

## A Geometrical Structural Model of 2:1 Trioctahedral Clay Minerals

2:1 삼팔면체 점토광물의 기하학적 구조모델

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**ABSTRACT:** This study introduces a new structural model of 1M 2:1 trioctahedral clay minerals or, more generally, 2:1 trioctahedral phyllosilicates. The structural model requires only the chemical formulae of the clay minerals as an input and uses the regression relation (Radoslovich, 1962) to calculate the *a*- and *b*-dimensions of the phyllosilicates with the given chemical formulae. The atomic coordinates of the constituent atoms are geometrically calculated for C2/m space group under the assumption that the interatomic distances are constant. To determine the *c*-dimension, this study calculates the binding energies of 1M 2:1 trioctahedral phyllosilicates as a function of *d*(001) and find the minimum energy producing *d*(001).

The structural model generates the cell dimensions, interaxial angles, interatomic distances, octahedral, tetrahedral and interlayer thickness, polyhedron deformation angles and atomic coordinates in the unit cell. The simulated structural parameters of phlogopite and annite are very close to the reported data by Hazen and Burnham (1973), suggesting that the structure simulation using only the chemical formulae is successful, and thus, that the structural model of this study overcomes the difficulties in the previous models by other investigators.

**요약:** 이 연구는 1M 2:1 삼팔면체 점토광물의 새로운 구조모델을 제시하고자함을 목적으로 한다. 오직 점토광물의 화학조성만을 입력자료로 필요로 하는 이 모델은 주어진 화학조성에 따라 Radoslovich (1962)의 regression 공식을 이용하여 *a*와 *b* 축 길이를 계산한다. *c* 축 길이는, 원자간 거리는 항상 일정하다는 가정아래, 구성원자의 단위포내 좌표를 C2/m 공간군에 대하여 계산한 다음, 여러 *d*(001)에 대하여 점토광물의 결합 에너지를 계산하여 최소에너지를 내는 *d*(001)으로부터 결정하였다.

이 구조모델은 단위포의 축 길이, 축간 각도, 원자간 거리, 팔면체층과 사면체 층의 두께 및 층간 두께, 다면체의 변형 각도 그리고 원자좌표를 계산해 낼 수 있다. 이러한 모델에 따라, phlogopite와 annite의 구조 자료를 계산한 결과는 Hazen과 Burnham (1973)이 보고한 구조자료와 상당히 일치하며, 이는 화학조성만을 이용한 1M 2:1 삼팔면체 점토광물의 구조자료 계산이 성공적이었음을 의미한다. 그 결과로, 이 연구에서 제시된 모델을 사용한다면 다른 연구자에 의해 제안된 이전의 구조모델의 어려움들을 극복할 수 있다.

### INTRODUCTION

Many naturally occurring clay minerals or phyllosilicates formed under relatively low temperatures and pressures generally occur as microcrystals having poor crystallinities and nonstoichiometric chemical compositions, which makes

the clay mineral separation difficult, and consequently, causes erroneous chemical analyses and provides insufficient structural parameters. Clay minerals significantly control the mineral assemblages and water chemistries of many geological systems, and determine the physical properties of clay-containing materials. Researchers in such

fields as aqueous geochemistry, low grade metamorphism and material science have investigated the clay minerals to understand their systems or materials better. However, the inaccurate chemical compositions and structural data are great disadvantages to those researchers, especially when they study the crystal chemistries, stabilities and other aspects of the clay minerals.

The purpose of this study is to develop a geometrical structural model of 2:1 trioctahedral clay minerals, which provides all the structural parameters as a function of the chemical compositions only. The structural model may help researchers understand the relations between the chemical constituents and the structural details, and thus, stabilities of 2:1 trioctahedral clay minerals.

A few researchers have tried to simulate the structures of phyllosilicates using geometrical analyses. Franzini and Schiaffino (1963), Donnay et al. (1964), Tepkin et al. (1969) and Appelo (1978) developed the structural models for 1M 2:1 trioctahedral phyllosilicates and Appelo (1978) and Yu (1990a) simulated the structures of 1M and 2M1 2:1 dioctahedral phyllosilicates. The structural models of these workers except Yu (1990a) require knowing the chemical compositions, cell dimensions and/or interaxial angles to accomplish the simulations. As mentioned earlier, however, the structural data used for the simulations, such as  $b$ ,  $c$  and  $\beta$  are not readily available, especially for nonstoichiometric clay minerals.

