DETERMINATION OF CHLORITE COMPOSITIONS BY X-RAY SPACINGS AND INTENSITIES

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Abstract – The cell dimensions and compositions of four chlorites whose crystal structures have been determined in detail are used to test existing graphs and regression equations designed to give tetrahedral and octahedral compositions. It is found that the thicknesses of the tetrahedral sheet, the 2:1 octahedral sheet, the interlayer sheet, and the space between the 2:1 layer and the interlayer can vary appreciably from specimen to specimen quite independently of tetrahedral composition. Total octahedral composition, the number of octahedral vacancies, cation ordering, and the distribution of trivalent cations and of charge between the two octahedral sheets must have effects on $d(001)$ that are additional to the effect of tetrahedral composition. Nevertheless, Brindley's $d(001)$ graph and a regression equation by Kepezhinskas both should give tetrahedral compositions with an average error of 10%, or about 0·1 Al^{IV}, for most trioctahedral chlorites. They are not valid for dioctahedral or di, trioctahedral species. Equations derived from the data of von Engelhardt and of Shirozu relating the b parameter to octahedral Fe, Mn content give results with an average error of 10%, or 0·1 Fe, Mn, for the four test chlorites provided Cr is included with the Fe, Mn, as does a regression equation by Kepezhinskas that contains terms for both the b parameter and $d(001)$. Methods using the $(00l)$ intensities or structure amplitudes give less consistent results for heavy atom contents than the spacing methods, but can be used to give approximate values for the asymmetry in distribution of heavy atoms between the 2:1 octahedral sheet and the interlayer.

INTRODUCTION

THE (001) and (060) X-ray spacings have been cited extensively in the literature as empirical measures of the tetrahedral and octahedral cation populations of chlorite minerals. Increasing substitution of Al for Si in the tetrahedral sites is said to decrease the layer thickness, measured by $d(001) = c \sin \beta$. Increasing substitution of the larger Fe^{2+} ion for Mg or Al in the octahedral sites tends to increase the lateral dimensions of the layers, as measured by the $d(060)$ value. An alternative method of determining octahedral compositions makes use of the greater scattering powers of Fe, Mn, Cr, and Ni relative to Mg and Al, as recorded in the relative $(00l)$ X-ray intensities.

Four trioctahedral chlorite structures have been refined in detail to date, and a di,trioctahedral chlorite has been refined to a lesser extent. Critical analysis of these structures shows that there are pitfalls in the use of the (001) and (060) X-ray spacings, although useful quantitative information can be obtained for most specimens. Relative $(00l)$ intensities yield less reliable results than the spacing method for octahedral compositions.

TETRAHEDRAL SPACING GRAPHS

Graphs or regression equations relating $d(001)$ to tetrahedral composition or to tetrahedral and octahedral composition have been given by von Engelhardt (1942); Bannister and Whittard (1945); Hey (1954); Brindley and Gillery (1956); Kovalev (1956); Nelson and Roy (1958); Shirozu (1958); Gillery (1959); Brindley (1961); Albee (1962), and Kepezhinskas (1965). The graph of Brindley (1961) for ferrous orthochlorites incorporates data from earlier workers and may be taken as representative. It is a straight line that can be expressed as

$$d(001) = 14·55 \text{ Å} - 0·29x \qquad (1)$$

where x is the number of Al atoms per four tetrahedral sites. Brindley states that a correction seems necessary for leptochlorites having more than 4·0% Fe_2O_3 and suggests the relationship

$$d(001) = 14·55 \text{ Å} - 0·29x - 0·05Fe^{3+}. \qquad (2)$$

Albee (1962) has recast the available analyses in a slightly different form. He gives a straight line that corresponds to

$$d(001) = 14·52 \text{ Å} - 0·14x \qquad (3)$$

where $x = Al^{IV} + Al^{VI} + Cr$ in atoms per 10 cations. This form of allocation recognizes that

