American Mineralogist, Volume 69, pages 122–127, 1984

The crystal structure of paragonite-$2M_1$

CHENG-YI LIN[1] AND S. W. BAILEY

Department of Geology and Geophysics
University of Wisconsin-Madison
Madison, Wisconsin 53706

Abstract

The structure of a near end member paragonite-$2M_1$ was refined in $C2/c$ symmetry to a residual of 4.5% with 698 non-zero independent reflections. Attempted refinement in Cc symmetry was not successful. Tetrahedral Si,Al cations are disordered, and the mean T–O distances are in accord with prediction. The small interlayer Na cation facilitates a larger tetrahedral rotation angle (16.2°), smaller b-repeat (8.898Å), and smaller interlayer separation (3.053Å) than observed for muscovite-$2M_1$. It also allows an offset of adjacent 2:1 layers across the interlayer gap that significantly reduces the β angle and is due to mutual repulsion between oxygen anions brought into proximity by tetrahedral tilting.

Introduction

Paragonite, the Na analogue of muscovite, is an abundant rock-forming mineral in low-grade and medium-grade metamorphic rocks. There is a solid solution between paragonite and muscovite and a slightly asymmetric unmixing solvus. Naturally occurring end member paragonite has not been reported.

The most abundant polytype for paragonite is $2M_1$, although the 3T form also has been recognized in nature and the 1M form can be made synthetically. The $2M_1$ and 3T paragonite polytypes may coexist with very similar compositions (Nakamura and Kihara, 1977). Burnham and Radoslovich (1964) refined the structures of coexisting natural sodian muscovite-$2M_1$ ($K_{0.65}Na_{0.35}$) and potassian paragonite-$2M_1$($Na_{0.85}K_{0.15}$) by single crystal X-ray techniques. Soboleva *et al.* (1976) used high voltage texture electron diffraction patterns to refine the structure of a fine grained synthetic paragonite-1M ($Na_{0.91}K_{0.09}$). Sidorenko *et al.* (1977a,b) applied the same technique for the refinement of natural fine grained $2M_1$ ($Na_{0.06}K_{0.10}Ca_{0.03}\square_{0.27}$) and 3T ($Na_{0.71}K_{0.16}Ca_{0.03}\square_{0.10}$) forms of paragonite. This paper reports refinement of a near end member paragonite-$2M_1$ ($Na_{0.92}K_{0.04}Ca_{0.02}\square_{0.02}$) structure by single crystal X-ray methods. The research was investigated in order to provide more accurate parameters of a paragonite without appreciable interlayer K or vacancies to serve as a reference for comparison with the structures of other Na-micas. Attention will be focused on the interlayer region.

Experimental

Several homogeneous paragonites of near end member composition (~4 mole% muscovite) were kindly furnished by Prof. Dr. Martin Frey of the University of Basel and Professor C. V. Guidotti of the University of Maine. A suitable but thin lath-shaped single crystal 0.32 × 0.25 × 0.018 mm in size was obtained from sample PVB 1705, originally collected by Prof. Dr. Peter Bearth of the University of Basel from a glaucophane-bearing metamorphosed eclogite from the ophiolite zone of Zermatt-Saas Fee in the Swiss Alps. The occurrence is described by Bearth (1973) and Bearth and Stern (1979). An electron microprobe analysis (Table 1) of this sample by C. A. Geiger of this department shows that only one mica is present and gives a resultant formula of ($Na_{0.916}K_{0.042}Ca_{0.018}\square_{0.024}$) ($Al_{1.990}Fe_{0.028}Mg_{0.013}Ti_{0.003})_{2.034}(Si_{2.939}Al_{1.061})O_{10}(OH)_2$.

