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Crystal structure of a new (21)-clinopyribole synthesized at high temperature and pressure

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ABSTRACT

A (21)-clinopyribole with the composition $K_{1.10}Na_{2.32}Ca_{1.52}Mg_{5.85}Al_{1.23}Si_{12.04}O_{34}(OH)_2$ has been synthesized at 10 GPa and 1250 °C in a multi-anvil apparatus. The unit-cell parameters are $a = 9.8390(9)$, $b = 26.6471(6)$, $c = 5.2665(5)$ Å, $\beta = 106.25(5)°$, and $V = 1325.6(4)$ Å^3. The structure (space group $A2/m$) consists of an alternating arrangement of single- and double-chain silicate slabs along the b axis, with a + + + + configuration. This phase possesses all the features predicted by Veblen and Burnham (1978b) for a mixed-chain silicate intermediate between pyroxenes and amphiboles. The single-chain portion of the structure corresponds to a clinopyroxene with the omphacite composition $Di_{55}Jd_{45}$, whereas the double chain portion is essentially a potassic richterite. The MS2 cation in the single-chain portion occupies a coordination environment that is similar to the M4 site in richterite, whereas the MD4 cation coordination in the double-chain portion is comparable to the M2 site in $C2/c$ omphacite. The observed unit-cell volume is 1.5% smaller than the equivalent mixture of $Di_{55}Jd_{45}$ + richterite, accounting, in part, for its high-pressure stability relative to its pyroxene and amphibole components.

INTRODUCTION

Because of their structural similarities, micas, amphiboles, and pyroxenes can be collectively grouped into a polysomatic series called biopyriboles (Johannsen 1911; Thompson 1970, 1978). All members of the biopyribole family can be considered as mixtures of pyroxene (P) ($CaMgSi_2O_6$ or $Mg_2Si_2O_6$) and mica/talc (M) [$Mg_3Si_4O_{10}(OH)_2$] sub-units stacked along the crystallographic **b** axis. All known biopyriboles that show long-range ordered stacking sequences fall into two series: $M_{(n-1)}P$ and $M_nPM_{(n-1)}P$ with talc or trioctahedral mica formed as $n \rightarrow \infty$ for both series. Members of the first series include single-chain pyroxenes (P) with $n = 1$, double-chain amphiboles (MP) with $n = 2$, and triple-chain silicates with $n = 3$ (MMP), such as (3)-jimthompsonite [the number in the parenthesis represents the chain sequence of the basic repeating unit (Konishi and Akai 1991; Grobéty 1996)] and (3)-clinojimthompsonite (Thompson 1970; Veblen and Burnham 1978a, 1978b; Droop 1994). Alkali-bearing MMP-type triple-chain silicates were synthesized by Drits et al. (1974) and Tateyama et al. (1978) under low P-T conditions. Members of the $M_nPM_{(n-1)}P$ stacking series contain mixed n-fold and $(n + 1)$-fold tetrahedral chains. Natural examples of these series are (32)-chesterite and a monoclinic analogue of (32)-chesterite with an (MMPMP) stacking sequence and $n = 2$ (Veblen and Burnham 1978a, 1978b; Droop 1994).

Aside from long-range ordered biopyriboles that form macroscopic crystals, short- range ordered biopyriboles may occur as domains of up to a few thousand angstrom-width within amphiboles and/or pyroxenes. These domains can show a wide variety of stacking sequences, including quadruple and higher order tetrahedral chains (Veblen and Buseck 1979; Yau et al. 1986; Schumacher and Czank 1987; Grobéty 1996). Natural wide-chain silicates have been found in low-pressure (~0.6 GPa) and low-to-medium temperature (300 ~ < 600–700 °C) ultramafic assemblages, low-temperature hydrothermal veins, and the alternation halo of a skarn ore deposit (e.g., Veblen and Burnham 1978a; Akai 1980; Yau et al. 1986; Schumacher and Czank 1987; Droop 1994; Grobéty 1996; Akai et al. 1997). They have been also found as a low-temperature weathering product of enstatite (Eggleton and Boland 1982). However, mixed chain biopyribole structures are not necessarily restricted to low-pressure and low-to-medium temperature conditions. Here we report results of the single crystal structure analysis of a mixed chain (21)-clinopyribole synthesized at 10 GPa and 1250 °C.

