# The crystal structure of a Mg-rich carpholite

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## Abstract

The crystal structure of a magnesium-rich carpholite with the chemical formula $(Mg_{0.795}Fe^{2+}_{0.203}Mn_{0.002})Al_2Si_2O_6(OH)_4$ and with the lattice constants $a = 13.714(2)$, $b = 20.079(2)$, $c = 5.105(1)$ (space group $Ccca$) has been refined by the least-squares method using 1163 reflections measured on a computer controlled automatic single-crystal diffractometer, using monochromatic $MoK\alpha$ radiation. The unweighted R-factor is 0.044. The structure very closely resembles that of ferrocarpholite and Mn-carpholite, thus suggesting the likelihood of complete miscibility between the three end-members. The inter-atomic bond distances and angles of the $SiO_4$-tetrahedra and the $AlO_6$-octahedra further demonstrate the crystal–chemical similarities between pyroxenes and Mn-carpholites, thereby emphasizing the similarity in bonding in all carpholites.

## Introduction

The comparatively recent discoveries of a large number of Fe- and Mg-rich carpholites in different parts of the world and their characteristic occurrence in geological units subjected to high pressure/low temperature metamorphism has aroused the interest of mineralogists and crystallographers in their structure and crystal–chemical relationships. Though the chemical compositions of carpholites can be represented by the end-members manganocarpholite, $MnAl_2Si_2O_6(OH)_4$, ferrocarpholite, $FeAl_2Si_2O_6(OH)_4$, and magnesiocarpholite, $MgAl_2Si_2O_6(OH)_4$, it has been observed that carpholites occur preferentially as binary solid solutions, the third component being generally less than 5% (Mottana and Schreyer, 1977; Viswanathan and Seidel, 1979). In order to understand the nature of the solid solutions and the crystal–chemical relationships a knowledge of the structure of the end-members is necessary. MacGillavry *et al.* (1956) first defined the basic structural principles of carpholites by determining the structure of an iron-rich carpholite, $(Fe^{2+}_{0.8},Mg_{0.2})(Al_{0.95}Fe^{3+}_{0.05})Si_2O_6(OH)_4$, by conventional film methods. Later Naumova *et al.* (1975) and recently Lindemann *et al.* (1979) determined the structure of an almost pure manganocarpholite by more modern automatic diffractometer methods, and arrived at almost identical results. Under these circumstances it was considered

relevant to determine the structure of the remaining end-member, magnesiocarpholite, and compare it with the others. Unfortunately good crystals of the almost pure magnesiocarpholite from central Crete (specimen 77/5, Viswanathan and Seidel, 1979) could not be obtained because it is finely intergrown with pyrophyllite and muscovite. Hence another magnesium-rich specimen which was collected by Dr. E. Seidel in southeast Sfinari, West Crete (specimen KRH 2, Viswanathan and Seidel, 1979) was chosen for structure determination.

## Experimental and results

A typical feature of most of the carpholite crystals is their acicular habit, often tending to become fibrous. The needle axis is parallel to the crystallographic $c$ axis. Specimens containing such magnesium-rich carpholites sometimes show such fibers bent during tectonic deformation. Most of the single crystals examined under the microscope appear as if they are made up of such fibers. Precession photographs of such crystals invariably showed splitting of reflections because of lack of parallel alignment of the fragile needles. Precession photographs of the crystal finally selected for the structure determination did not show any such effects. It had a needle shape with an approximate triangular cross section, the lengths of the sides of the triangle being $0.105 \times$

0.076 × 0.057 mm. Precession and Weissenberg photographs indicated the space group to be *Ccca*. The lattice constants determined with a Guinier powder pattern are $a = 13.714(2)$; $b = 20.079(2)$; $c = 5.105(1)$Å.

The chemical analysis was carried out by Dr. E. Seidel. The elements Si, Ti, Al, Fe, P, K and Ca were determined by X-ray fluorescent methods, and Mn, Mg, Na, Ca and Fe by atomic absorption methods. Ferrous iron was determined by oxidation to ferric iron and $H_2O$ by the Penfield method. Dr. Seidel corrected the chemical analysis for the presence of a few small inclusions of quartz and arrived at the formula $(Mg_{0.795}Fe^{2+}_{0.203}Mn_{0.002})Al_2Si_2O_6(OH)_4$ for the investigated quartz free crystal (see Viswanathan and Seidel, 1979, for further details).