Cell dimensions of a = 5.128(2)Å, b = 8.898(3)Å, c = 19.287(9)Å, and β = 94.35(3)° were obtained by least squares refinement of 15 reflections on a Nicolet $P2_1$ automated single crystal diffractometer. These also indicate a near end member composition. Data for 5449 reflections were obtained out to 2θ = 60° in all eight octants of the limiting sphere. The $2\theta:\theta$ variable scan technique with monochromatic Mo$K\alpha$ radiation was used. Crystal and electronic stability were checked after every 50 reflections by monitoring a standard reflection. Integrated intensities were corrected for Lp and absorption effects and symmetry-averaged to 698 non-zero independent monoclinic reflections. The absorption correction was produced by the empirical ψ scan technique in which the data are compared to complete ψ scans (10° increments of ϕ) for selected reflections spaced at 2θ

---

[1] Present address: Department of Geology, Nanjing University, China.

0003–004X/84/0102–0122$02.00

Table 1 Electron microprobe analysis (wt.%).

	1	2	3	4	mean	atoms		
SiO_2	46.10	45.90	45.36	46.45	45.953	Si	2.939	4.00
						Al^{IV}	1.061	
Al_2O_3	40.51	40.53	40.79	40.06	40.473	Al^{VI}	1.990	2.034
TiO_2	0.05	0.06	0.06	0.12	0.073	Ti	0.003	
FeO	0.56	0.50	0.49	0.58	0.533	Fe^{2+}	0.028	
MgO	0.15	0.12	0.11	0.15	0.133	Mg	0.013	
MnO	0.01	0.00	0.00	0.00	0.003	Mn	--	
CaO	0.24	0.29	0.29	0.25	0.267	Ca	0.018	0.976
BaO	0.03	0.00	0.00	0.02	0.013	Ba	--	
K_2O	0.63	0.45	0.45	0.52	0.513	K	0.042	
Na_2O	7.36	7.39	7.34	7.46	7.388	Na	0.916	
H_2O (diff.)	4.36	4.76	5.11	4.39	4.651			

intervals of 5°. There were no violations of the *C*-centering or *c*-glide extinctions.

Refinement

Least squares refinement with program ORFLS was initiated in *C2/c*, the ideal space group of the $2M_1$ structure. Scattering factors appropriate for 50% ionization were taken from Cromer and Mann (1968). Unit weights were used throughout refinement because experience in this laboratory has shown them to be superior to sigma weights for the intensity distribution found in layer silicates, where there is a great differential in intensity between $k = 3n$ and $k \neq 3n$ indices. Atomic coordinates for the structure of potassian paragonite (Burnham and Radoslovich, 1964), kindly furnished by C. W. Burham, were used as the initial coordinates for several cycles of refinement. Fixed isotropic B values were used at first and no cation ordering was assumed in the choice of scattering factors. Variable isotropic B values were used, followed by variable anisotropic values. Refinement proceeded smoothly from an initial residual of 0.157 to a final *R* of 0.045. On a final difference map, all atom positions were close to zero density (range 0.02 to 0.06 electrons/Å^3) and the position of the proton of the OH group was visible as a peak of 0.24 electrons/Å^3. The position of the hydrogen was not refined. Tables 2–6 report the experimental data, final atomic coordinates, thermal ellipsoid orientations, bond lengths, and other important structural features.[2]

Because refinement in the ideal space group *C2/c* indicated no ordering of the tetrahedral cations, refinement in subgroup *Cc* also was attempted. The procedure used for margarite-$2M_1$ and muscovite-$2M_1$ by Guggenheim and Bailey (1975) was followed. Only one ordering pattern of Si and Al in tetrahedral sites is possible in *Cc* symmetry that is consistent with Si,Al disorder in sites T(1) and T(2) of the *C2/c* space group. This is the ordering pattern found in margarite-$2M_1$. Non-centric atomic coordinates for this pattern were derived by use of distance-least-squares program OPTDIS, and refinement of these coordinates was attempted with program ORFLS. One octahedral cation was held constant in position in order to fix the origin in this noncentrosymmetric *Cc* space group. This refinement was not successful. Although the Al-rich tetrahedra remained larger than the Si-rich tetrahedra, individual T–O bond lengths differed by as much as 0.25Å within the same tetrahedron and convergence ceased near *R* = 10%.