both tetrahedral and octahedral cations may affect $d(001)$, but does not take into account the possibility that a full complement of 4·0 tetrahedral and 6·0 octahedral cations may not be present. Lapham (1958) gives curves for the effect of octahedral and tetrahedral Cr on $d(007)$. Kepezhinskas (1965) has shown a statistical relationship between the basal spacing and total tetrahedral and octahedral

analysis, and the unit cell parameters determined by least squares refinement of X-ray powder data. Major differences from the reported data were found both in composition (primarily Si, Al) and in certain cell parameters (primarily b) for the "corundophilite" and "prochlorite" specimens. Application of equations (1–5) to the new data gives the following results:

Chlorite	$d(001)$		Tetrahedral Al			$Al^{IV} + Al^{VI} + Cr$	
	Obs.	Equation (4)	Probe	Equation (1)	Equation (5)	Probe	Equation (3)
Kämmererite	14·326 Å	14·358 Å	0·85	0·77	0·85	1·67	1·39
Corundophilite	14·270	14·299	0·98	0·97	1·00	1·80	1·79
Ripidolite	14·166	14·176	1·09	1·32	1·28	2·34	2·52
Prochlorite	14·143	14·272	1·52	1·40	1·34	2·57	2·69
			Av. Errors: 9·9%		7·8%		7·5%

composition, of the form

$$d(001) = 13·496\,kX + 0·223\,Si - 0·0064\,Al^{VI}$$
$$+ 0·107\,Fe^{3+} - 0·001\,Fe^{2+} + 0·0103\,Mg. \quad (4)$$

Cr and Mn behave like Fe^{3+} and Fe^{2+}, respectively. This equation can be combined with equation (10) for the b parameter (see next section) and converted to Å units to give an equation for tetrahedral Al (x) similar in form to equations (1–3), as follows

$$d(001) = 14·648\,\text{Å} - 0·378x. \quad (5)$$

Detailed structural refinements have been reported for kämmererite from Erzincan, Turkey (Brown and Bailey, 1963), ripidolite from the Tazawa mine, Japan (Shirozu and Bailey, 1965), prochlorite from Washington, D.C. (Steinfink, 1958, a, 1961), and corundophilite from Kenya (Steinfink, 1958, b). Chemical analyses have been reported previously for all specimens except the ripidolite. The variety names used here are those cited in the original publications. According to the classification of Foster (1962), however, the ripidolite would be brunsvigite, the corundophilite would be sheridanite, and the prochlorite would be ferric sheridanite

Because both the tetrahedral and octahedral compositions vary appreciably in these four trioctahedral chlorites, they may be used to test the reliability of equations (1–5). Preliminary testing using the published compositions and cell parameters, however, yielded poor agreement. For this reason samples of all four chlorites were obtained from the original sources. The compositions were determined by electron microprobe analysis, adjusted to give the same ratio of ferrous and ferric iron as present in the original wet chemical

The agreement between compositions determined by electron microprobe and those calculated from the revised $d(001)$ values now can be considered reasonable for all of the equations tested. Only the prochlorite specimen contains enough ferric iron to test the correction factor in equation (2). For this specimen the correction is in the wrong direction, as the corrected value for Al^{IV} of 1·15 is in poorer agreement with the probe analysis of 1·52 than is the uncorrected value of 1·40 from equation (1).

The average unweighted errors in composition, assuming the probe analyses to be correct, range from 7 to 10%, although there are individual errors ranging from 0 to 21%. The close agreement between observed and calculated values for several specimens probably is fortuitous. This is suggested by comparison of the results from the interrelated equations (4 and 5) from Kepezhinskas. For the kämmererite and corundophilite specimens the Al^{IV} values calculated by equation (5) agree closely with the observed values, but the $d(001)$ values calculated by equation (4) differ by 0·03 Å from the observed values. For the ripidolite specimen, on the other hand, the calculated $d(001)$ value differs from the observed by only 0·01 Å, whereas there is a discrepancy of 17% in observed and calculated Al^{IV} values. The reason for individual discrepancies obtained by any of the spacing equations can be appreciated better by breaking down the (001) spacing into its component sheet thicknesses for each specimen.