EXPERIMENTAL PROCEDURES

The (21)-clinopyribole crystal used in this study was synthesized at 10 GPa and 1250 °C (experiment no. JKW58) for 12 hours from a mixture of high purity oxides and carbonates using a multi-anvil apparatus. The starting material had a composition (wt%) SiO_2 57.4, Al_2O_3 5.2, MgO 18.5, CaO 7.6, Na_2O 5.3, K_2O 4.3, H_2O 1.4 with water added as brucite. In this bulk composition, idiomorphic (21)-clinopyribole crystals up to 180 × 80 μm coexist with potassic amphibole and small amounts of diopside. The average chemical composition of the largest (21)-

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clinopyribole crystal of the experimental charge, determined by electron microprobe (n = 15), is (wt%) SiO_2 57.7(2), Al_2O_3 5.1(2), MgO 18.8(2), CaO 6.8(2), Na_2O 5.7(2), K_2O 4.1(2). The standards used for electron microprobe analysis were pure synthetic SiO_2 for Si, pure synthetic Al_2O_3 for Al, pure synthetic MgO for Mg, natural wollastonite for Ca, synthetic sodic pyroxene for Na, and natural orthoclase for K. When normalized to 34 O atoms + 2 OH the resulting stoichiometry is $K_{1.10}Na_{2.32}Ca_{1.52}Mg_{5.85}Al_{1.23}Si_{12.04}O_{34}(OH)_2$ with Σcation = 24.06.

A single-crystal fragment (0.08 × 0.07 × 0.07 mm), cut from the largest (21)-clinopyribole crystal, was chosen for the X-ray study based on optical examination, precession photography, and X-ray diffraction peak profiles. The X-ray precession photographs showed that the crystal has monoclinic symmetry and an *A*-centered lattice. Detailed X-ray diffraction experimental procedures are similar to those described by Yang et al. (1999). The unit-cell parameters are a = 9.8390(9), b = 26.6471(6), c = 5.2665(5) Å, β = 106.25(5)°, and V = 1325.6(4) Å^3, which are comparable to those reported by Finger et al. (1998) for the (21)-clinopyribole crystal synthesized in a different run [a = 9.8525(6), b = 26.6818(7), c = 5.269(1) Å, and β = 106.27(1)°].

The initial structure model of (21)-clinopyribole was taken from that of Finger and Yang (unpublished data). A total of 1263 reflections with $I > 2\sigma(I)$ was used in the structure refinements. The atomic site nomenclature suggested by Veblen and Burnham (1978b) is adopted. The sites belonging to the single chain part are denoted by "S" and those belonging to the double chain part by "D". These letters are inserted after the site names; for example, OS1 is in the single chain and OD1 is in the double chain. The first six atoms in Table 1 belong to the single chain part and the rest belong to the double chain part. For the structure refinement, we assumed 12 Si atoms per formula unit (apfu) and (K + Na + Ca + Mg + Al) normalized from the microprobe analysis to 12. The following schema of the atomic site occupancies were used for the initial refinements: all tetrahedral TS, TD1, and TD2 sites were occupied by Si, the octahedral MS1, MD1, MD2, and MD3 sites by (Mg + Al), the MS2 site by (Ca + Na), the MD4 sites by (Ca + Na + K), and the A site by K. The refinement showed no Al occupancy in the MD1 and MD3 sites. Difference Fourier maps at convergence of the refinement revealed two slightly positive peaks: one was ~1.0 Å away from OD3, and the other was ~0.3 Å away from MD4. The first peak indicated the position for H and the second one suggested a splitting of the MD4 site, as observed in all amphiboles where large (Na, K, Ca) and small (Li, Mg, Mn, Fe) cations may substitute at the M4 site (e.g., Oberti et al. 1995 and references therein). An MD4-site splitting model was then introduced with 0.06 (= 7.06–7) Mg apfu assigned to the split MD4' site. Yet, the refinement of the positional coordinates of this site failed to converge. Thus, such a consideration was rejected in the subsequent refinements. An A-site disorder model was taken into account as well, and Fourier maps indicate that K is completely ordered at the central (2/*m*) position. A Raman spectrum of the same crystal used for the X-ray diffraction study displayed no splitting of the O-H stretching band at 3740 cm^{-1}, which further supported a complete ordering of K at the 2/*m* position (Della Ventura and Robert 1990). For the final refinements, the MD1 and MD3 sites were assumed to be fully occupied by Mg; the ratios of Mg/Al in the MS1 and MD2 sites were allowed to vary with the total Al amount constrained to that determined from microprobe analysis. Likewise, the ratios of Ca/Na in the MS2 and MD4 sites were refined as well, with the amounts of K and Mg in the MD4 site fixed. The final R_w and R factors are 0.038 and 0.037, respectively. The resulting crystal-chemical formula can thus be expressed as