Discussion of the structure

Many of the structural features of paragonite-$2M_1$ are very similar to those found in other dioctahedral micas and need not be discussed further. These features include the shapes of the individual tetrahedra and octahedra, the tetrahedral and octahedral sheet thicknesses, and the mean T–O and M–O,OH distances (Tables 5 and 6).

Tetrahedral positions and bond lengths

The angle of tetrahedral rotation of 16.2° (Table 6) is several degrees larger than reported for muscovite (11.3° in the structure by Rothbauer (1971)). This is correlated with the observations that the *b* repeat of paragonite-$2M_1$ (8.898Å) is smaller than that of muscovite-$2M_1$ (9.105Å) and that the interlayer separation is smaller (3.053Å *vs.* 3.480Å). Radoslovich (1963) pointed out that in muscovite the interlayer K is too large for its 6-coordinated hole after full tetrahedral rotation has taken place to relieve the lateral misfit between the tetrahedral and octahedral sheets. As a result the interlayer K prevents rotation from proceeding to its full extent; the octahedral sheet is stretched laterally to compensate for the incomplete rotation, and adjacent 2:1 layers are propped apart by 0.8Å by the K relative to pyrophyllite. Verification of this effect was provided by Burns and White (1963) who showed that the *b* repeat distance decreases as K is leached from muscovite. Na is 0.36Å smaller in ionic radius than K, and allows both greater tetrahedral rotation to relieve the lateral misfit and a closer approach of adjacent layers. The basal oxygen surfaces are still not in contact, however, as judged by the $(c\sin\beta)/2$ value of 9.62Å in paragonite-$2M_1$ relative to 9.20Å in pyrophyllite-1Tc where there is no interlayer cation and the surfaces should be in contact.

The tetrahedral rotation value of 16.2°, the mean Na–O value of 2.62Å, and the interlayer separation of 3.053Å are quite close to the values given by Burnham and Radoslovich (1964) for potassian paragonite (15.9°,

---

[2] Table 2 of observed and calculated structure amplitudes and Table 4 of thermal ellipsoid orientations may be obtained by ordering document AM-83-236 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D.C. 20009. Please remit $5.00 in advance for the microfiche.

Table 3. Atomic parameters for paragonite-$2M_1$ in *C*2/*c*, with esd's in parentheses

Atom	x	y	z	$B_{equiv.}$	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
T(1)	0.9528(3)	0.4288(2)	0.1409(1)	0.93	0.0050(4)	0.0017(2)	0.00114(4)	−0.0003(2)	0.0002(1)	0.00005(8)
T(2)	0.4401(3)	0.2578(2)	0.1409(1)	0.95	0.0056(5)	0.0016(2)	0.00116(5)	0.0001(3)	0.0002(1)	0.00002(8)
M(1)	0.2500	0.7500	0.0000							
M(2)	0.2499(3)	0.0832(2)	−0.00002(10)	0.90	0.0051(5)	0.0015(2)	0.00112(4)	−0.0006(3)	−0.0001(1)	0.00012(8)
Na	0.0000	0.0941(5)	0.2500	2.85	0.0218(18)	0.0095(7)	0.0021(1)	−0.0041(66)	0.0025(4)	0.0013(2)
O(1)	0.9574(7)	0.4439(7)	0.0554(2)	1.11	0.0051(13)	0.0020(4)	0.0014(1)	0.0008(6)	−0.0001(3)	0.00001(20)
O(2)	0.3795(7)	0.2516(4)	0.0554(2)	1.08	0.0074(12)	0.0015(4)	0.0013(1)	−0.0002(6)	0.0002(3)	0.00008(20)
OH	0.9518(7)	0.0628(4)	0.0512(2)	1.11	0.0061(12)	0.0024(4)	0.0013(1)	−0.0008(6)	0.0004(3)	−0.0005(2)
O(3)	0.3739(8)	0.0914(5)	0.1743(2)	1.50	0.0134(14)	0.0027(4)	0.0015(1)	−0.0007(6)	0.0004(3)	0.0002(2)
O(4)	0.7491(8)	0.2960(4)	0.1628(2)	1.48	0.1221(14)	0.0029(4)	0.0015(1)	−0.0001(7)	0.0004(4)	0.0005(2)
O(5)	0.2475(8)	0.3818(4)	0.1748(2)	1.45	0.0111(14)	0.0026(4)	0.0016(1)	0.0009(7)	0.0007(3)	0.00001(20)
H	0.8866	0.1458	0.0706							