The intensity data were collected with a STOE four circle automatic single-crystal diffractometer with MoKα radiation and a graphite monochromator. Altogether 5694 reflections were measured in the 2θ-range 0–65°, which were then reduced to 1301 symmetry-independent reflections. The data were then corrected for Lorentz, polarization and absorption effects ($\mu = 13.0$) using the ABSORB routine, which is available in the X-RAY 76 crystallographic programs (Stewart, 1976). Of the 1301 reflections only 1163 were considered for final refinement as the others had F less than $3\sigma(F)$ and hence were considered as unobserved[1]. The refinement was carried out with the ORFLS program (Busing *et al.*, 1962).

In order to work out a trial and error model of the structure of carpholite under investigation two important observations were considered: first, the similarity of the powder pattern of the mineral under study with that of a manganocarpholite, which clearly suggested that the structural principles must be the same. Second, the striking needle shape of the crystals indicated the presence of $SiO_3$ chains in the structure of Mg-carpholites. Though Mg and Al can occupy six-coordinated positions one can conclude from the crystal–chemical and charge balance considerations (Viswanathan and Seidel, 1979) that the $Mn^{2+}$ position will probably be occupied by divalent Mg, the aluminum atoms occupying the same position as in manganocarpholite. However for a preliminary refinement of the structure an exact knowledge

of their positions was considered irrelevant, as Mg and Al possess approximately the same scattering factors. Hence refinement was initiated assuming average structure factors for magnesium and aluminium, and using the atomic coordinates given by Naumova *et al.* (1975) as starting parameters. After five cycles of refinement of scale factors and atom parameters the discrepancy index, R, was reduced to 0.12. Calculation of inter-atomic distances revealed long bonds comparable to those of Mg–O at the position occupied by Mn in manganocarpholite and shorter ones comparable to those of Al–O at the other positions in question. Scattering factors for $Mg^{2+}$ and $Al^{3+}$ from the *International Tables of Crystallography* (Vol. 4, 1974, Kynoch Press, England), were introduced for these sites, respectively, with 20 percent $Fe^{2+}$ substituting for Mg. Unit weights were used throughout the refinement. The final residuals arrived at using isotropic and anisotropic temperature factors were 0.060 and 0.044, respectively. Atomic coordinates (Table 1) and the bond lengths and angles about the cations (Table 2 and 3) are derived from parameters obtained following refinement of anisotropic temperature factors. Atomic coordinates and bond lengths of the Mn-carpholite (Naumova *et al.*, 1975) are also given in the tables for comparison. The temperature factors are listed in Table 4.

## Discussion

The atomic parameters of magnesium-rich carpholite agree better with those of the Mn end-member (Naumova *et al.*, 1975 and Lindemann *et al.*, 1979) than with those of the Fe-rich end-member (MacGillavry *et al.*, 1956). A calculation of the bond distances and angles of the $SiO_4$ tetrahedra showed that they deviate from acceptable values in the latter case, which must be attributed mainly to the inaccurate determination of the z-coordinates of silicon and oxygens.

The structure of magnesium-rich carpholite is very similar to that of manganocarpholite; it also consists of pyroxene-like slabs having the composition $Si_4Al_2O_{12}(OH)_4$ (Viswanathan and Seidel, 1979) which cause it to be fibrous. Such slabs are linked to each other by pyroxene-like octahedral metal layers which are oriented perpendicular to the slabs. Smaller magnesium atoms, instead of manganese, occupy the outer octahedra of the metal layers (Fig. 1). As a result, the pyroxene-like slabs are brought closer to each other along [010] and [100], thus explaining

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[1] To receive a copy of the observed and calculated structure factors, order Document AM-81-174 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D.C. 20009. Please remit $1.00 in advance for the microfiche.