This paper introduces a new structure synthesis method for 2:1 trioctahedral clay minerals which requires only the chemical compositions as input data. The synthesis provides all the structural details, including the cell dimensions, interaxial angles, interatomic distances, octahedral, tetrahedral and interlayer thicknesses, polyhedron deformation angles and atomic coordinates in the unit cell. The geometrical analyses of the structure and the binding energy calculation of the 2:1 trioctahedral clay minerals generate these structural details.

### ASSUMPTIONS FOR THE STRUCTURE SYNTHESIS

The work of many investigators on the structure of the phyllosilicates leads to the following assumptions, which cause no significant error during the structure simulation:

1. The octahedra are stretched and flattened into trigonal antiprism because of repulsion between the octahedral cations. The octahedral cations maintain an ideal hexagonal configuration when they are projected on (001).
2. The  $b$ -dimension is determined by the octahedral layer only, because the octahedron is more ionic than the tetrahedron and edge sharing octahedra are more rigid with respect to rotation and tilting than the more covalent corner-sharing tetrahedra.
3. The tetrahedra rotate to fit the  $a$ -dimension.
4. All the cations in the each cationic site are randomly distributed enough that we may consider the interatomic distance between the cation and anion as the average of the interatomic distances. The distance is a function of the fraction of each cation in each cationic site.
5. Interatomic distances remain constant, no matter what kind of distortion and deformation occurs, except the interatomic distances between the interlayer cations and the basal oxygens, which are determined by the Coulomb, Pauli repulsion and London forces between the layers.
6. The space group of 1M 2:1 trioctahedral clay minerals is  $C2/m$ .

### b-DIMENSION AND INTERATOMIC DISTANCE CALCULATIONS

Given the chemical composition, the  $b$ -dimension is calculated with a regression equation. A few researchers have predicted the  $b$ -dimension of phyllosilicates with regression analyses of the  $b$ -dimension as a function of chemical composition (Faust, 1957; Radoslovich, 1962; Veitch and Radoslovich, 1963). This study uses Radoslovich's equation (Radoslovich, 1962):

$$b = 8.925 + 0.099K - 0.069Ca + 0.062Mg + 0.116Fe^{2+} + 0.098Fe^{3+} + 0.166Ti \quad \text{for mica and}$$

$$b = 8.944 + 0.096Mg + 0.096Fe^{3+} + 0.037Al_{tet} \quad \text{for}$$

smectite, (1)

in which the element symbols represent the numbers of the cations in an  $O_{10}(\text{OH})_2$  formula.

The interatomic distances in cationic sites are obtained by averaging the interatomic distances of the occupying cations according to their mole fractions:

$$r_i = \sum_j f_{j,i} r_j, \quad (2)$$

where  $r_i$  is the interatomic distances in the  $i$ th cationic site,  $f_{j,i}$  is the mole fraction of  $j$ th cation in the  $i$ th site and  $r_j$  is the interatomic distance between the  $j$ th cation and an oxygen bonding to it. The interatomic distances between the cations and oxygens are obtained from the effective ionic radii (Shannon, 1976) and reported interatomic distances in clay minerals. Table 1 lists the interatomic distances adopted in this study.

**Table 1.** Interatomic distances used in the structural model of 1M 2:1 trioctahedral clay minerals.

Atomic Pair	Layer	Interatomic Distance(A)
Si-O	Tetrahedral	1.610
Al-O	Tetrahedral	1.745
Fe <sup>3+</sup> -O	Tetrahedral	1.840
Al-O	Octahedral	1.920
Fe <sup>3+</sup> -O	Octahedral	2.000
Fe <sup>2+</sup> -O	Octahedral	2.130
Mg-O	Octahedral	2.060