2.640Å, and 3.078Å, respectively) and are all in the direction expected for a specimen closer to the ideal end member composition. The differences relative to the $2M_1$, 3T, and 1M paragonite structures determined by high voltage texture electron diffraction patterns reflect in part the larger determinative errors in the latter structures. The tetrahedral rotation values for these three structures range from 15.7° to 19.1°, the mean Na–O bond lengths

Table 5. Calculated bond lengths and angles, with esd's in parentheses

Bond lengths (Å)		Bond angles (°)	
	Tetrahedron T(1)		
T(1)-O(1)	1.655(5)		
-O(3)	1.647(5)		
-O(4)	1.653(4)		
-O(5)	1.655(5)		
mean	1.653		
O(1)-O(3)	2.704(6)	O(1)-T(1)-O(3)	110.0(2)
-O(4)	2.738(6)	-O(4)	111.7(2)
-O(5)	2.702(7)	-O(5)	109.4(2)
O(3)-O(4)	2.711(6)	O(3)-T(1)-O(4)	110.4(2)
-O(5)	2.673(6)	-O(5)	108.1(2)
O(4)-O(5)	2.661(6)	O(4)-T(1)-O(5)	107.1(2)
mean	2.698	mean	109.5
	Tetrahedron T(2)		
T(2)-O(2)	1.654(5)		
-O(3)	1.661(5)	T(1)-O(3)-T(2)	124.6(2)
-O(4)	1.644(5)	-O(4)-	134.2(2)
-O(5)	1.649(4)	-O(5)-	124.7(2)
mean	1.652	mean	127.8
O(2)-O(3)	2.702(6)	O(2)-T(2)-O(3)	109.2(2)
-O(4)	2.728(6)	-O(4)	111.6(2)
-O(5)	2.709(6)	-O(5)	110.2(2)
O(3)-O(4)	2.670(6)	O(3)-T(2)-O(4)	107.8(2)
-O(5)	2.664(6)	-O(5)	107.2(2)
O(4)-O(5)	2.709(6)	O(4)-T(2)-O(5)	110.7(2)
mean	2.697	mean	109.5
	Interlayer inner	cation outer	
Na-O(3)	2.496(4)	3.425(4)	
-O(4)	2.718(5)	3.438(6)	
-O(5)	2.657(5)	3.248(5)	
mean	2.624	3.370	
H--O(H)	0.904	∢H-O(H) to (001)	24.4°

Bond lengths (Å)		Bond angles (°)	
	Octahedron M(1)		
M(1)-O(1)	2.253x2	O(1)-M(1)-O(2)	81.1(2)x2
-O(2)	2.249x2	-OH	79.6(2)x2
-OH	2.160x2	O(2)-M(1)-OH	79.6(2)x2
mean	2.221	mean [shared M(2)]	80.1
O(1)-O(2)	3.421(5)x2	O(1)-M(1)-O(2)	98.9(2)x2
-OH	3.392(5)x2	-OH	100.4(2)x2
O(2)-OH	3.388(5)x2	O(2)-M(1)-OH	100.4(2)x2
mean(unshared)	3.400	mean (unshared)	99.9
	Octahedron M(2)		
M(2)-O(1)	1.908(4)		
	1.923(4)		
-O(2)	1.907(4)		
	1.930(4)		
-OH	1.891(4)		
	1.891(4)		
mean	1.908		
O(1)-O(2)	2.759(5)	O(1)-M(2)-O(1)	92.2(2)
	2.767(5)		92.3(2)
-OH	2.754(6)	-OH	92.5(2)
	2.795(6)		94.8(2)
O(2)-OH	2.759(5)	O(2)-M(2)-OH	92.5(2)
	2.795(5)		94.8(2)
mean(unshared)	2.772	mean (unshared)	93.2
O(1)-O(1)	2.430(9)	O(1)-M(2)-O(1)	78.8(1)
O(2)-O(2)	2.430(8)	O(2)-M(2)-O(2)	78.6(2)
OH - OH	2.353(8)	OH -M(2)- OH	77.0(2)
mean[shared M(2)]	2.404	mean [shared M(2)]	78.1
O(1)-O(2)	2.927(6)	O(1)-M(2)-O(2)	98.9(2)
-OH	2.825(5)	-OH	96.1(2)
O(2)-OH	2.824(6)	O(2)-M(2)-OH	96.1(2)
mean[shared M(1)]	2.859	mean [shared M(1)]	97.0

