_o) - 1.5\ (\text{field strength}) - 221.5. \qquad (4)$$

This equation may be used to predict the amount of tetrahedral rotation in micas from chemical composition data. Previous techniques for predicting α requires both chemical composition and lattice parameter data. Substitution of various misfits and field strengths into equation (4) shows that the relative contribution of the latter is much greater for small misfits. Barium mica is an extreme case where the interlayer cation contributes appreciably to α.

PREDICTION OF MICA STRUCTURES

The relative developed in the last sections may be utilized to predict the structure of micas from chemical composition data. First, α can be estimated using equation (4), then the interlayer structure can be approximated from equation (1). Finally, the approximate structure of the octahedral and tetrahedral sheets can be estimated using the equations derived by Donnay *et al.*, (1964b).

Other prediction techniques employ the Radoslovich (1961) formula

$$\alpha = \text{arc cos}\left(\frac{b\ (\text{observed})}{b\ (\text{unrestrained tetrahedral sheet} = b_t)}\right)$$

to calculate α. There are several methods available for calculating the unrestrained dimension of the tetrahedral sheet: Radoslovich and Norrish (1962), Brown and Bailey (1963), Donnay *et al.*, (1964b). Donnay *et al.*, (1964b) have constructed nomograms for predicting α from the measured b cell-edge and estimated T-O distances.

The prediction equations derived in this investigation do not depend on a determination of the cell edges. Since the data for fluor-polylithionite was not used in the calculation of equation (4), the usefulness of this equation and equation (1) can be illustrated with this mica. Taking the chemical composition as $KAlLi_2Si_4O_{10}F_2$, the structural parameters are estimated as $\alpha = 2.90°$, $\Delta = 0.12$ Å, in close agreement with the measured values $\alpha = 3.0°$, $\Delta = 0.135$ Å. (Takeda *et al.*, 1967; Takeda, personal communication). From the measured b cell-edge, Donnay *et al.*, (1964b) estimate that α is 12° for fluor-polylithionite. It is quite apparent that the Donnay *et al.* method is in error for polylithionite; the nomogram also predicts α values for fluorophlogopite, barium mica, and phengite which are larger than observed.

	Fluorophlogopite	*Barium Mica*	*Phengite*
α (calc-nomogram)	~7.2°	~8.5°	~10.0°
α (obs)	5.88°	4.73°	6.03°
α (equation (4))	6.4°	5.3°	4.2°

Bailey *et al.*, (1967), have shown that the agreement between α (calc) and α (obs) is much better than this for all the other micas. The cause of the discrepancy is directly related to the accuracy with which b (ideal) can be estimated. This is especially true for small rotations where α is extremely sensitive to the magnitude of b (obs)/b_t. Furthermore, for small rotations the interlayer cation is very nearly in 12-fold coordination; this is revealed by the small difference (Δ) between the outer and inner interlayer cation-oxygen distances at these angles. Hence, for small ditrigonal distortions, the basal tetrahedral O-O edges become shared edges that may be shortened in response to interlayer cation-tetrahedral cation repulsion. The shortening is probably inversely proportional to α, modified, of course, by the magnitude of interlayer thickness and the valency of the interlayer cation. Phengite and barium mica exhibit about 0.06 Å shortening of the basal 0-0 distances with respect to the basal-apical 0-0 distances; the discrepancy between α (calc) and α (obs) is largest for these two micas. On the other hand, fluorophlogopite exhibits only about a 0.03 Å shortening so the discrepancy is not as large. The same effect is also observed in lithium fluormica which has a shortening of about 0.05 Å; α (calc) = 9.0°, while α (obs) = 6.2°. The discrepancy is not as noticeable for high rotations, because α is not as sensitive to the magnitude of b (obs)/b_t.

The following calculation illustrates the results obtainable using the Radoslovich (1961) formula when the observed barium mica basal 0-0 distance (x) is used to calculate b (ideal).

$$b \text{ (ideal)} = 2\sqrt{3}\,(\text{0-0(basal)}) = 2\sqrt{3}\,(2.652\text{Å}) = 9.187 \text{ Å}$$

$$\alpha \text{ (calc)} = 4.5°$$

$$\alpha \text{ (obs)} = 4.73°$$

The agreement is very good, showing that the Radoslovich formula, and, accordingly, the Donnay *et al.*, (1964b) predictive equations will work only if accurate approximations can be obtained for the basal 0-0 distances, especially for small ditrigonal distortion–α less than about 7°.

SUMMARY

A critical examination of all refined mica structures has revealed a linear relationship between α and the difference Δ between the mean outer and inner interlayer cation-oxygen distances. The equation calculated for this line may be used to estimate the interlayer structure and bonding of micas. Using an approach based on the Donnay *et al.*, (1964b) technique it was shown that the linear dependency of interlayer structure on tetrahedral rotation can be understood simply by considering the mathematics of rotation of ideal tetrahedra.

Since a great deal of speculation has centered around the cause of tetrahedral rotation in micas, we have attempted to quantify the various factors involved. Multiple regression analysis demonstrated that on the average the primary control of the tetrahedral sheet rotation is the tetrahedral-octahedral sheet misfit and not the interlayer cation; actually, the contributions from the interlayer cation and the misfit vary for different micas depending on the magnitude of the misfit and the field strength of the interlayer cation. Barium mica, for example, is one case where the interlayer cation contributes appreciably to α.

Finally, it was shown that by using the above mathematical formulations α and Δ may be calculated knowing only the chemical composition of the mica. Furthermore, it was pointed out that shortening of the basal 0-0 edges in the tetrahedral sheet leads to erroneous values of α when using the Radoslovich (1961) formula for micas which have low values of α.

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