$$2[^{M2}(Ca_{0.552}Na_{0.448})^{M1}(Mg_{0.439}Al_{0.561})Si_2O_6] \text{ (Pyroxene part)}$$
$$+$$
$$^{A}K^{M4}(Ca_{0.416}Na_{1.424}K_{0.100}Mg_{0.060})$$
$$^{M1,3}Mg_3{}^{M2}(Mg_{1.892}Al_{0.108})Si_8O_{22}(OH)_2 \text{ (Amphibole part)}$$

TABLE 1. Atomic coordinates and displacement factors of (21)-clinopyribole

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_2	β_{eq}
MS1	1/2	0.2188(1)	1/2	0.0019(2)	0.0003(1)	0.0069(7)	0	0.0015(3)	0	0.74(7)
MS2	1/2	0.3482(1)	1/2	0.0040(2)	0.0004(1)	0.0120(7)	0	–0.0003(3)	0	1.38(6)
TS	0.7817(1)	0.2800(0)	0.4774(2)	0.0021(1)	0.0003(1)	0.0065(4)	0.0000(0)	0.0011(1)	–0.0001(1)	0.72(2)
OS1	0.6110(3)	0.2751(1)	0.3820(5)	0.0026(3)	0.0006(1)	0.0114(11)	0.0000(1)	0.0011(4)	–0.0007(2)	1.24(6)
OS2	0.8527(3)	0.3330(1)	0.5653(5)	0.0047(3)	0.0003(1)	0.0136(11)	–0.0002(1)	0.0039(5)	–0.0004(2)	1.28(6)
OS3	0.8460(3)	0.2438(1)	0.7430(5)	0.0024(3)	0.0004(1)	0.0089(10)	–0.0001(1)	0.0016(4)	0.0003(1)	0.93(6)
MD1	0	0.4398(1)	0	0.0025(2)	0.0003(1)	0.0071(7)	0	0.0017(3)	0	0.80(4)
MD2	0	0.1205(1)	0	0.0023(2)	0.0003(1)	0.0084(8)	0	0.0009(3)	0	0.83(8)
MD3	0	0	0	0.0022(3)	0.0003(1)	0.0072(9)	0	0.0010(4)	0	0.75(5)
MD4	0	0.3132(1)	0	0.0033(2)	0.0004(1)	0.0100(6)	0	0.0004(2)	0	1.13(5)
TD1	–0.2792(1)	0.0579(1)	0.0241(2)	0.0019(1)	0.0003(1)	0.0057(4)	0.0000(1)	0.0010(2)	0.0000(1)	0.66(2)
TD2	0.2898(1)	0.1168(1)	0.4803(2)	0.0018(1)	0.0003(1)	0.0070(4)	0.0000(1)	0.0011(1)	0.0000(1)	0.71(2)
OD1	–0.1103(3)	0.0584(1)	0.1085(5)	0.0020(3)	0.0003(1)	0.0092(10)	0.0001(1)	0.0020(4)	0.0001(1)	0.81(6)
OD2	0.1194(3)	0.1160(1)	0.3919(5)	0.0019(3)	0.0003(1)	0.0075(10)	0.0000(1)	0.0008(4)	0.0003(1)	0.82(6)
OD3	0.1092(4)	0	0.3937(7)	0.0025(4)	0.0004(1)	0.0100(15)	0	0.0011(6)	0	1.01(8)
OD4	0.3690(3)	0.1687(1)	0.5554(5)	0.0037(3)	0.0004(1)	0.0130(11)	–0.0003(1)	0.0025(5)	–0.0002(2)	1.22(6)
OD5	0.3486(3)	0.0860(1)	0.2565(5)	0.0022(3)	0.0004(1)	0.0092(10)	–0.0001(1)	0.0004(4)	–0.0003(1)	1.01(6)
OD6	–0.6554(3)	0.0809(1)	–0.2498(5)	0.0020(3)	0.0005(1)	0.0095(10)	0.0000(1)	0.0022(4)	0.0003(2)	0.98(6)
OD7	–0.3366(4)	0	–0.0200(8)	0.0026(4)	0.0003(1)	0.0104(15)	0	0.0009(6)	0	1.02(8)
AD	1/2	0	1/2	0.0082(3)	0.0005(1)	0.0204(9)	0	–0.0064(4)	0	2.56(5)
HD	0.200(6)	0	0.461(11)							2.1(1.0)

