Ideal wollastonite and the structural relationship between the pyroxenoids and pyroxenes

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ABSTRACT

A hypothetical ideal wollastonite with regular octahedra and T3 tetrahedron is presented and used to compare and contrast the pyroxenes and pyroxenoids. While clinopyroxenes have close-packed arrangements of oxygen anions, several lines of evidence demonstrate that pyroxenoids do not. One such line is the number of tetrahedra in a single tetrahedral chain per octahedra in a single associated octahedral chain (interior to the octahedral band), referred to as the “single-chain T:O ratio,” which is 1:1 in pyroxenes but 3:2 in wollastonite and always greater than 1:1 in other MSiO3 pyroxenoids. Because the Si-tetrahedron is extremely resistant to distortion, this forces marked distortion in at least one pyroxenoid octahedral site.

The octahedral layers in pyroxenes and pyroxenoids are compared by placing them in the context of a fully occupied, closest-packed sheet of idealized octahedra, and it is shown that they are fundamentally different.

The new mineral yangite is analyzed from the perspective developed in this study. It is structurally similar to the pyroxenoids, but the structure is a new type because it contains double tetrahedral chains and mixed polyhedral layers containing double chains of tetrahedra and bands of octahedra of width two. The tetrahedral chains are wollastonite-type chains and the wollastonite-type double chain is shown to have important differences from the amphibole double chain. A possible explanation for the existence of this crystal structure based on a hydrogen bond between Pb and O is presented.

Keywords: Clinopyroxene, pyroxenoid, chain silicate, yangite, wollastonite, diopside, close-packing

INTRODUCTION

The new mineral yangite, a new type of chain silicate with double tetrahedral chains and ideal formula PbMnSi3O8·H2O, is described elsewhere in this issue (Downs et al. 2016). This companion paper compares and contrasts the pyroxenoids and pyroxenes to develop some new approaches to characterizing and understanding members of the pyroxenoid group. To do so, this study compares hypothetical ideal pyroxenoids and pyroxenes—specifically the relationships between their tetrahedral and octahedral structural subunits, their anion packing arrangements, their octahedral arrangements, and the compositions of their “polyhedral layers,” as defined below. The octahedral arrangement of a hypothetical pyroxenoid with T-chain repeat unit length of 11 is predicted. Finally, the new approaches are applied to see how yangite compares with the pyroxenoids and provide an understanding of why its structure is adopted.

Numerous papers have discussed the structural relationship between the pyroxenes and pyroxenoids, with a particular emphasis on the description of pyroxenoids as polyomes built from pyroxene and “wollastonite-like” (Angel and Burnham 1991) modules. By the 1980s, it was known that clinopyroxene (Cpx) and pyroxenoid (Pxd) intergrowths take place along face poles (1TT) and (001) in Cpx and Pxd, respectively (cf. Ried 1984). During that decade, the existence of isostructural portions of the two structures that would allow seamless intergrowth was debated. By the early 1990s, it was determined that such portions did exist (cf. Veblen 1991; Angel and Burnham 1991). Figures 1a and 1b illustrate isostructural planar portions of diopside (Thompson and Downs 2008) and rhodonite (Peacor et al. 1978), looking down face poles (1TT) and (001), respectively.

Many other discussions of the relationship between the pyroxenes and pyroxenoids focus on tetrahedral chain (T-chain) geometry and repeat length because T-chain repeat length in described pyroxenoids is variously 3, 5, 7, or 9 (cf. Klein and Dutrow 2008). Prewitt and Peacor (1964) and Liebau (1956) noted that octahedral cation size determines T-chain type, with decreasing cation size corresponding to increasing T-chain repeat unit length. These topics will be addressed in detail later in the paper. Ohashi and Finger (1978) concluded that the distribution of octahedral cations between the different sites within the octahedral layers determine both structure type and the range of solid solutions. Both Prewitt and Peacor (1964) and Ohashi and Finger (1978) described pyroxenoids as having distorted closest-packed arrangements of oxygen anions.

This report analyzes pyroxenoids and pyroxenes in terms of several different structural subunits, defined here. For the purposes of this paper, a polyhedral layer is a unit that is one polyhedron thick in one direction, called the “stacking vector,” and infinite in dimension in all directions perpendicular to the stacking vector. Layered structures, such as the pyroxenoids and pyroxenes, can be described as composed of one or more types