It can be seen from the following chart that the thicknesses of the tetrahedral sheet, the 2:1 octahedral sheet, the interlayer sheet, and the space between the 2:1 layer and the interlayer can vary appreciably from specimen to specimen quite independently of tetrahedral composition. Other

Sheet thicknesses	Kämmererite	Corundophilite	Ripidolite	Prochlorite
2:1 tet. sheet	2 × 2·259 Å	2 × 2·297 Å	2 × 2·252 Å	2 × 2·278 Å
2:1 oct. sheet	2·149	2·055	2·182	2·108
Σ = total layer	6·667 Å	6·649 Å	6·686 Å	6·664 Å
Interlayer sheet	2·026	1·912	1·975	1·898
Interlayer O–OH	2 × 2·8165	2 × 2·854	2 × 2·752	2 × 2·790
Σ = $d(001)$	14·326 Å	14·269 Å	14·165 Å	14·142 Å

factors, such as total octahedral composition, number of octahedral vacancies, cation ordering, and the distribution of trivalent cations and of charge between the two octahedral sheets must have effects on $d(001)$ that are additional to the effect of tetrahedral composition. For example, the O–OH space between the 2:1 layer and the interlayer sheet decreases nearly linearly in proportion to the octahedral $Fe + Cr + Mn + Ni$ present in these specimens (Fig. 1). This effect has been noted previously by Hayashi and Oinuma (1967) from the positions of the OH absorption bands in infrared patterns of Fe-rich chlorites. Synthetic chlorites tend to have larger (001) spacings than natural chlorites of similar composition, and Gillery (1959) attributes this difference to an uneven distribution of cations between the two octahedral sheets in the synthetic products. Crowley and Roy (1960) have found that increasing pressure during synthesis decreases $d(001)$, possibly as a result of Si,Al ordering. Octahedral vacancies also may affect the (001) spacing, as in the oxidized prochlorite specimen that has only 5·41 total octahedral cations according to microprobe analysis.

Despite the discrepancies noted above, the use of $d(001)$ graphs or regression equations will give reasonable tetrahedral compositions for most trioctahedral chlorites. This is attested by the agreement noted above for the four test chlorites and also by the fit of the points to the empirical lines in the publications cited. The examples cited serve as a warning that other sorts of structural variations may have noticeable effects on $d(001)$ and that agreement better than 7–10% between observed and calculated Al^{IV} values should not be expected unless these structural variations can be taken into account.

All of the equations cited above were derived for trioctahedral chlorites and should not be applied to dioctahedral species. Eggleton and Bailey (1967) found that trioctahedral $d(001)$ graphs predicted Al^{IV} values that were too high by 0·3–0·6 atoms for several analyzed dioctahedral chlorites. For a particular di,trioctahedral structure refined by these authors this discrepancy appears due primarily to a closer approach of the basal oxygens to the hydroxyl group of the interlayer than is found in trioctahedral species. This specimen of sudoite from the Tracy mine, Michigan,
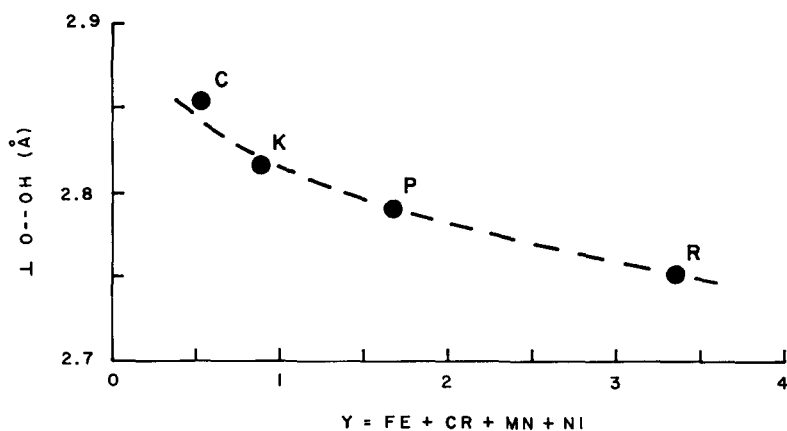