Note: Atomic site nomenclature suggested by Veblen and Burnham (1978b) is adopted here: Atomic sites belonging to the single chain part are denoted by "S" and those belonging to the double chain part by "D". These letters are inserted after the site names; for example,OS1 is in the single chain and OD1 is in the double chain. The first six atoms belong to the single chain part and the rest belong to the double chain part.

Final atomic positional coordinates and displacement parameters are presented in Table 1 and selected interatomic distances in Table 2. The observed and calculated structure factors are given in Table 3.[1]

RESULTS AND DISCUSSION

The most remarkable feature of the (21)-clinopyribole structure is that it is characterized by an alternating arrangement of single- and double-chain silicate slabs (MPP with $n = 1$) along the **b**-axis, with a + + + + configuration, i.e., all octahedra point in the +**c** direction (Fig. 1) [see Veblen et al. (1977) for an explanation of this stacking terminology]. The single-chain portion of the structure corresponds to a clinopyroxene with the omphacite composition of $Di_{55}Jd_{45}$, whereas the double chain portion is essentially a postassic richterite. The existence of the MPP structure consisting of alternating single and double chains was predicted by Veblen and Burnham (1978b), Veblen and Buseck (1979), and Thompson (1981). Veblen and Buseck (1979) suggested that formation of the MPP structure could occur during a reaction between enstatite and anthophyllite by analog with chesterite, which was found in the reaction between anthophyllite and jimthompsonite. Even more interesting is that, based on their studies of low-Ca biopyribole structures, Veblen and Burnham (1978b) postulated that "the existence of chesterite and the unnamed mineral, consisting of mixed double and triple chains, suggests that other mixed-chain silicates intermediate between the pyroxenes and the amphiboles will be found. The most likely phases would be PMP's with space groups $A2_1ma$ or $A2/m$ or their subgroups, and having $b \approx 27$ Å." Apparently, the (21)-clinopyribole structure we report in this paper possesses all the features predicted by Veblen and Burnham (1978b).

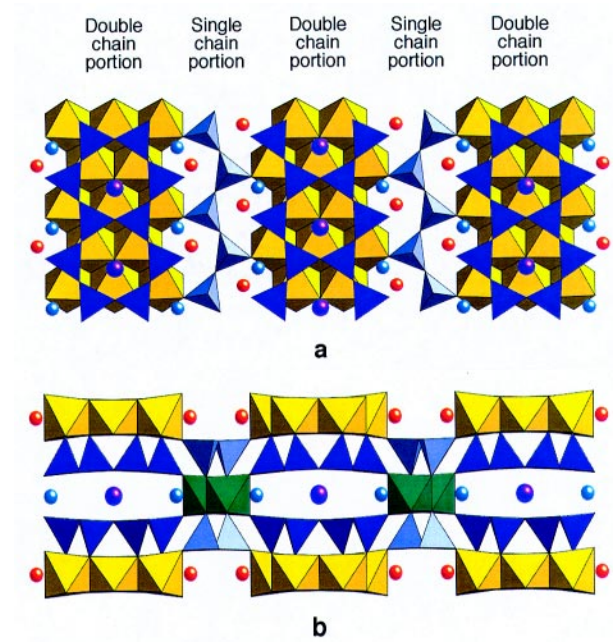

FIGURE 1. Crystal structure of synthetic (21)-clinopyribole: (**a**) viewed along **a*** and (**b**) along **c***.