Table 6. Other structural features of paragonite-$2M_1$

Tetrahedral rotation	α		16.2°	
Tetrahedral angle	τ	T(1)	110.4°	
		T(2)	110.3°	
Octahedral rotation	ω		8.3°	
Octahedral flattening	ψ	M(1)	62.1°	
		M(2)	57.0°	
		Na	54.4°	
Octahedral distortion*			RMS	$(\sigma\theta)^2$
		M(1)	7.24	107.7°
		M(2)	5.43	58.9
Sheet thickness: tetrahedral			2.243Å	
octahedral			2.078Å	
Interlayer separation			3.053Å	
Basal oxygen corrugation Δz			0.226Å	
Intralayer shift			$+ 0.374a_{2,3}$	
Layer offset			$+ 0.045a_{1,1}$	
Resultant shift			$- 0.285a_1$	

*RMS octahedral distortion parameter is defined by Dollase (1969) as the rms-deviation of the 15 octahedral angles from their ideal values. $(\sigma\theta)^2$ is defined by Robinson et al. (1971) as $\sum_{i=1}^{12}(\theta_i-90°)^2/11$, where θ_i is the observed O-M-O angle.

from 2.56Å to 2.62Å, and the interlayer separations from 3.00 to 3.06Å. The predicted rotation angle for the paragonite of this chemical composition is 13.7° according to the equation of McCauley and Newnham (1971) and using their suggested bond length values. The difference between the observed and predicted angles suggests that the latter study needs revision to incorporate newly refined mica structure data and new values for bond lengths.

The mean T–O bond lengths (Table 5) for T(1) and T(2) are nearly identical; hence, tetrahedral Si and Al show long-range disorder in paragonite-$2M_1$, just as in muscovite-$2M_1$. The observed mean T–O values of 1.652Å and 1.653Å are in excellent agreement with the value of 1.652Å predicted by the regression equation of Hazen and Burnham (1973) for micas. Mean T–O values for the other four paragonite structures reported in the literature are 1.666Å ($2M_1$ structure by Sidorenko *et al.* (1977a)), 1.652Å ($2M_1$ by Burnham and Radoslovich (1964)), 1.659Å (1M by Soboleva *et al.* (1976)), and 1.646Å (3T by Sidorenko *et al.* (1977b)). Drits (1975) noted that T–O bond lengths tend to be slightly greater for trioctahedral layer silicates than for dioctahedral forms, but Zvyagin and Soboleva (1979) believed that the paragonites were exceptions to this generalization. They explained that the larger T–O bonds observed in the paragonites studied by electron diffraction were a result of attraction of the basal oxygens by the small Na ions imbedded in the ditrigonal cavities. This was considered to cause both a large rotation angle and a lengthening of the T–O bonds. This effect is not substantiated by the present study.