### OCTAHEDRAL LAYER SIMULATION

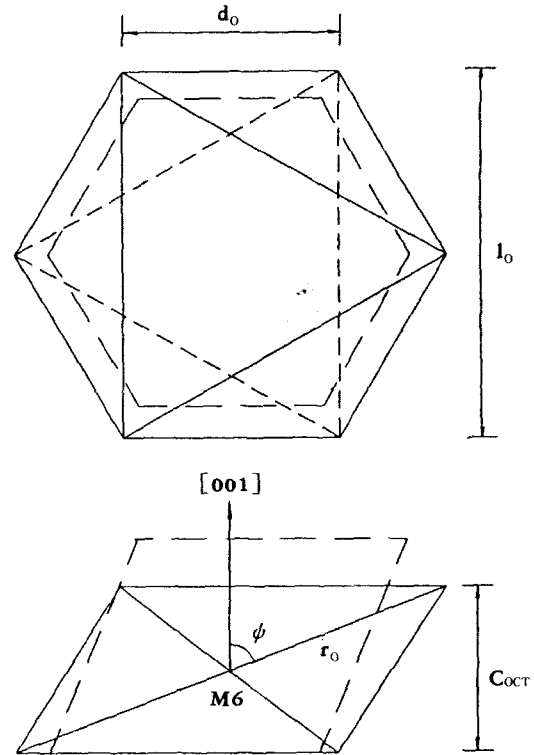
Fig. 1 shows an ideal and flattened octahedron. From Fig. 1, the projected octahedral edge length,  $d_o$ , on (001) is calculated by

$$d_o = l_o / 2\sin(60^\circ) = l_o / \sqrt{3}, \quad (3)$$

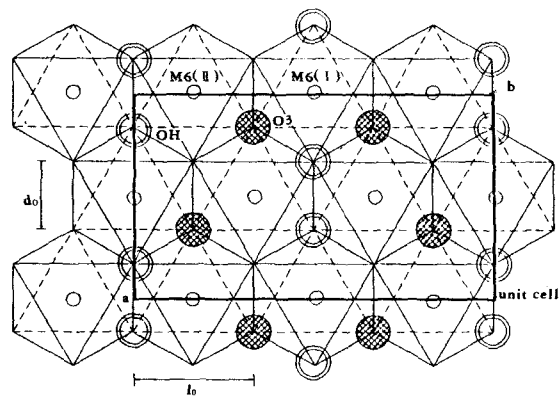
where  $l_o$  is the octahedral edge length, given by  $b/3$ . If we define "octahedral flattening angle",  $\psi$ , as the angle between [001] and the line connecting opposite vertices of the octahedron (Donnay et al., 1964), the angle becomes

$$\psi = \sin^{-1} \left( \frac{l_o}{r_o \sqrt{3}} \right), \quad (4)$$

where  $r_o$  is the interatomic distance between the octahedral cation and the apical oxygen, calculated



**Fig. 1.** Ideal (solid line) and flattened (broken line) octahedron.



**Fig. 2.** Atomic configurations in the octahedral layer, projected on (001).

Then, the octahedral thick-

ness,  $c_{oct}$ , is given by

$$c_{oct} = 2r_o \cos \psi. \quad (5)$$

The coordinates of the octahedral atoms are calculated with the values obtained from equations (3), (4) and (5). Fig. 2 illustrates the atomic configurations in the octahedral layer, projected on (001). The atomic coordinates become as the below:

For the octahedral cation, M6(I) and M6(II),

$$\begin{aligned} x_{M6(I)} &= 0.0 \\ y_{M6(I)} &= 0.5 \\ z_{M6(I)} &= 0.5 \end{aligned}$$

$$\begin{aligned} x_{M6(II)} &= 0.0 \\ y_{M6(II)} &= 1/6 \\ z_{M6(II)} &= 0.5. \end{aligned}$$

For the bridging oxygen (or apical oxygen), O3, and the hydroxyl ion, OH,

$$\begin{aligned} x_{O3} &= \frac{2d_o}{a} + \frac{c(1/2 - z_{O3})\cos\beta}{a} \\ y_{O3} &= 1/6 \\ z_{O3} &= 1/2 - c_{oct}/2c' \end{aligned}$$

$$\begin{aligned} x_{OH} &= \frac{d_o}{2a} + \frac{c(1/2 - z_{OH})\cos\beta}{a} \\ y_{OH} &= 0.0 \\ z_{OH} &= z_{O3}. \end{aligned}$$

In the above equations, x, y and z represent the atomic coordinates, a and c the cell dimensions,  $\beta$  the interaxial angles and  $c' = c \sin \beta$ .