The comparison of the single-chain portion of (21)-clinopyribole with the *C*2/*c* omphacite structure and the double-chain portion with the richterite structure reveals the following noticeable features: (1) The silicate tetrahedral chain is more kinked in the single-chain portion (<OS3-OS3-OS3 = 165.7°) than in *C*2/*c* omphacite with a similar composition (sample number SBB 61) (<O3-O3-O3 = 170.1°) (Oberti and Caporuscio 1991), whereas it is significantly less kinked in the double-chain portion (<OD5-OD6-OD5 = 173.9°) than in potassic richterite and Si-bearing potassic richterite (<O5-O6-O5 = 168.7–170.2°) (Papike et al. 1969; Oberti et al. 1992; Robert et al. 1993); (2) because of the alternating arrangement of two types of silicate chains along the **b** direction, the cations located at the interface between the single- and double-chain portions, namely the MS2 and MD4 cations, show interesting coordinations. Specifically, among eight oxygen atoms that are coordinated to the MS2 cation, only two of them are from the single chain portion (Table 2); the six others are from the double chain portion. For the MD4 cation, only two out of eight bonded oxygen atoms are from the double chain portion and the rest are from the single chain portion. In other words, the MS2 cation in the single-chain portion actually occupies a coordination environment that is more similar to the M4 site in richterite than the M2 site in diopside, whereas the MD4 cation coordination in the double-chain portion is more comparable to the

[1]For a copy of Table 3, document item AM-01-073, contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. Deposit items may also be available on the American Mineralogist web site (http://www.minsocam.org or current web address).

TABLE 2. Selected interatomic distances (Å) in (21)-clinopyribole

MS1-OS1(×2)	2.009(3)	TS-OS1	1.618(3)
MS1-OS1(×2)	2.052(3)	TS-OS2	1.586(3)
MS1-OD4(×2)	1.934(3)	TS-OS3	1.671(3)
Avg.	1.998	TS-OS3	1.662(3)
	Avg.		1.634
MS2-OS1 (×2)	2.399(3)		
MS2-OD4 (×2)	2.379(3)		
MS2-OD5 (×2)	2.871(3)		
MS2-OD6 (×2)	2.552(3)		
Avg.	2.550		
MD1-OD1 (×2)	2.044(3)	TD1-OD1	1.596(3)
MD1-OD2 (×2)	2.071(3)	TD1-OD5	1.627(3)
MD1-OD3 (×2)	2.092(3)	TD1-OD6	1.622(3)
Avg.	2.069	TD1-OD7	1.637(3)
		Avg.	1.621
MD2-OD1 (×2)	2.142(3)		
MD2-OD2 (×2)	2.073(3)	TD2-OD2	1.610(3)
MD2-OS2 (×2)	2.008(3)	TD2-OD4	1.582(3)
Avg.	2.074	TD2-OD5	1.667(3)
		TD2-OD6	1.673(3)
MD3-OD1 (×4)	2.067(2)	Avg.	1.633
MD3-OD3 (×2)	2.051(4)		
Avg.	2.062	AD*2/m*-OD5 (×4)	2.837(3)
		AD*2/m*-OD6 (×4)	3.138(3)
MD4-OD2 (×2)	2.374(3)	AD*2/m*-OD7 (×2)	2.589(4)
MD4-OS2 (×2)	2.401(3)	AD*2/m*-OD7 (×2)	3.542(4)
MD4-OS3 (×2)	2.707(3)	Avg. of 10	2.908
MD4-OS3' (×2)	2.530(3)	Avg. of 12	3.014
Avg.	2.503		

M2 site in diopside rather than the M4 site in richterite (Fig. 2).

The average of the MS2-O bond length (2.550 ± 0.003 Å) is significantly longer than that of the MD4-O bond length (2.503 ± 0.003 Å), but the average of the four shortest M-$O_{non\text{-}bridging}$ bond lengths for the two cation sites are nearly the same (MS2-$O_{non\text{-}bridging}$ = 2.389 Å vs. MD4-$O_{non\text{-}bridging}$ = 2.386 Å). Thus, the major difference between the average MS2-O and MD4-O bond lengths reflects the difference in the M-$O_{bridging}$ distances, which is primarily a result of the configurations of the silicate chains, as the more kinked chains tend to provide a tighter coordination for the M2 site in pyroxenes or M4 in amphiboles. In the (21)-clinopyribole structure, the double silicate chain is 8.1° straighter than the single chain. It is, therefore, reasonable to expect the average MD4-$O_{bridging}$ bond length (2.618 ± 0.003 Å) to be shorter than the average MS2-$O_{bridging}$ bond length (2.712 ± 0.003 Å). Of course, the compositional difference between the MS2 and MD4 sites could also have some effect on the difference in the average M-O distances for the two sites, but it should be minor relative to the effects of the chain configurations.

