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Incommensurate modulated crystal structure of a lillianite homologue 4L-(Pb)4(Cu,Sb)8(Pb,Sb)8Se24

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The synthetic 4 L-(Pb)₄(Cu,Sb)₈(Pb,Sb)₈Se₂₄ crystallizes in the superspace group $Cmc2_1(\alpha00)000$ with a = 4.165 Å, b = 14.085 Å, c = 19.82 Å and the modulation vector q = 0.6882(3) a^* . The mixed Pb/Sb sites are coordinated octahedrally by the Se atoms, almost every third Pb/Sb position is replaced by Cu that prefers a tetrahedral coordination of Se atoms. This phenomenon can be described by a combination of a positional and occupational modulation.

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