Fig. 1. Relation of octahedral atoms of $Fe + Cr + Mn + Ni$ to perpendicular O–OH distance between 2:1 layer and interlayer sheet. C = Corundophilite. K = Kämmererite, P = Prochlorite, R = Ripidolite.

has a thin dioctahedral 2 : 1 layer and a rather thick trioctahedral interlayer sheet. For specimens with two dioctahedral sheets, a thinner interlayer sheet can be predicted. This would create an additional source of error in usage of the $d(001)$ graphs.

OCTAHEDRAL SPACING GRAPHS

Von Engelhardt (1942); Brindley and MacEwan (1953); Hey (1954); Shirozu (1958); Radoslovich (1962); and Kepezhinskas (1965) have studied the dependence of $d(060)$ or of the b parameter on octahedral composition. Von Englehardt's graph is slightly curved at high Fe concentrations, primarily due to the inclusion of the 1 : 1 layer silicate cronstedtite as the Fe end member. If this point is excluded and kX units corrected to Å units, his data up to 4·0 Fe^{2+} atoms per 6·0 octahedral positions fit a straight line of the form

$$b = 9·22 \text{ Å} + 0·028 Fe^{2+}. \qquad (6)$$

The graph of Shirozu (1958) shows a linear relation

hedral sheets and of some Mg or Fe^{3+} in chlorites effectively buffers the b parameter against variations, except those due to substitutions by much larger cations such as Fe^{2+} and Mn^{2+}.

The same four chlorites used to test the $d(001)$ equations can be used to test the equations above relating b to octahedral Fe content. The results, listed below, show that von Engelhardt's revised equation (6), Shirozu's equation (7a), and its revision (7b) by Brindley give reasonable results for all four specimens, but only if all the transition metals are included in the comparison. The average unweighted errors range from 8 to 13 per cent for these methods. The results given by the Hey (8) and Radoslovich (9) equations are in poor agreement with the probe analyses. Shirozu (1958) points out that his calibration standards did not contain much Fe^{3+}, and it should be noted that the greatest absolute deviation using his equation (7a) is for the Fe^{3+}-rich prochlorite specimen. The effect of the 0·59 octahedral vacancies in this specimen is not known.

Chlorite	b_{obs}	Octahedral Fe atoms				
		Probe analysis	Engelhardt	Shirozu	Hey	Radoslovich
				Fe²⁺,Mn	Total Fe	
		Fe^{2+} Equation (6)	(7a)	(7b)	(8)	Fe^{2+} (9)
Corundophilite	9·235 Å	$Fe_{0·37}Cr_{0·15}Ni_{0·01}$	0·54	0·64	0·68	1·18	0·17
Kämmererite	9·247	$Cr_{0·75}Fe_{0·14}$	0·96	0·95	1·00	1·61	0·57
Prochlorite	9·267	$Fe_{1·66}Mn_{0·02}$	1·68	1·46	1·54	2·32	1·23
Ripidolite	9·336	$Fe_{3·30}Mn_{0·05}$	4·14	3·23	3·41	4·79	3·53
		Av. Errors: 8·4%		11·1%	12·7%	71·2%	34·0%

between the b parameter and Fe^{2+},Mn of the form

$$b = 9·210 \text{ Å} + 0·039(Fe^{2+},Mn). \qquad (7a)$$

Brindley (1961) has drawn a slightly different line through Shirozu's data points to give

