MS15-2-1 $Cu_{0.9}Pb_{1.2}Sb_{2.9}Se_6$, an incommensurably modulated $^{4'4}$L-lillianite
#MS15-2-1

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Abstract
Lillianites are a structural family derived from the crystal structure of the mineral lillianite $Pb_3Bi_2S_6$ and belong to the sulfosalts.[1,2] The structures are built up by tilted and distorted NaCl type slabs that are interconnected by cations in bicapped trigonal prisms formed by anions (see Fig. 1). The numbers N1 and N2 in the symbol ^{N1,N2}L denote the number of edge-sharing octahedra across the NaCl type slabs.[3]
^{4,4}L-type $Cu_{0.9}Pb_{1.2}Sb_{2.9}Se_6$ can be described as an incommensurably modulated structure with the (3+1)-dimensional superspace group $Cmc2_1(\alpha 00)000$ with unit-cell dimensions a = 4.155(6) Å, b = 14.081(5) Å, and c = 19.842(11) Å, and a modulation vector of 0.68379(16) a^*.
The crystal structure features combined positional and occupational modulation on two sites where octahedral vacancies are either occupied by Sb atoms or Cu atoms that are displaced towards an edge of the octahedra, thus adopting a distorted tetrahedral coordination (see Fig. 2). The feature induces positional modulation of different extent of all other atoms in the structure.
In addition to the structure determination at ambient conditions, temperature induced structural changes were investigated. While cooling to 120 K had no effect on the symmetry, the satellite reflections disappear above 250 °C as the copper atoms lose their long-range order.

References
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Fig. 1: Projection along [001].

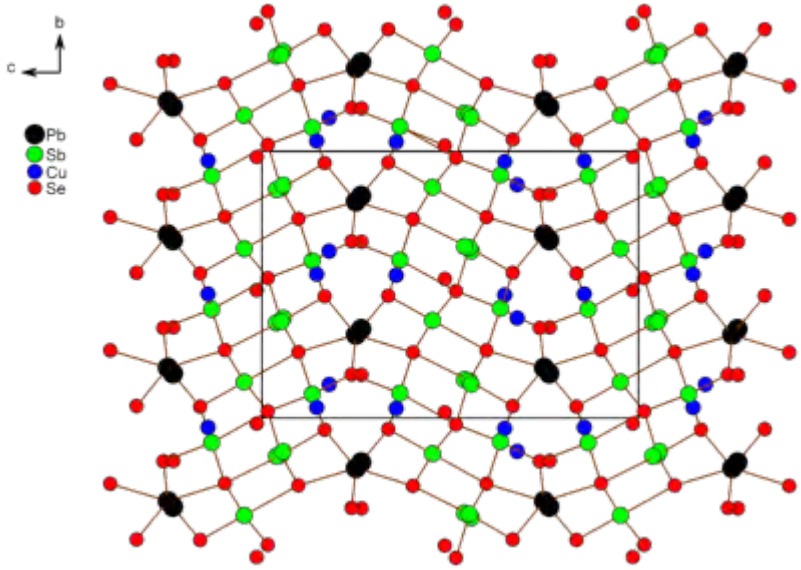

Fig. 2: Cutout of the modulated site.