### TETRAHEDRAL LAYER SIMULATION

Fig. 3 shows an ideal tetrahedron having the edge length and height of

$$l_t = 2\sqrt{2} r_t / \sqrt{3} \quad \text{and} \quad (6)$$

$$c_{tet} = 4r_t/3 + 0.025. \quad (7)$$

Where  $r_t$  is the interatomic distance between the tetrahedral cation and oxygen, obtained with equation (2). In a real structure, the distance between the tetrahedral cation and apical oxygen is about 0.025 Å longer than the distance between the tetrahedral cation and

the basal oxygen. Thus, this correction is included in equation (7).

The lateral dimension of an undeformed tetrahedral layer is generally larger than that of an octahedral layer. The rotation of the tetrahedra relieves this lateral size misfit between the tetrahedral layer and octahedral layer. Fig. 4 illustrates how the tetrahedral rotation relieves the size misfit. From Fig. 4, the rotation angle,  $\alpha$ , is calculated by

$$\alpha = \cos^{-1} \left( \frac{a}{2l_t} \right), \quad (8)$$

where a represents the a-dimension, which equals to  $b/\sqrt{3}$ .

Fig. 5 shows the positions of the tetrahedral cations, basal oxygens and apical oxygens, projected on (001). The atomic coordinates of the tet-

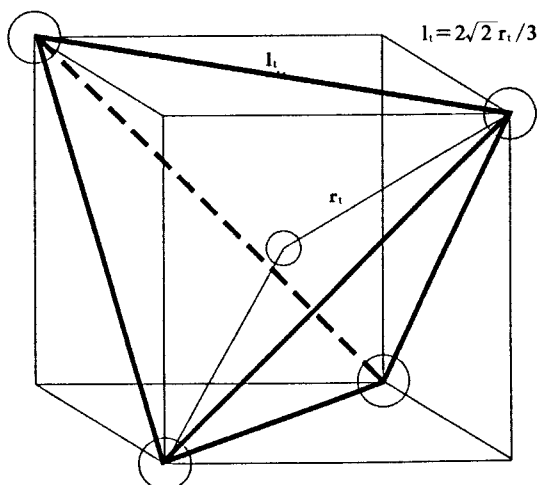


Fig. 3. Ideal tetrahedron.

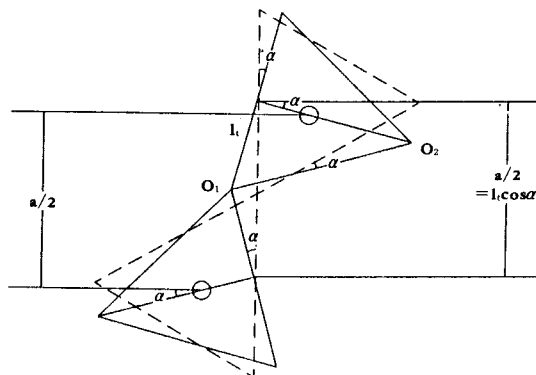


Fig. 4. Tetrahedral rotation to fit the a-dimension.

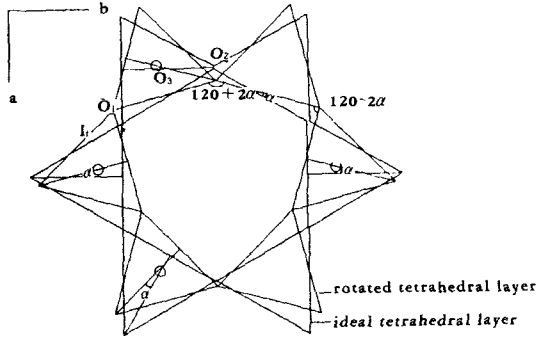


Fig. 5. Atomic configurations in the tetrahedral layer, projected on (001).

rahedral cation and basal oxygens are calculated with the results from equations (6), (7) and (8) and the octahedral atomic coordinates:

For the tetrahedral cation, M4,

$$x_{M4} = x_{O3} + \frac{c(z_{O3} - z_{M4})\cos\beta}{a},$$

$$y_{M4} = y_{O3}.$$

$$z_{M4} = z_{O3} - (r_1 + 0.025)/c'.$$

For the basal oxygen, O1 ,

$$x_{O1} = x_{O3} - \frac{l_1 \sin\alpha}{2\sqrt{3}a} + \frac{l_1 \cos\alpha}{2a} + \frac{c(z_{O3} - z_{O1})\cos\beta}{a},$$

$$y_{O1} = y_{O3} - \frac{l_1 \cos\alpha}{2\sqrt{3}b} - \frac{l_1 \sin\alpha}{2b},$$