$$b = 9·210 \text{ Å} + 0·037(Fe^{2+},Mn). \qquad (7b)$$

Hey (1954) gives separate factors for total Fe and Mn^{2+} as follows

$$b = 9·202 \text{ Å} + 0·028 Fe + 0·047 Mn. \qquad (8)$$

Radoslovich (1962) gives

$$b = 9·23 \text{ Å} + 0·03 Fe^{2+}(\pm 0·0285). \qquad (9)$$

Tetrahedral Al and Cr and octahedral Mg, Cr, and Fe^{3+} were not found to have significant effects on the b parameter by Radoslovich. The data were insufficient for testing the effect of Mn^{2+}. Radoslovich suggests that the presence of two octa-

Kepezhinskas (1965) has reported a statistical effect of tetrahedral Si on the b parameter, in addition to the effects of octahedral Mg, Al, Fe^{2+}, and Fe^{3+},

$$b = 9·3274 \text{ kX} - 0·0094 Mg - 0·0195 Si - 0·022 Al^{VI}$$
$$+ 0·0208 Fe^{3+} + 0·0241 Fe^{2+}. \qquad (10)$$

Cr and Mn behave like Fe^{3+} and Fe^{2+}, respectively. This equation can be combined with the previous equation (4) for $d(001)$ by Kepezhinskas to give two alternative equations for the determination of total ferruginosity F (equivalent to heavy atom content), as follows

$$F = 560·82b - 5156·05 \qquad (11)$$

or

$$F = 527·025b - 39·461d(001) - 4283·797 \qquad (12)$$

where b and $d(001)$ are in kX units. Ferruginosity is

defined as

$$F = \frac{2Fe_2O_3 + 2Cr_2O_3 + FeO + MeO + NiO}{2Fe_2O_3 + 2Cr_2O_3 + FeO + MnO + NiO + MgO} \tag{13}$$

expressed in atomic percentages.

The results of calculating the b parameter and ferruginosity by these equations are shown below for the same four chlorites, after interconversion of KX and Å units.

| Chlorite | b parameter | | Ferruginosity | | |
	Obs.	Calcld.	Probe Analysis	Equation (11)	Equation (12)
Corundophilite	9·235 Å	9·240 Å	10·1%	12·7%	11·5%
Kämmererite	9·247	9·254	14·9	19·4	15·6
Prochlorite	9·267	9·285	38·4	30·6	32·3
Ripidolite	9·336	9·330	71·7	69·2	68·7
			Av. Errors:	19·9%	9·7%

Equation (12) gives consistent ferruginosity results for all four specimens. The calculated b values compare well with the observed values, except for the prochlorite specimen that is Fe^{3+}-rich and has appreciable octahedral vacancies. The agreement between observed and calculated b values is much better than is given by an equation by Brindley and MacEwan (1953). The latter equation also takes into account both tetrahedral and octahedral substitutions, but yields calculated b values that are too small by 0·04–0·10 Å for the test specimens (treating Cr as Fe^{3+}).

INTENSITIES OF BASAL REFLECTIONS

Brown (1955) and Brindley and Gillery (1956) have calculated structure amplitudes for the $(00l)$ reflections of chlorite on the basis of different contents and distributions of octahedral heavy atoms $(Fe + Mn + Cr)$. The two octahedral sheets are separated along Z by $c/2$. For this reason the scattered contributions from the two sheets are exactly in phase for the even orders of $(00l)$ so that these F values vary as a function of total heavy atom content, irrespective of distribution between sheets. If the heavy atoms are distributed symmetrically between the two octahedral sheets, the odd order F values are independent of octahedral composition due to exact cancellation of the scattered contributions from the two sheets. The odd order F values are then entirely due to the contributions from the tetrahedral sheets. For an asymmetric distribution of heavy atoms the odd order F values have an added contribution that is a function of the difference in scattering power between the two octahedral sheets. Experimental

determination of the ratios of structure amplitudes for different $(00l)$ reflections theoretically should permit determination of total heavy atom content as well as degree of asymmetry.

