

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

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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 Cu^{2+} . The square-planar 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.