$$z_{O1} = z_{O3} - c_{tet}/c'.$$

For the basal oxygen, O2,

$$x_{O2} = x_{O3} + \frac{l_1 \cos\alpha}{\sqrt{3}a} + \frac{c(z_{O3} - z_{O2})\cos\beta}{a},$$

$$y_{O2} = 0.5,$$

$$z_{O2} = z_{O1}.$$

### INTERLAYER SIMULATION AND C-DIMENSION CALCULATION

The atomic coordinates of the interlayer cation, MI, is fixed to the values of  $x_{MI}=0.0$ ,  $y_{MI}=0.0$  and  $z_{MI}=0.0$ . The interaxial angle,  $\beta$ , is calculated by

$$\beta = 90^\circ + \tan^{-1}(d_o/c'). \quad (9)$$

The c-dimension of the phyllosilicates is the sum of the thicknesses of the octahedral layer, tetrahedral layer and interlayer. Unknown is only the interlayer thickness for the c-dimension calculation. The interlayer thickness is a function of the interatomic distance between the interlayer cation and the basal oxygen. One may try to calculate the interlayer thickness from the reported interatomic distances from Shannon (1973) or other mica structure analyses, just as we do in the octahedral and tetrahedral structure simulation. However, the almost completely ionic character of the bonding between the interlayer cation and oxygen makes the bond distance variable, unlike the octahedral and tetrahedral bondings which have about 60% covalency at maximum. Thus, one should avoid using a constant interatomic distance in simulating the interlayer structure.

The binding energy calculation is useful in determining the c-dimensions of phyllosilicates, because the phyllosilicates must have the minimum energy producing c-dimensions or d(001), which we observe in nature. For a arbitrarily given c-dimension, all the structural details can be generated according to the above structural model. For a series of such structural models having different c-dimensions, the binding energies can be calculated and the minimum energy producing c-dimension or d(001) can be found. Yu(1990b) discussed the details of the binding energy calculation theory. This study adopts the binding energy calculation procedures of Yu (1990b) and determine the c-dimension of 2:1 trioctahedral phyllosilicates. Table 2 summarizes the geometrical structural model of 1M 2:1 trioctahedral phyllosilicate, having space group C2/m.

### RESULTS AND DISCUSSION

The structural parameters of phlogopite and annite are obtained according to the structural model summarized in Table 2. The chemical compositions of the phlogopite and annite are  $KMg_3(AlSi_3)O_{10}(OH)_2$  and  $K_{0.993}Al_{0.103}Fe^{3+}_{0.218}Fe^{2+}_{2.542}Mg_{0.137}(Al_{1.19}Si_{2.81})O_{10}(OH)_2$ , respectively.

**Table 2.** Structural model for 1M 2:1 trioctahedral phyllosilicates, space group C2/m.

Required Data: Chemical composition

Cell Dimension Calculation:

$$b = 8.925 + 0.099K - 0.069Ca + 0.062Mg + 0.116Fe^{2+} + 0.098Fe^{3+} + 0.166Ti$$

$$a = b/\sqrt{3}$$

c = the minimum energy producing c-dimension

Interatomic Distance, Edge Length, Deformation Angle and Thickness Calculations:

$$r_i = \sum f_{i,j} r_j$$

$$l_o = b/3$$

$$d_o = l_o/\sqrt{3}$$

$$l_t = 2\sqrt{2} r_i/\sqrt{3}$$

$$\psi = \sin^{-1}\left(\frac{l_o}{r_o\sqrt{3}}\right)$$

$$\alpha = \cos^{-1}\left(\frac{a}{2l_t}\right)$$

$$c_{oct} = 2r_o \cos\psi$$

$$c_{tet} = 4r_t/3 + 0.025$$

$$c' = c \sin\beta$$

Atomic Coordinates Calculation:

M1  $x_{M1} = 0.0$   
 $y_{M1} = 0.0$   
 $z_{M1} = 0.0$

M6(I)  $x_{M6(I)} = 0.0$   
 $y_{M6(I)} = 0.5$   
 $z_{M6(I)} = 0.5$

M6(II)  $x_{M6(II)} = 0.0$   
 $y_{M6(II)} = 1/6$   
 $z_{M6(II)} = 0.5$

M4  $x_{M4} = x_{O3} + \frac{c(z_{O3} - z_{M4})\cos\beta}{a}$

$$y_{M4} = y_{O3}$$

$$z_{M4} = z_{O3} - (r_t + 0.025)/c'$$

O1  $x_{O1} = x_{O3} - \frac{l_1 \sin\alpha}{2\sqrt{3}a} + \frac{l_1 \cos\alpha}{2a} + \frac{c(z_{O3} - z_{O1})\cos\beta}{a}$

$$y_{O1} = y_{O3} - \frac{l_1 \cos\alpha}{2\sqrt{3}b} + \frac{l_1 \sin\alpha}{2b}$$

$$z_{O1} = z_{O3} - c_{tet}/c'$$

O2  $x_{O2} = x_{O3} + \frac{l_1 \cos\alpha}{\sqrt{3}a} + c(z_{O3} - z_{O2})\cos\beta/a$

$$y_{O2} = 0.5$$

$$z_{O2} = z_{O1}$$

**Table 2 Cont'd.**

O3  $x_{O3} = 2d_o + \frac{c(1/2 - z_{O3})\cos\beta}{a}$

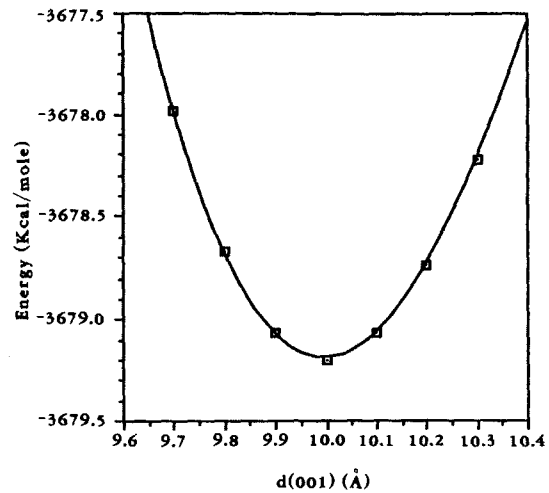
$$y_{O3} = 1/6$$

$$z_{O3} = 1/2 - c_{oct}/2c'$$

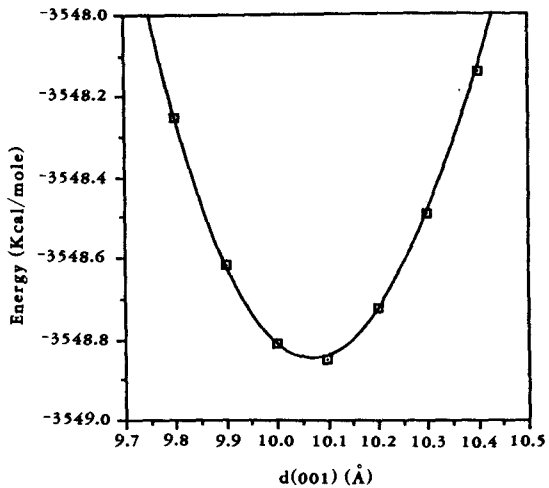
OH  $x_{OH} = \frac{d_o}{2a} + \frac{c(1/2 - z_{OH})\cos\beta}{a}$

$$y_{OH} = 0.0$$

$$z_{OH} = z_{O3}$$



**Fig. 6.** Binding energy variation of phlogopite as a function of d(001).



**Fig. 7.** Binding energy variation of annite as a function of d(001).

To determine the minimum energy producing  $d(001)$ , the binding energies are calculated as a function of  $d(001)$ . The binding energy calculation uses the same parameters and constants as those in Yu(1990b), except  $\rho$  and Pauli radii of K and oxygens. This study chooses  $\rho=0.156 \text{ \AA}^{-1}$  and the Pauli radii of 1.5, 1.079 and 1.086  $\text{\AA}$  for K, the basal oxygen and the apical oxygen, respectively.

Figs. 6 and 7 respectively show the binding energy variations of the phlogopite and annite as a function of  $d(001)$ . The minimum energy producing  $d(001)$ 's are respectively 10.00 and 10.08  $\text{\AA}$  for the phlogopite and annite. Tables 3 and 4 compare the structural parameters generated with the structural model using the minimum energy producing  $d(001)$ 's with the reported ones of Hazen and Burnham(1973) for phlogopite and annite, respectively.