Petruk (1964) has presented similar information in graphical form using experimental $(00l)$ intensities from randomly oriented powders rather than structure amplitudes. The degree of asymmetry in octahedral heavy atom distribution is determined from the ratio I_{003}/I_{005} and the total heavy atom content from the ratio $(I_{002} + I_{004})/I_{003}$. In using the latter ratio for cases of asymmetrical heavy atom distributions the observed value of I_{003} must be corrected to the value it should have for a symmetrical distribution. This is given by

$$I_{\text{symm}} = I_{\text{obs}}$$
$$\times \frac{(55\cdot5)^2}{[55\cdot5 - (\text{degree of asymmetry} \times 12\cdot3)]^2}. \tag{14}$$

Oinuma, Shimoda and Sudo (1972) have plotted the relative intensities of the first three chlorite basal reflections on a triangular diagram to show graphically the effect of varying numbers of octahedral heavy atoms and of varying degrees of asymmetry. Their preferred graph is designed for randomly oriented diffractometer mounts with Cu X-radiation. It includes the spectrum of compositional possibilities from trioctahedral through dioctahedral species.

The published structure amplitudes (F) for the four test chlorites have been used to evaluate the Brindley and Gillery tables. Odd orders of $(00l)$ were used to determine the degree of asymmetry and even orders for total heavy atom content. Alternatively, Schoen's recommendation (1962) of using the ratio F_{003}/F_{001} for asymmetry and the absolute value of F_{002} for total heavy atom content was tested also. In order to evaluate Petruk's curves and the Oinuma et al., graph the published structure amplitudes were converted to intensities (I) by the equation

$$I = F^2 \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cdot \cos \theta}.$$

Chlorite	Degree of asymmetry					Total heavy atoms				
	Structure	B & G	Petruk	Schoen	O,S,S	Probe Analysis	B & G	Petruk	Schoen	O,S,S
Corundophilite	0·0	−0·29	−0·10	−0·19	−0·20	0·53	0·23	0·26	0·60	0·67
Kämmererite	−0·7	−0·55	−0·89	−0·33	−0·33	0·89	0·52	0·99	0·75	0·75
Prochlorite	+0·65	+0·46	+0·60	+0·38	+0·40	1·68	2·47	1·66	2·50	2·45
Ripidolite	+0·6	+0·42	+0·84	+0·04	0·0	3·35	4·99	2·88	4·35	4·60
						Av. Errors: 48·6%	19·3%	26·9%	31·3%	

The results are listed above.

Both the Brindley and Gillery tables and Petruk's curve give values of asymmetry (defined as the number of heavy octahedral atoms in the 2 : 1 layer minus those in the interlayer hydroxide sheet) that are approximately in agreement with those determined from the structural refinements, although not in detail. The best values for total heavy atom content are those given by Petruk's curve, but even these deviate from the microprobe analyses by an average of 19%. There are at least two reasons why these intensity methods fail to give better agreement with analysis both for asymmetry and heavy atom content.

(1) The calculated F and I values are based on ideal z parameters of the atoms. The actual z parameters differ from the ideal as a result of the compositional and structural variations in sheet thicknesses documented in a previous section of this paper.

(2) The values for asymmetry and heavy atom content are very sensitive to small changes in F or I. Experimental errors of ± 5 per cent must be expected in individual F or I values. Applying this error to the Brindley and Gillery table for F_{007} as an example, a true F value of 40 should give 0·00 asymmetry but F values of 38 and 42 would give $+0·33$ and $-0·33$, respectively. Likewise in the table for F_{002}, a true F value of 80 would give a total Fe content of 4·00 atoms but values of 76 and 84 would give values of 3·56 and 4·40 atoms, respectively.

CONCLUSIONS

Based on comparison with the four test chlorites, both tetrahedral Al and total octahedral heavy atoms can be estimated by X-ray spacing methods with an average error of about 10%, although individual determinations may be in error up to 20%. A 10% error for these specimens corresponds approximately to 0·1 atoms of Al^{IV} or Fe^{2+}.