Table 1. Fractional atomic coordinates of Mg- and Mn-carpholites

| Atom[a] | Mg-carpholite | | | Mn-carpholite (Naumova et al., 1975) | | |
|---|---|---|---|---|---|---|
| | x | y | z | x | y | z |
| Mg(Fe,Mn) | 0 | 0.8754(1)[b] | $\frac{3}{4}$ | 0 | 0.8727 | $\frac{3}{4}$ |
| Al(1) | 0.1909(1) | $\frac{3}{4}$ | $\frac{3}{4}$ | 0.1933 | $\frac{3}{4}$ | $\frac{3}{4}$ |
| Al(2) | 0 | 0.9614(1) | $\frac{1}{4}$ | 0 | 0.9614 | $\frac{1}{4}$ |
| Si | 0.1935(1) | 0.8798(1) | 0.4172(2) | 0.1941 | 0.8794 | 0.4130 |
| (OH)(1) | 0.0997(2) | 0.8099(1) | 0.8794(5) | 0.1035 | 0.8072 | 0.8872 |
| (OH)(2) | 0.0684(2) | 0.9657(1) | 0.9276(5) | 0.0687 | 0.9670 | 0.9312 |
| O(1) | 0.2060(2) | 0.7997(1) | 0.4313(4) | 0.2063 | 0.8000 | 0.4332 |
| O(2) | 0.0803(2) | 0.8993(1) | 0.4099(5) | 0.0825 | 0.8993 | 0.3983 |
| O(3) | 0.2485(2) | 0.9129(1) | 0.6707(5) | 0.2448 | 0.9114 | 0.6709 |

[a] The oxygens have been labelled as in pyroxene structure (Clark et al., 1969).
[b] Standard erros x $10^{-4}$ are in parentheses.

the contraction of the unit cell with the substitution of $Mg^{2+}$ for $Fe^{2+}$ or $Mn^{2+}$.

The finer structural details of the magnesium-rich carpholite confirm the crystal–chemical similarities already observed between pyroxenes and manga-nocarpholites (Viswanathan and Seidel, 1979). The dimensions of the $SiO_4$ tetrahedra (Table 2) are comparable to those of Mn-carpholite. Whether the average value of the Si–O bonds (Papike et al., 1969) or the shortest Si–O(2) bond is considered (Clark et al.,

Table 2. Bond lengths (Å) and angles (°) of silicate tetrahedra

| Atoms | Mg-carpholite | Mn-carpholite | Atoms | Mg-carpholite | Mn-carpholite |
|---|---|---|---|---|---|
| Si-O(1) | [a]1.618(3) | [b]1.624 | Si-O(3)-Si | 131.88(16) | 132.72(16) |
| -O(2) | 1.602(3) | 1.597 | | | |
| -O(3) | 1.631(3) | 1.635 | O(3)-O(3)-O(3) | 178.10(15) | 173.57(15) |
| -O(3) | 1.639(3) | 1.630 | | | |
| | Mean 1.623 | 1.622 | | | |
| O...O distances | | | Angles at Si | | |
| O(2)-O(1) | 2.642(3) | 2.651(3) | O(2)-O(1) | 110.28(16) | 110.76(16) |
| O(2)-O(3) | 2.662(4) | 2.669(4) | O(2)-O(3) | 110.80(15) | 111.30(15) |
| O(2)-O(3) | 2.677(4) | 2.655(4) | O(2)-O(3) | 111.38(15) | 110.68(15) |
| O(1)-O(3) | 2.707(3) | 2.715(3) | O(1)-O(3) | 112.85(14) | 112.88(14) |
| O(1)-O(3) | 2.646(3) | 2.622(3) | O(1)-O(3) | 108.67(13) | 107.40(13) |
| O(3)-O(3) | 2.553(4) | 2.565(4) | O(3)-O(3) | 102.64(15) | 103.52(16) |
| | Mean 2.648 | 2.646 | | 109.44 | 109.42 |

a. Numbers in paranthesis represents one estimated standard deviation ($\sigma$) and refers to the last decimal place.

b. Standard errors are not available.

Table 3. Interatomic distances (Å) and angles (°) of coordinating octahedra about the cations

