

Structural mechanisms of solid solution and cation ordering in augite-jadeite pyroxenes: I. A macroscopic perspective

**TIZIANA BOFFA BALLARAN,^{1,*} MICHAEL A. CARPENTER,² M. CHIARA DOMENEGHETTI,³ AND
VITTORIO TAZZOLI¹**

¹Dipartimento di Scienze della Terra, Università di Pavia, via Ferrata 1, 27100 Pavia, Italy

²Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.

³Centro di studio per la Cristallografia e la Cristallochimica, via Ferrata 1, 27100 Pavia, Italy

ABSTRACT

Single-crystal and powder X-ray diffraction data were collected to characterize the macroscopic solid-solution and cation-ordering behavior in the system augite-jadeite (low acmite content). We examined 28 natural pyroxenes with compositions on the join augite-jadeite and with different degrees of order. Annealing experiments were carried out to obtain crystals with different degrees of order ($P2/n$) and complete disorder ($C2/c$) at compositions between 35 and 60% Jd. Three synthetic $C2/c$ pyroxenes with composition $\text{Di}_{80}\text{Jd}_{20}$, $\text{Di}_{60}\text{Jd}_{40}$, and $\text{Di}_{50}\text{Jd}_{50}$ were also examined.

The long-range order parameters Q_{M1} and Q_{M2} of the M1 and M2 sites were obtained by a minimization procedure combining single-crystal X-ray diffraction data and chemical analyses. For both $C2/c$ and $P2/n$ pyroxenes, the a , b , c lattice parameters and unit-cell volume, as well as tetrahedral and octahedral mean bond distances depend linearly on composition. Only the angle β of ordered omphacites slightly deviates from the linear trend of the $C2/c$ samples. The out-of-plane tilting of the basal face of tetrahedra is sensitive to the different degrees of order.