Beta angle and interlayer region

Each 2:1 layer of the $2M_1$ structure ideally has a stagger or intralayer shift of $a/3$ of the upper tetrahedral sheet relative to the lower tetrahedral sheet. Adjacent layers are positioned so that the directions of stagger alternate regularly by angles of +120°, −120°, +120° . . . . If the hexagonal rings of adjacent layers exactly superimpose around the interlayer cation there is a resultant shift of $-a/3$ between layer 1 and layer 3 to give a resultant beta angle of 95°. In most K-micas the observed resultant shift and β angle are larger than ideal as a consequence of octahedral flattening and rotation and of M(1) being larger than M(2). These structural effects cause the stagger within each layer to be appreciably larger than $a/3$, and in addition there is a small offset of adjacent layers around the interlayer K. In the paragonite of this study the intralayer staggers are $+0.374a$ instead of $0.333a$, quite similar to those in the $2M_1$ K-micas, but adjacent 2:1 layers are offset around the interlayer Na by $+0.045a_1$ = 0.23Å. This offset is five times the magnitude of the offset reported for muscovite-$2M_1$ by Rothbauer (1971), and is opposite in direction so that β is reduced in size rather than increased, (β = 94.35° relative to 95.74°).

A similar reduction in β angles has been noted in the other paragonite structures in the literature. Soboleva *et al.* (1977) explain the observed offsets of layers around the interlayer Na as the overall result of mutual repulsion between tetrahedral cations of adjacent layers, interaction of the H proton with the interlayer cation, and mutual repulsion of oxygen anions across the interlayer gap. Although the first factor is strongest it does not provide the required lateral offset, which must be due to the second and third factors. The authors attribute the positive direction of layer offset observed in paragonite-1M to a relatively small corrugation of the basal oxygen surface (Δz = 0.10Å) so that the interaction of the H proton (directed toward the vacant M(1) site) with the interlayer cation becomes dominant in the 1M form. According to this explanation the more corrugated basal surfaces found in most other dioctahedral micas would accentuate repulsion between the closest oxygens of adjacent layers and would tend to displace the upper layer in the opposite direction (along $-\mathbf{a}_1$ rather than $+\mathbf{a}_1$) relative to the lower layer.

The explanation above requires modification because the H proton has been shown to be quite pliant in position in dioctahedral micas due to its repulsion by the interlayer cation. It is not likely to be able to cause an offset of an entire 2:1 layer by 0.23Å. For paragonite-1M, discussed by Soboleva *et al.* (1977), it is also true that the symmetry precludes any resultant shift of the Na by the H proton, because the 2-fold rotation axis through the Na relates a H^+ below to an oppositely directed H^+ at an equal distance above. For the paragonite-$2M_1$ of this study the H^+ protons are on the same side of the Na and would tend to repel it along $-\mathbf{b}_1$ (Fig. 1) if forceful enough. No such effect is noted. Instead the corrugation of the basal oxygen surfaces (Δz = 0.23Å) due to tetrahedral tilting around the vacant M(1) site places O(3) atoms of adjacent layers in closest contact (3.102Å), and repulsion between

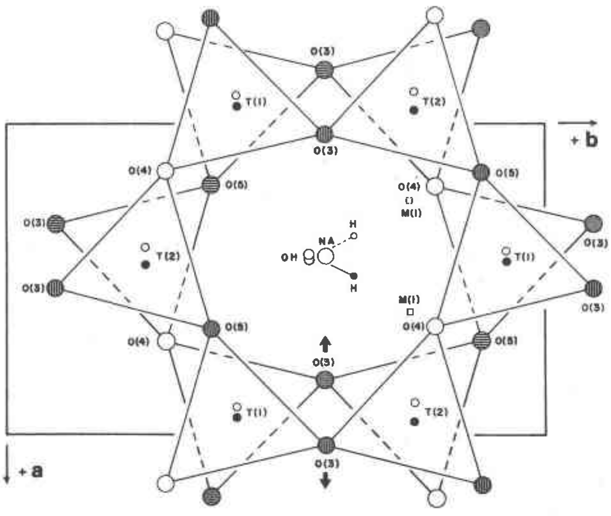

Fig. 1. Projection of interlayer region between layers 1 and 2 onto (001). Tetrahedral tilting around vacant M(1) sites moves O(4) atoms (unshaded) away from median plane at $z = 0.25$. Repulsion between O(3) atoms in closest contact offsets upper layer along $+\mathbf{a}$. Cations above median plane shown as solid circles.