Tetrahedral Al is estimated best by $d(001)$ equation (1) from Brindley (1961) or equation (5) from Kepezhinskas (1965). An estimate of $Al^{IV} + Al^{VI} + Cr$ can be obtained with equal accur-

acy from equation (3) from Albee (1962). Some caution must be used in such estimates because structural factors and octahedral composition may affect $d(001)$ quite independently of tetrahedral Al content. For example, the four test chlorites do not show a linear variation of $d(001)$ with Al^{IV}, primarily as a result of the closer approach of the 2 : 1 layer and the interlayer with increasing heavy atom content (Fig. 1). The corundophilite and ripidolite specimens have comparable Al^{IV} values, yet $d(001)$ for ripidolite is 0·1 Å smaller than that for corundophilite because of the large iron content of the former.

Total octahedral heavy atoms are estimated best by b parameter equation (6) derived from the data of von Engelhardt (1942), by equations $(7a)$ and $(7b)$ from the data of Shirozu (1958), or by regression equation (12) from Kepezhinskas (1965). Methods using the relative intensities or structure amplitudes of the basal reflections are not as accurate as the spacing methods because of (1) variation in the z parameters of the atoms independent of heavy atom content and (2) the extreme sensitivity of F and I to heavy atom content. Such methods are at present the only means short of structural analysis, however, for determining any asymmetry in the distribution of heavy atoms between the 2 : 1 octahedral sheet and the interlayer. Best results for asymmetry were obtained using the tables of Brindley and Gillery (1956) or the curve of Petruk (1964).

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Résumé – Les dimensions de la maille et les compositions de quatre chlorites dont les structures cristallines ont été déterminées d'une façon précise, sont utilisées pour tester les abaques et les équations de régression dont on dispose et qui sont destinées à donner les compositions tétraédriques et octaédriques. On a trouvé que les épaisseurs de la couche tétraédrique, de la couche octaédrique 2 : 1 et de la couche interlamellaire et que la distance entre la couche 2 : 1 et la couche interlamellaire peuvent varier d'une façon appréciable d'un échantillon à l'autre d'une façon tout à fait indépendante de la composition tétraédrique. La composition octaédrique totale, le nombre de lacunes octaédriques, l'arrangement des cations, et la distribution des cations trivalents et de la charge entre les deux couches octaédriques doivent avoir un effet sur d(001) qui s'ajoute à l'effet de la composition tétraédrique. Néanmoins, l'abaque d(001) de Brindley et une équation de régression proposée par Kepezhinskas devraient toutes les deux donner les compositions tétraédriques avec une erreur moyenne de 10%, soit environ 0,1 Al^{IV}, pour la plupart des chlorites trioctaédriques. Elles ne sont pas valables pour les minéraux dioctaédriques ou di, trioctaédriques. Les équations tirées des données de Von Engelhardt et de Shirozu reliant le paramètre b à la teneur en Fe, Mn octaédrique donnent des résultats entachés d'une erreur moyenne de 10%, soit 0,1 Fe, Mn, pour les quatre chlorites étudiées, à condition que Cr soit inclus dans Fe, Mn, ceci au même titre qu'une équation de régression proposée par Kepezhinskas et qui contient des termes à la fois pour le paramètre b et d(001). Les méthodes utilisant les intensités (001) ou les amplitudes de structure donnent des résultats moins satisfaisants pour les teneurs en atomes lourds que la méthode des espacements, mais elles peuvent être utilisées pour obtenir une valeur approchée de l'asymétrie de la distribution des atomes lourds entre les couches octaédriques 2 : 1 et interlamellaire.