The *c* dimension of chain silicates is usually informative of the chain configurations in terms of kinking angles and tetrahedral distortions. For (21)-clinopyribole, its *c* dimension (5.266 Å) is longer than that of omphacite (~5.250 Å) (e.g., Matsumoto et al. 1975; Rossi et al. 1983; Oberti and Caporuscio 1991; Mottana et al. 1999), but shorter than that of richterite (~5.285Å) (Papike et al. 1969; Oberti et al. 1992; Robert et al. 1993). The longer *c* dimension and the more kinked angle found in the single chain of (21)-clinopyribole suggest a more distorted SiO_4 tetrahedron in the single-chain portion. In fact, the quadratic elongation (QE) and angle variance (AV) (Robinson et al. 1971) for the SiO_4 tetrahedron in the single chain of (21)-clinopyribole are 1.0073 and 31.2, respectively, whereas they are 1.0053 and 22.9 for the SiO_4 tetrahedron in *C*2/*c* omphacite (Oberti and Caporuscio 1991). The same reasoning can be applied to explain why the SiO_4 tetrahedra of the double chains in (21)-clinopyribole are less distorted than those in richterite: the respective QE and AV values are 1.0026 and 11.2 for TD1 and 1.0071 and 30.7 for TD2 in (21)-clinopyribole, whereas they are 1.0027 and 11.7 for T1 and 1.0073 and 31.2 for T2 in potassic richterite (Oberti et al. 1992).

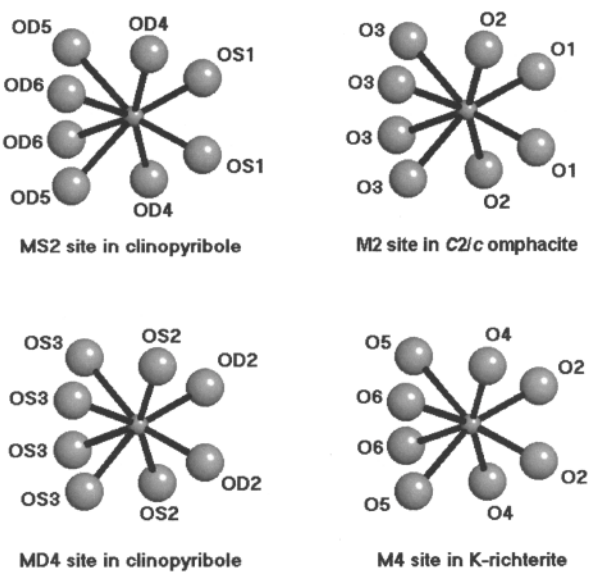

FIGURE 2. Comparison of cation coordinations in *C*2/*c* omphacite, K-richterite, and (21)- clinopyribole. Note the similarity between the MS2 site in (21)-clinopyribole and the M4 site in K-richterite, and that between the MD4 site in (21)-clinopyribole and the M2 site in *C*2/*c* omphacite.

Finger et al. (1998) noted that the unit-cell volume of (21)-clinopyribole is appreciably smaller at ambient conditions than the equivalent mixture of $Di_{55}Jd_{45}$ + richterite. Using unit-cell volumes of 439.1 $Å^3$ for diopside (Levien and Prewitt 1981), 401.8 $Å^3$ for jadeite (Cameron et al. 1973), and 922.7 $Å^3$ for potassic richterite (Robert et al. 1993), the calculated volume for the (21)-clinopyribole composition is 1345.1 $Å^3$, which is 1.5% larger than the observed volume. Hence, the high-pressure stability of (21)-clinopyribole relative to its pyroxene and amphibole components is, in part, due to its more closely packed structure.