| $(MO_6)$-octahedron | Mg-rich carpholite | Mn-rich carpholite | $(Al(1)O_6)$-octahedron | Mg-rich carpholite | Mn-rich carpholite | $(Al(2)O_6)$-octahedron | Mg-rich carpholite | Mn-rich carpholite |
|---|---|---|---|---|---|---|---|---|
| M-(OH)(1) [2] | 2.008(3)* | 2.076(3) | Al(1)-(OH)(1) [2] | 1.857(3) | 1.840(3) | Al(2)-O(2) [2] | 1.852(3) | 1.862(3) |
| M-O(2) [2] | 2.111(3) | 2.199(3) | Al(1)-O(1) [2] | 1.920(2) | 1.922(2) | Al(2)-(OH)(2) [2] | 1.896(3) | 1.892(3) |
| M-(OH)(2) [2] | 2.233(3) | 2.330(3) | Al(1)-O(1) [2] | 1.963(3) | 1.959(3) | Al(2)-(OH)(2) [2] | 1.961(3) | 1.969(3) |
| Mean | 2.117 | 2.202 | Mean | 1.913 | 1.907 | Mean | 1.903 | 1.908 |
| **O...O distances** | | | **O...O distances** | | | **O...O distances** | | |
| (OH)(1)-(OH)(1) [1] | 3.037(4) | 3.189(4) | (OH)(1)-(OH)(1) [1] | 2.746(3) | 2.714(3) | O(2) -O(2) [1] | 2.740(4) | 2.741(4) |
| (OH)(1)-O(2) [2] | 3.006(3) | 3.138(3) | (OH)(1)-O(1) [2] | 2.720(4) | 2.729(4) | O(2) -(OH)(2) [2] | a2.805(4) | a2.765(4) |
| (OH)(1)-O(2) [2] | 3.235(4) | 3.364(4) | (OH)(1)-O(1) [2] | 2.812(3) | 2.757(3) | O(2) -(OH)(2) [2] | a2.573(4) | a2.650(4) |
| (OH)(1)-(OH)(2) [2] | 3.166(3) | 3.287(3) | (OH)(1)-O(1) [2] | b2.686(4) | b2.645(4) | O(2) -(OH)(2) [2] | 2.717(3) | 2.725(3) |
| O(2) -(OH)(2) [2] | 2.965(4) | 3.061(4) | O(1) -O(1) [2] | 2.437(3) | 2.459(3) | OH(2)-(OH)(2) [2] | 2.900(4) | 2.890(4) |
| O(2) -(OH)(2) [2] | a2.573(4) | a2.650(4) | O(1) -O(1) [2] | 2.824(3) | 2.832(3) | OH(2)-(OH)(2) [2] | c2.441(4) | c2.429(4) |
| (OH)(2)-(OH)(2) [1] | a2.608(4) | a2.656(4) | O(1) -O(1) [1] | 2.722(3) | 2.764(3) | OH(2)-(OH)(2) [1] | a2.608(4) | 2.656(4) |
| Mean | 2.961 | 3.070 | Mean | 2.702 | 2.694 | Mean | 2.685 | 2.693 |
| **Angles at M** | | | **Angles at Al(1)** | | | **Angles at Al(2)** | | |
| (OH)(1)-(OH)(1) [1] | 98.23(13) | 100.37(13) | (OH)(1)-(OH)(1) [1] | 95.35(13) | 95.07(13) | O(2) -O(2) [1] | 95.41(14) | 94.80(14) |
| (OH)(1)-O(2) [2] | 93.68(10) | 94.39(10) | (OH)(1)-O(1) [2] | 92.12(11) | 93.00(11) | O(2) -(OH)(2) [2] | 96.87(12) | 94.87(12) |
| (OH)(1)-O(2) [2] | 103.48(10) | 103.76(10) | (OH)(1)-O(1) [2] | 96.21(11) | 94.24(11) | O(2) -(OH)(2) [2] | 86.69(11) | 89.80(12) |
| (OH)(1)-(OH)(2) [2] | 96.43(09) | 96.32(09) | (OH)(1)-O(1) [2] | 89.31(10) | 88.21(11) | O(2) -(OH)(2) [2] | 90.84(10) | 90.67(10) |
| O(2) -(OH)(2) [2] | 86.02(10) | 85.00(10) | O(1) -O(1) [2] | 77.72(10) | 78.64(10) | OH(2)-(OH)(2) [2] | 97.51(12) | 96.89(12) |
| O(2) -(OH)(2) [2] | 72.58(10) | 71.56(10) | O(1) -O(1) [2] | 93.29(10) | 93.69(10) | OH(2)-(OH)(2) [2] | 78.51(11) | 77.96(11) |
| (OH)(2)-(OH)(2) [1] | 71.46(11) | 69.52(10) | O(1) -O(1) [1] | 87.79(11) | 89.73(12) | OH(2)-(OH)(2) [2] | 83.38(13) | 84.85(13) |
| Mean | 89.51 | 89.33 | Mean | 90.04 | 90.03 | Mean | 89.97 | 90.00 |

*Numbers in paranthesis represents one estimated standard deviation (σ) and refers to the last decimal place.

a. Edges shared between $(MO_6)$-octahedron and $(Al(2)O_6)$-octahedron.

b. Edges shared between $(Al(1)O_6)$-octahedra.

c. Edges shared between $(Al(2)O_6)$-octahedra.