them shifts the upper tetrahedral sheet in the $+\mathbf{a}_1$ direction of the 2M$_1$ cell by an average of $0.045a = 0.23$Å (Fig. 1). For paragonite-1M the resultant offset of layers along $+\mathbf{a}_1$ of the 1M cell is smaller both because the different geometry of layer stacking causes repulsion along the $-\mathbf{a}_2$ and $-\mathbf{a}_3$ pseudohexagonal axes at the same time (with a smaller resultant along $+\mathbf{a}_1$) and because adjacent O(3) atoms do not approach as closely (3.196Å) across the interlayer gap as for paragonite-2M$_1$ (3.102Å). Although the interlayer geometry is the same for muscovite-2M$_1$ as for paragonite-2M$_1$ the large size of the interlayer K apparently blocks any significant layer offset. The dominance of the interlayer cation size in muscovite-2M$_1$ is illustrated by the variability in direction of the small offsets found in different specimens ($-0.005a_1$ per layer by Rothbauer (1971), $-0.005a_1$ by Güven (1971), but $+0.001a_1$ by Burnham and Radoslovich (1964), $+0.002a_1$ by Gatineau (1963), and $+0.002a_1$ by Birle and Tettenhorst (1968)—all as quoted by Bailey (1980) but taking into account that his values are for total offset per unit rather than per layer). These values are measured on orthogonal projections between the positions of the tetrahedral cations in adjacent layers.

The large decrease in interlayer separation in paragonite-2M$_1$ (3.053Å) relative to muscovite-2M$_1$ (3.480Å) reduces the normally thick trigonal antiprism around K to an octahedron of nearly ideal shape around Na (ψ = 54.4°). The mean Na–O bond length of 2.624Å is still considerably larger than predicted (2.38Å) from the effective ionic radii of Shannon (1976). The same is true of the observed mean Na–O bonds in the other paragonite structures (range 2.56Å to 2.64Å). The deviation between observed and predicted values is due partly to the corrugation of the basal oxygen surface that creates an irregular interlayer cavity. The O(3) atoms that approach each other most closely across the interlayer gap also coordinate most closely with the Na (2.496Å). The O(4) atoms that have been depressed or elevated away from the mean plane of their neighbors by tetrahedral tilting in turn are farthest from the Na (2.718Å), whereas the O(5) atoms are intermediate in approach. An irregular interlayer cavity due to the corrugation effect also exists around K in muscovite-2M$_1$, but the differences between individual K–O bond lengths are much smaller (Δ = 0.04Å) than in paragonite-2M$_1$ (Δ = 0.22Å). The closest observed approach of Na–O(3) = 2.496Å is in accord with the observation that in micas the bond lengths to the interlayer cation tend to be at least 0.1Å larger than the sums of the ionic radii for six-fold coordination. This deviation increases with decreasing tetrahedral twist and increasing effective coordination number for the cation.

Acknowledgments

We are indebted to Prof. Dr. Martin Frey of the University of Basel and Professor C. V. Guidotti of the University of Maine for provision of the specimen studied and to C. A. Geiger for an electron probe analysis. This research was supported in part by grant EAR-8106124 from the National Science Foundation and in part by grant 13157-AC2-C from the Petroleum Research Fund, administered by the American Chemical Society.

References

Bailey, S. W. (1980) Structures of layer silicates. Chap. 1 in G. W. Brindley and G. Brown, Eds., Crystal Structures of Clay Minerals and their X-ray Identification, p. 1–123. Mineralogical Society, London.

Bearth, P. (1973) Gesteins- und Mineralparagenesen aus den Ophiolithen von Zermatt. Schweizerische Mineralogische und Petrographische Mitteilungen, 53, 299–334.