High-pressure phases with sites suitable for large alkali elements, such as K and Na, are rare. The synthesis and discovery of the present Ca-bearing (21)-clinopyribole not only demonstrate how a fundamental and important role crystal-chemistry can play in mineral research, but also show that many other exotic phases may be found as we further explore the composition-temperature-pressure space. Moreover, they provide us with profound insights into biopyribole crystal chemistry. In particular, together with structural data for pyroxenes, amphiboles, and biopyriboles, the determination of the (21)-clinopyribole structure enables us to postulate the existence of other four possible chain silicates, as illustrated in Table 4, which includes the ideal chemical compositions, approximate unit-cell parameters, and possible space groups for those phases. Among the postulated phases in Table 4, two are Ca-bearing and two are Ca-free. The postulated Ca-bearing triple-train silicates have been observed as intergrowth microstructures in Ca-containing clinopyroxenes (such as augite and diopside) that have been altered to other minerals (Veblen and Buseck 1979; Nakajima and Ribbe 1980). The two postulated Ca-free (21)-clinopyriboles should be structurally similar to the (21)-clinopyribole we report here. Intriguingly, based on X-ray diffraction data, Avgustinik and Vigdergauz (1948) and Sueno et al. (1980) proposed the presence of the ordered (21)-polysome (the MPP structure) as a product of the thermal breakdown of talc. Additional evidence for the existence of the (21)-pyribole composed of single and double chains was provided by Konishi and Akai (1991) and Grobéty (1996) from TEM measurements on heated talc and retrograde hydration of anthophyllite. However, the observed MPP structures were reported to occur only within a very short ordered sequence (less than 10 repeated units).

In addition to the Ca-free and Ca-bearing systems listed in Table 4, our data, along with those reported by Drits et al. (1974) and Tateyama et al. (1978), also indicate a Na-bearing system for biopyriboles. A possible chemical formula for a Na-bearing (21)-clinopyribole may be derived from our data as

TABLE 4. Comparison of chain-silicate crystal data

	Ca-free system		Ca-bearing system	Type of chains
	Orthorhombic	Monoclinic	Monoclinic	
	Orthopyroxene	Clinopyroxene	Diopside	Single
Composition	$(Mg,Fe)_2Si_2O_6$		$Ca_2Si_2O_6$	
a (Å)	18.3	9.6	9.75	
b (Å)	8.9	8.9	8.92	
c (Å)	5.3	5.3	5.3	
β (°)		109	105.5	
Space group	*Pbca*	*C2/c*	*C2/c*	
	Anthophyllite	Cummingtonite	Tremolite	Double
Composition	$(Mg,Fe)_7Si_8O_{22}(OH)_2$		$Ca_2Mg_5Si_8O_{22}(OH)_2$	
a (Å)	18.56	9.53	9.8	
b (Å)	18.2	18.3	18.0	
c (Å)	5.3	5.3	5.3	
β (°)		102	104.5	
Space group	*Pnma*	*C2/m*	*C2/m*	
	Jimthompsonite	Clinojimthompsonite	**Postulated(?)**	Triple
Composition	$(Mg,Fe)_{10}Si_{12}O_{32}(OH)_4$		$Ca_2(Mg,Fe)_8Si_{12}O_{32}(OH)_4$	
a (Å)	18.6263	9.874	~9.8	
b (Å)	27.2303	27.24	~27.0	
c (Å)	5.2970	5.316	~5.3	
β (°)		109.47	~106	
Space group	*Pbca*	*C2/c*	*C2/c*	
	Chesterite	**Unnamed mineral**	**Postulated(?)**	Double and triple
Composition	$(Mg,Fe)_{17}Si_{20}O_{54}(OH)_6$		$Ca_4(Mg,Fe)_{13}Si_{20}O_{54}(OH)_6$	
a (Å)	18.614	9.867	~9.8	
b (Å)	45.306	5.31	~45.0	
c (Å)	5.2966	5.292	~5.3	
β (°)		109.7	~106	
Space group	$A2_1ma$	*A2/m*, *Am*, or *A2*	*A2/m*, *Am*, or *A2*	
	Postulated(?)	**Postulated(?)**	Clinopyribole	Single and double
Composition	$(Mg,Fe)_{11}Si_{12}O_{34}(OH)_2$		$K(Ca,Na)_4(Mg,Al)_7Si_{12}O_{34}(OH)_2$	
a (Å)	~18.5	~9.8	9.8525	
b (Å)	~27.0	~27.0	26.6818	
c (Å)	~5.3	~5.3	5.269	
β (°)		~109	106.27	
Space group	$A2_1ma$ *or Amma*	*A2/m*	*A2/m*	

$\square Na_4Mg_3Al_4Si_{12}O_{34}(OH)_2$, whereas the chemical compositions determined for Na-bearing MMP-type triple-chain biopyriboles are $Na_2Mg_8[Si_{12}O_{30}(OH)_2](OH)_2$ (Drits et al. 1974) and $Na_2Mg_4Si_6O_{16}(OH)_2$ (Tateyama et al. 1978).

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