1969), one comes to the conclusion that there is no replacement of silicon by aluminum in the tetrahedra in both the carpholites for which accurate structure data are now available.

The SiO$_4$-tetrahedra are distorted in the same way as in Mn-carpholites and resemble to some extent those in aluminum-rich pyroxenes such as spodumene and jadeite. The bridging Si–O bonds are longer than the non-bridging ones. This is further evidence that the differences in the Si–O bonds are inherent in the Si–O chain. The Si–O(2) bonds are also the shortest as in clinopyroxenes. The noteworthy differences between the Si–O tetrahedra of pyroxenes and carpholites are to be observed in two of

Table 4. Temperature factors and r.m.s. displacements. Anisotropic temperature factors were not available for Mn-carpholites.

| Atom | Mg-rich Isotropic $B(Å^2)$[a] | Mn-rich Isotropic $B(Å^2)$ | Mg-rich | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | r.m.s. displacement (Å) | | | Anisotropic (x $10^5$) | | | | | |
| | | | +a | +b | +c | | | | | | |
| Mg(Fe,Mn) | 0.65 | 0.43 | 0.107 | 0.111 | 0.063 | 118(7) | 59(3) | 307(26) | 0 | 27(8)[b] | 0 |
| Al(1) | 0.55 | 0.30 | 0.103 | 0.102 | 0.055 | 112(7) | 50(3) | 234(27) | 0 | 0 | 12(6) |
| Al(2) | 0.48 | 0.44 | 0.100 | 0.107 | 0.044 | 104(7) | 55(3) | 149(27) | 0 | -12(9) | 0 |
| Si | 0.47 | 0.25 | 0.095 | 0.103 | 0.047 | 96(4) | 50(2) | 168(17) | 4(2) | 6(5) | 7(4) |
| (OH)(1) | 1.02 | 0.96 | 0.113 | 0.136 | 0.094 | 153(14) | 82(6) | 669(55) | 19(7) | 0(1) | 4(12) |
| (OH)(2) | 0.72 | 0.65 | 0.103 | 0.113 | 0.075 | 113(13) | 61(6) | 424(48) | -4(7) | -5(15) | 4(10) |
| O(1) | 0.66 | 0.70 | 0.118 | 0.100 | 0.064 | 145(13) | 47(6) | 329(47) | -0(6) | 25(15) | 20(10) |
| O(2) | 0.72 | 0.66 | 0.099 | 0.121 | 0.073 | 108(12) | 66(6) | 424(48) | 12(7) | -3(15) | 29(10) |
| O(3) | 0.72 | 0.43 | 0.112 | 0.123 | 0.063 | 138(15) | 68(7) | 333(52) | -10(6) | -61(15) | 1(11) |

a Equivalent isotropic temperature factors.

b Paranthesised figures represent the estimated standard deviations (esd) in terms of the least units, thus 0.00027(8) indicates an esd of 0.00008.
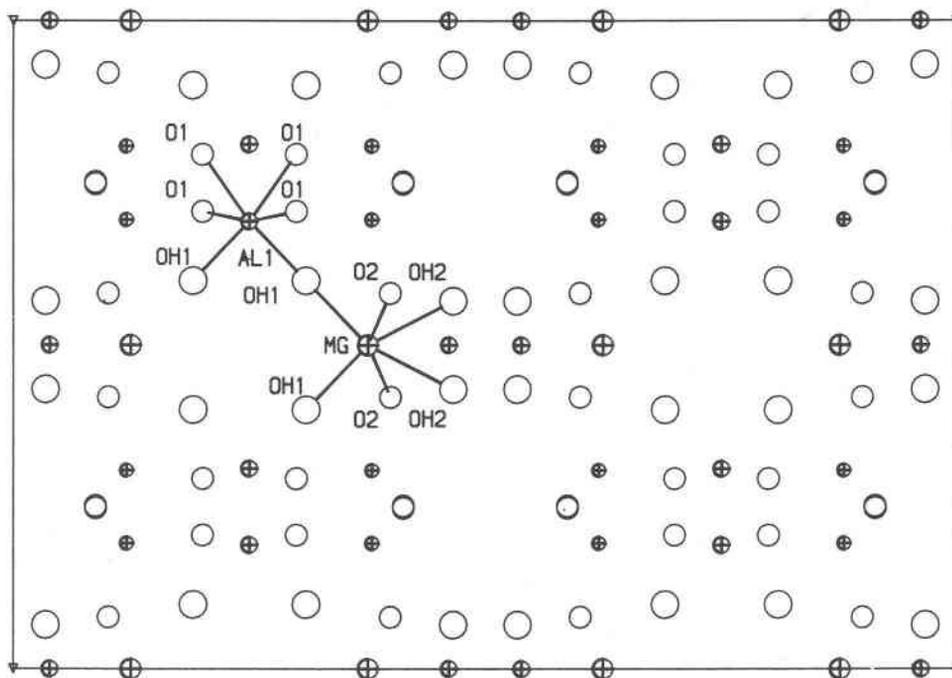
Fig. 1. A (001)-projection of the structure of Mg-carpholite. ⊕—Si; ⊕—Al; ⊕—Mg; ○—O; ○—(OH).