Kurzreferat – Die Zelldimensionen und Zusammensetzungen von vier Chloriten, deren Kristallgefüge in Detail bestimmt worden sind, wurden verwendet um bestehende Kurven und Regressionsgleichungen, ausgelegt für tetraedrische und oktaedrische Zusammensetzungen, zu überprüfen. Es wurde gefunden, dass sich die Dicken der tetraedrischen Tafel, der 2:1 oktaedrischen Tafel, der Zwischenschichttafel, sowie der Abstand zwischen der 2:1 Schicht und der Zwischenschicht von Probe zu Probe beträchtlich von einander unterscheiden können, und zwar ganz unabhängig von der tetraedrischen Zusammensetzung. Die gesamte oktaedrische Zusammensetzung, die Zahl von oktaedrischen Leerstellen, Kationenordnung, und die Verteilung von dreiwertigen Kationen und von Ladung zwischen zwei oktaedrischen Tafeln müssen Wirkungen auf $d(001)$ ausüben, die zusätzlich zu der Wirkung tetraedrischer Zusammensetzung sind. Trotzdem sollten sowohl Brindleys $d(001)$ Kurve und eine Regressionsgleichung von Kepezhinskas tetraedrische Zusammensetzungen mit einem Durchschnittsfehler von 10%, oder etwa 0,1 Al^{IV}, für die meisten trioktaedrischen Chlorite geben. Sie gelten nicht für dioktaedrische oder di, trioktaedrische Sorten. Aus den Daten von von-Engelhardt und Shirozu abgeleitete Gleichungen, die den b Parameter auf oktaedrischen Fe, Mn Gehalt beziehen, geben Resultate mit einem Durchschnittsfehler von 10%, oder 0,1 Fe, Mn für die vier Test-Chlorite, vorausgesetzt Cr wird mit Fe, Mn miteinbezogen. Das gleiche trifft zu auf eine Regressionsgleichung von Kepezhinskas die Ausdrücke für den b Parameter sowie $d(001)$ enthält. Methoden unter Verwendung der $(00l)$ Intensitäten oder Gefügeamplituden geben weniger übereinstimmende Ergebnisse für Gehalte an schweren Atomen als die Abstandsmethoden, können jedoch dazu verwendet werden um ungefähre Wert für die Asymmetrie in der Verteilung von schweren Atomen zwischen der 2:1 oktaedrischen Tafel und der Zwischenschicht zu erhalten.

Резюме — Для проверки существующих графиков и уравнений регрессии, построенных для выявления тетраэдрального и октаэдрального составов, используются размеры и состав зерен четырех хлоритов, структура кристаллов которых была детально определена. Нашли, что толщина тетраэдрального слоя; 2:1 октаэдрального слоя; промежуточного слоя и расстояние между 2:1 слоем и прослойкой может от образца к образцу значительно варьировать совершенно независимо от тетраэдрального состава. Общий октаэдральный состав; количество октаэдральных ваканций; расположение катионов; распределение тривалентных катионов и заряда между двумя октаэдральными слоями, добавочно влияющими на тетраэдральный состав, должны также влиять на $d(001)$. Несмотря на это, график Бриндлей $d(001)$ и уравнение регресси Кепежинсказкого должны давать тетраэдральный состав со средней 10%-ой ошибкой, или около 0,1 Al^{IV}, для большинства тетраэдральных хлоритов. Это не относится к диоктаэдральным и ди, триоктаэдральным образцам. Уравнения, построенные на данных фон Энгельгарта и Широдзу, относящие параметр b к октаэдральному содержанию Fe, Mn дают результаты со средней 10%-ой ошибкой, или 0.1 Fe, Mn для четырех хлоритов под испытанием при условии, что Cr включается вместе с Fe, Mn, как это приведено в уравнении регрессии Кепежисказкого, включающее члены как для параметра b так и для $d(001)$. Методы, применяющие интенсивности $(0,0,1)$ или амплитуды структуры, дают менее согласованные результаты на содержание тяжелых атомов, чем методы расстояния, но их можно использовать для получения *приблизительных значений несимметричного распределения тяжелых атомов между 2:1 октаэдральными слоями и промежуточным слоем.*