Polysomatism and polysomatic series: A review and applications

David R. Veblen

For deposit: Appendix 1

APPENDIX 1. THE RELATIONSHIP BETWEEN PYROXENOID P-SLABS AND THE CLINOPYROXENE STRUCTURE

Angel (1986b) asserted that the P-slabs in pyroxenoid structures such as rhodonite, pyroxmangite, pyroxferroite, and ferrosilite III do not have the pyroxene structure. In this appendix, I show that this conclusion is incorrect, by using three separate lines of argument: (1) an appropriate transformation from clinopyroxene to pyroxenoidlike unit cell basis vectors results in C-centered P-slabs, not body-centered slabs as suggested by Angel, (2) when transformed into a unit cell similar to that for clinopyroxene, the atomic positions in the pyroxenelike part of the pyroxmangite structure are very similar to those of clinopyroxenes, and (3) projections of the real clinopyroxene and pyroxenoid structures show that the shifts between layers of tetrahedral chains are essentially the same in the P-slabs and completely unlike the shifts shown in the idealized projections of Angel (1986b, Fig. 2). These arguments are also summarized briefly in the text of this paper.

Angel (1986b) based his assertion that the P-slabs in pyroxenoids possess a structure that is different from that of clinopyroxene on a transformation of unit cell basis vectors in which $\mathbf{b}$ of clinopyroxene is rewritten as $\mathbf{b}$ - $\mathbf{c}$, thus making $\mathbf{b}$ analogous to that axis in the pyroxenoids. Angel (1986b) noted that this transformed unit cell for clinopyroxene is body-centered, rather than C-centered. We can write Angel's transformation formally as the unit-cell transformation matrix

$$T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$$

The inverse of the transpose of this matrix, $(T^T)^{-1}$, does indeed transform the C-centering vector [1/2, 1/2, 0] to [1/2, 1/2, 1/2], demonstrating Angel's claim that this transformation is from a C-centered unit cell to a body-centered cell:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}.$$

Nonetheless, this transformation is not the appropriate one for transforming (and comparing) clinopyroxene with the P-slabs in pyroxenoids. As noted by Czank and Simons (1983), Ried (1984), Angel et al. (1984), Angel (1986b), and Veblen (1985a), it is the $\{11\overline{1}\}$ planes of clinopyroxene (e.g., johannsenite) that are parallel to (001) of pyroxenoids when the two structures intergrow. It is therefore these planes that must be structurally analogous for coherent intergrowth, and this leads to more appropriate transformation matrices (depending on which of the $\{11\overline{1}\}$ planes is chosen) of the type

$$T' = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix}.$$

The inverse of the transpose of this matrix leaves the C-centering vector [1/2, 1/2, 0] unchanged, indicating that the clinopyroxene structure is still C-centered when transformed into this new unit cell. It can be noted that this unit cell corresponds to the orientation of the P-slabs in pyroxenoids and, because it is C-centered, it is compatible with the C-centered unit cells that are now commonly employed for describing the pyroxenoid structures (e.g., Ohashi and Finger, 1975). However, its relationship to the standard clinopyroxene unit cell is not simple, because, for example, **c** is reversed relative to the skew of the octahedral strips (see Thompson, 1981, for an explanation of skew in terms of ducks). Furthermore, the relationship between the **a** axes of the clinopyroxene and the pyroxenoid is similar to that between the **a** axes of clinopyroxene and clinoamphibole, and β of the clinopyroxene in this cell setting is acute, just as it is when referred to standard C-centered amphibole axes (see Fig. 4 of Thompson, 1978).

It can be shown by transforming the atomic coordinates of clinopyroxene from the standard unit cell to the cell given by T ' that the clinopyroxene structure is very similar to

2

that of the P parts of rhodonite, pyroxmangite, etc. Alternatively, a portion of the pyroxenelike part of one of these pyroxenoids can be transformed into a unit cell analogous to the conventional clinopyroxene unit cell. I will follow the latter approach here, transforming part of the pyroxmangite structure refined by Ohashi and Finger (1975) into a clinopyroxenelike unit cell. First, the origin is shifted to the center of symmetry at the fractional coordinates (0, 1, 1/2) in the pyroxmangite unit cell by subtracting this vector from the fractional coordinates of the relevant atoms in pyroxmangite. The new **a** axis is given by the vector obtained by subtracting the position vector of an M3 atom from that of an M2 atom two tetrahedral layers away: [-1.0024, 0.1007, -0.2933]. The new **b** is found by subtracting the position vector of an M3 atom from that of an M2 atom in an adjacent chain of the same octahedral layer: [-0.0024, -0.8993, -0.2933]. The new **c** is given by the vector between an M3 atom and an M2 atom within the same chain: [0.0024, -0.1007, 0.2933]. It should be noted that this transformation not only changes but also effectively reverses the direction of **a** (and also **b**, in order to maintain a right-handed coordinate system). This reversal takes into account the fact that the "ducks" of the octahedral strip (see Thompson, 1981a) swim in the +**c** direction in the pyroxenoid (Ohashi and Finger, 1975) but in the -**c** direction in the standard unit-cell setting for clinopyroxene (Burnham et al., 1967). The matrix representing this unit-cell transformation is thus

$$T'' = \begin{bmatrix} -1.0024 & 0.1007 & -0.2933 \\ -0.0024 & -0.8933 & -0.2933 \\ 0.0024 & -0.1007 & 0.2933 \end{bmatrix}.$$

When the pyroxmangite metric tensor is transformed by this matrix and its transpose, the metric tensor for this new cell yields the unit-cell parameters given and compared to those of johannsenite in Table 1. While not identical, the unit cell is close to that for many

3

clinopyroxenes, with the most notable deviations being on the order of a few percent. The deviation from monoclinic shape of this clinopyroxenelike unit cell in the P-slab region of pyroxmangite is slight, as can be seen from the α and γ values of 89.82° and 89.78°.

The atomic coordinates of the pyroxmangite can be transformed into the clinopyroxenelike unit cell by multiplying them by the inverse of the transpose of T ". The results are shown in Table 1, which compares the atomic coordinates of the metal atoms in the pyroxenelike region of pyroxmangite with their atomic positions within one unit cell of johannsenite (Freed and Peacor, 1967). The agreement is quite close, the differences presumably resulting primarily from distortions required by mating of the P and W slabs and by substantially different occupancies of M2 (pyroxene nomenclature). It is clear that alternate layers of silicate chains are not shifted by $c/2$ in the pyroxenoid relative to the pyroxene, as claimed by Angel (1986b), and that this region of pyroxmangite is essentially identical to the clinopyroxene structure.

A final way that can be used to show the structural relationship between the P-slab regions of pyroxenoids and the clinopyroxene structure is to examine projections of the structures onto (100), as done by Angel (1986b, his Fig. 2) and Angel and Burnham (1991). Angel's (1986b) projections purport to indicate the relationship between back-to-back silicate chains in clinopyroxene and pyroxenoid, but the projections clearly are for an idealized structure. Close examination indicates that they assume, for example, that clinopyroxene has a metrically orthorhombic unit cell. Figure 14 shows projections of analogous fragments from the real johannsenite and pyroxmangite structures, showing that the real structures are not at all like those asserted by Angel (1986b, Fig. 2). Included in Figure 14 are the M1 polyhedra (pyroxene nomenclature) that control the shift between the back-to-back chains in both structures; indeed, it can be seen that the linkage of the chains via these polyhedra forces the two structures to have similar relative shifts between the

4

back-to-back chains. The very strong similarity between the real clinopyroxene structure and the pyroxenelike part of this real pyroxenoid are obvious.