Table 3 and 4 show that the difference between the simulated structural parameters and the reported ones are within experimental error. The x-coordinate difference of O2 in Table 4 for annite is 0.0137, which seems to be a significant error. If we convert the coordinate difference to the actual distance difference, however, the 0.0137 difference in x-coordinate represent only 0.0738  $\text{\AA}$  difference along the a-direction which is identical to 0.0072 difference in z-coordinate. Thus, the x-coordinate difference of O2 in annite is not so significant as the number itself represents. In conclusion, the results of this study show that the structure simulation is successful only with the chemical formulae of 2:1 trioctahedral phyllosilicates, and thus, one does not need any structural parameter to simulate the complete structure as in previously suggested models.

**Table 3.** Comparison of the simulated with the reported structural parameters of phlogopite (Hazen and Burnham, 1973).

	Simulated			Hazen and Burnham			Difference		
Atomic Coordinates:									
	x	y	z	x	y	z	$ \Delta x $	$ \Delta y $	$ \Delta z $
M1	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
M6( I )	.0000	.5000	.5000	.0000	.0000	.5000	.0000	.0000	.0000
M6( II )	.0000	.1667	.5000	.0000	.1685	.5000	.0000	.0018	.0000
M4	.5730	.1667	.2281	.5752	.1668	.2254	.0022	.0001	.0027
O1	.8278	.2299	.1733	.8248	.2307	.1677	.0030	.0008	.0056
O2	.5177	.0000	.1733	.5180	.0000	.1675	.0003	.0000	.0058
O3	.6317	.1667	.3950	.6297	.1664	.3902	.0020	.0003	.0048
OH	.1317	.0000	.3950	.1330	.0000	.4008	.0013	.0000	.0058
Cell Dimensions and Interaxial Angle:									
a		5.3174			5.3078			0.0106 (Å)	
b		9.2100			9.1901			0.0199 (Å)	
c		10.1539			10.1547			0.0008 (Å)	
$\beta$		100.05			100.08			0.03 (°)	
Deformation Angles:									
$\psi$		59.36			58.96			0.4 (°)	
$\alpha$		7.9			7.5			0.4 (°)	
Interatomic Distances:									
$r_o$		2.060			2.064			0.004 (Å)	
$r_t$		1.644			1.649			0.005 (Å)	

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**Table 4.** Comparison of the simulated with the reported structural parameters of annite (Hazen and Burnham, 1973).

	Simulated			Hazen and Burnham			Difference		
Atomic Coordinates:									
	x	y	z	x	y	z	$\Delta x$	$\Delta y$	$\Delta z$
MI	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
M6(I)	.0000	.5000	.5000	.0000	.5000	.5000	.0000	.0000	.0000
M6(II)	.0000	.1667	.5000	.0000	.1668	.5000	.0000	.0001	.0000
M4	.5746	.1667	.2239	.5703	.1665	.2254	.0043	.0002	.0015
O1	.8064	.2500	.1693	.8031	.2457	.1670	.0033	.0043	.0023
O2	.5564	.0000	.1693	.5427	.0000	.1684	.0137	.0000	.0009
O3	.6301	.1667	.3902	.6291	.1674	.3894	.0010	.0007	.0008
OH	.1301	.0000	.3902	.1239	.0000	.3931	.0062	.0000	.0029
Cell Dimensions and Interaxial Angle:									
a		5.3900			5.3860			0.0040 (Å)	
b		9.3358			9.3241			0.0117 (Å)	
c		10.2339			10.2683			0.0344 (Å)	
$\beta$		100.11			100.63			0.52 (°)	
Deformation Angles:									
$\psi$		58.36			58.20			0.16 (°)	
$\alpha$		0.00			1.5			1.5 (°)	
Interatomic Distances:									
$r_o$		2.110			2.101			0.009 (°)	
$r_i$		1.650			1.659			0.009 (°)	

Although the simulated structures are very close to the reported ones, a few more refinements in the structural model and energy calculation may improve the results. For example, the chemical formulae of phlogopite and annite used in this study are idealized ones, which are a little different from those reported by Hazen and Burnham (1973). The structural model of this study ignores F, Mn and Ti in the octahedral layer, which certainly cause somewhat erroneous results. In the binding energy calculation, there are possibilities for the improvements of ionicity estimation, Pauli repulsion energy parameter determination and van der Waals energy calculation. Future research will treat the above aspects of the possible refinements.

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