

## Structure of synthetic $\text{Li}_2(\text{Mg,Cu})\text{Cu}_2[\text{Si}_2\text{O}_6]_2$ : A unique chain silicate related to pyroxene

HIROYUKI HORIUCHI,<sup>1</sup> AKIHIRO SAITO,<sup>1</sup> TOSHINAGA TACHI,<sup>2</sup> AND HIROSHI NAGASAWA<sup>2</sup>

<sup>1</sup>Mineralogical Institute, Faculty of Science, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

<sup>2</sup>Department of Chemistry, Faculty of Science, Gakushuin University, 1-5-1 Mejiro, Toshima-ku, Tokyo 171, Japan

### ABSTRACT

A unique Cu-bearing chain silicate,  $\text{Li}_2(\text{Mg,Cu})\text{Cu}_2[\text{Si}_2\text{O}_6]_2$ , was synthesized, and the structure was determined by single-crystal X-ray diffraction techniques. The structure was found to be triclinic, space group  $P\bar{1}$ , with unit-cell parameters  $a = 5.7068(7)$ ,  $b = 7.4784(9)$ ,  $c = 5.2193(3)$  Å,  $\alpha = 99.911(8)$ ,  $\beta = 97.436(8)$ ,  $\gamma = 84.52(1)^\circ$ , and  $Z = 1$ . The arrangement of zweier single chains,  $[\text{Si}_2\text{O}_6]$ , differs significantly from chain arrangements in the pyroxene and pyroxenoid structures, and the “I-beam” description of the pyroxene structure is not applicable. The structure may be classified as a new derivative type of the pyroxene structure, with an “oblique I-beam”. Cu atoms are coordinated by four O atoms in a square-planar arrangement with 1.94–2.00 Å for Cu–O and two O atoms with longer Cu–O distances of 2.41–2.92 Å, consistent with the crystal-field stabilization of the  $d^9$  electronic structure of  $\text{Cu}^{2+}$ . The square-planar  $\text{CuO}_4$  units form a  $[\text{Cu}_n\text{O}_{2n+2}]$  ribbon with  $n = 3$  in the structure, which is also found in Cu-bearing chain silicates such as shattuckite and planchéite with  $n > 3$ . Mg is octahedrally coordinated by O atoms, but the configuration is affected by the partial replacement by Cu.