the O–Si–O angles. In the former the O(1)–O(2) angle is considerably greater than the tetrahedral angle of 109.47°, whereas in the latter the O(3)–Si–O(3) angle is considerably smaller. When the angles, $<$(SiOSi) and $<$(000)$_{br}$ are plotted in Figure 8 of Meagher (1980) the carpholites plot in the low energy trough, where many pyroxenes also plot.

The dimensions of the Al(1) and Al(2) octahedra (Table 3) are comparable to those of Mn-carpholite. The octahedral edges shared by adjacent Al octahedra are very short. As expected the two bonds Al(1)–(OH)(1) and Al(2)–O(2) are shorter than the other Al–O bonds. The Al(1) octahedra are slightly bigger and Al(2) octahedra slightly smaller than those of manganese variety. The size of Al(2) octahedra is probably influenced by the size of the outer cation (Mg, Fe or Mn) as observed by Okamura et al. (1974) in the case of Al-rich clinopyroxene.

Mg-rich carpholite differs from Mn-rich carpholite mainly in the environment of the large cation. (Mg,Fe)–O bonds are shorter in keeping with the smaller ionic radius of magnesium. In order to achieve this the Mg-atoms are shifted along the $b$ axis towards the coordinating O(2) and (OH)(2) (Fig. 1). The (OH)(1) ions in turn are shifted towards the

Mg atoms. In order to keep the Al(1)–(OH)(1) bonds approximately the same as in Mn-carpholite, the Al(1) atoms, being constrained to the 2-fold axis, shift away from each other along the $a$ axis, thereby increasing the Al(1)–Al(1) distance from 3.003Å to 3.024Å. However, these changes in no way reduce the distortions in the octahedra of the larger cation. In fact if the metal–anion bonds are compared (Table 3) we note that the M–(OH)(1) bonds are the shortest and the M–(OH)(2) are the longest in both minerals. These distortions should be attributed to the repulsion between $Al^{3+}$ and $Mg^{2+}(Fe^{2+},Mn^{2+})$ ions and to the excess negative charges on the coordinating anions, (OH)(1) and O(2). Thus these data show that the M octahedra in iron-rich carpholites are not more symmetrical than those in orthopyroxenes or garnets, as had been suggested by Seifert (1979).

It is interesting to compare the mean M–O distances with the values 2.173Å, 2.137Å and 2.077Å given by Papike et al. (1969) for $Mn^{2+}$–O, $Fe^{2+}$–O and Mg–O respectively in amphiboles. Assuming a linear combination these distances for the Mg-rich and Mn-carpholite should be 2.089Å and 2.173Å respectively. However, the observed bonds are some-

what longer (Table 3) attesting to the similarity of bonding of these metal atoms to the surrounding anions.

Summarizing, it can be said that the bonding is almost identical in all carpholites and that the principles which govern their structures must also be identical. Hence considerable solid solutions may be expected between the three end-members.

The isotropic temperature factors are small and are comparable with those of Mn-carpholite (Naumova *et al.*, 1975). The root-mean-square equivalents (Table 4) show systematically low values for the displacements along the $c$ axis, which may appear to be due to problems with the absorption correction. However, as the absorption coefficient is small and as the routine used for the absorption correction is a reliable one, such values cannot be due to any error in the temperature factor. The values suggest that the thermal ellipsoids of all atoms are oblate triaxial ones with the shortest axes oriented approximately parallel to the $c$ axis. As no other reliable anisotropic temperature factors[2] are available at the moment for Mn-carpholites, it is not possible to draw any useful conclusions from the observed trend.

## Acknowledgments

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[2] The temperature factors given by Lindemann *et al.* (1979) appear to be too large for the metal atoms and too small for some anions to be considered useful.

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