Bearth, P. and Stern, W. (1979) Zur Geochemie von Metapillows der Region Zermatt-Saas. Schweizerische Mineralogische und Petrographische Mitteilungen, 59, 349–373.

Birle, J. D. and Tettenhorst, R. (1968) Refined muscovite structure. Mineralogical Magazine, 36, 883–886.

Burnham, C. W. and Radoslovich, E. W. (1964) Crystal structures of coexisting muscovite and paragonite. Carnegie Institute of Washington Year Book 63, 232–236.

Burns, A. F. and White, J. L. (1963) The effect of potassium removal on the *b*-dimension of muscovite and dioctahedral soil micas. Proceedings of the International Clay Conference 1963, Stockholm, 1, 9–16, Pergamon Press, London.

Cromer, D. T. and Mann, J. B. (1968) X-ray scattering factors computed from numerical Hartree-Fock wave functions. Acta Crystallographica, A24, 321–324.

Dollase, W. A. (1969) Crystal structure and cation ordering of piemontite. American Mineralogist, 54, 710–717.

Drits, V. A. (1975) Structural and crystallochemical peculiarities of layer silicates. In The Crystallochemistry of Minerals in the Solution of Geologic Problems, p. 35–51 (in Russian). "Nauka", Moscow.

Gatineau, L. (1963) Localisation des remplacements isomorphiques dans la muscovite. Comptes Rendus Hebdomadaires des

Seances, Academie des Sciences, Paris, 256, 4648–4649.

Guggenheim, S. and Bailey, S. W. (1975) Refinement of the margarite structure in subgroup symmetry. American Mineralogist, 60, 1023–1029.

Güven, N. (1971) The crystal structures of $2M_1$ phengite and $2M_1$ muscovite. Zeitschrift für Kristallographie, 134, 196–212.

Hazen, R. M. and Burnham, C. W. (1973) The crystal structure of one-layer phlogopite and annite. American Mineralogist, 58, 889–900.

McCauley, J. W. and Newnham, R. E. (1971) Origin and prediction of ditrigonal distortion in micas. American Mineralogist, 56, 1626–1638.

Nakamura, H. and Kihara, K. (1977) Coexistence of $2M_1$ and 3T muscovites and paragonites in low-grade metamorphic rocks of the Sanbagawa metamorphic belt, Japan. Mineralogical Journal, 8, 343–348.

Radoslovich, E. W. (1963) The cell dimensions and symmetry of layer lattice silicates, IV. Interatomic forces. American Mineralogist, 48, 76–99.

Robinson, R., Gibbs, G. V., and Ribbe, P. H. (1971) Quadratic elongation: a quantitative measure of distortion in coordination polyhedra. Science, 172, 567–570.

Rothbauer, R. (1971) Untersuchung eines $2M_1$-Muskovits mit Neutronenstrahlen. Neues Jahrbuch für Mineralogie, Monatshefte, 143–154.

Shannon, R. D. (1976) Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides. Acta Crystallographica, A32, 751–767.

Sidorenko, O. V., Zvyagin, B. B., and Soboleva, S. V. (1977a) Refinement of the crystal structure of $2M_1$ paragonite by the method of high-voltage electron diffraction. Soviet Physics, Crystallography, 22, 554–556 (English transl.).

Sidorenko, O. V., Zvyagin, B. B., and Soboleva, S. V. (1977b) The crystal structure of 3T paragonite. Societ Physics, Crystallography, 22, 557–560 (English transl.).

Soboleva, S. V., Sidorenko, O. V., and Zvyagin, B. B. (1977) Crystal structure of paragonite 1M. Soviet Physics, Crystallography, 22, 291–293 (English transl.).

Zvyagin, B. B. and Soboleva, S. V. (1979) Variabilité des longueurs de liaisons Si, Al_t–O dans les silicates lamellaires. Bulletin de Mineralogie, 102, 415–419.

Manuscript received, July 16, 1982;
accepted for publication, July 5, 1983.