

$\text{Sr}_5\text{CuPb}_3\text{O}_{12}$	$hP34$	$(189) P-62m - k_i^2 g f^3 e c$
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$\text{Sr}_5\text{Pb}_3\text{CuO}_{12}$ [2]

Structural features: Three infinite chains of edge-linked PbO_6 octahedra are interconnected via common vertices with distorted CuO_4 tetrahedra (partial disorder).

Yamaura K. et al. (2001) [1]

$\text{CuO}_{12.62}\text{Pb}_3\text{Sr}_5$

$a = 1.01297$, $c = 0.35598$ nm, $c/a = 0.351$, $V = 0.3163$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$6k$	$m..$	0.2371	0.4432	$\frac{1}{2}$		single atom Pb
O2	$6i$	$..m$	0.1383	0	0.2529	0.109	
O3	$6i$	$..m$	0.9592	0	0.4238	0.109	
Pb4	$3g$	$m2m$	0.3407	0	$\frac{1}{2}$		octahedron O_6
O5	$3f$	$m2m$	0.1747	0	0	0.771	
O6	$3f$	$m2m$	0.4619	0	0		coplanar triangle Pb_2Sr
Sr7	$3f$	$m2m$	0.7019	0	0		monocapped trigonal prism O_7
Cu8	$2e$	$3.m$	0	0	0.164	0.5	
Sr9	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		tricapped trigonal prism O_9

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, neutrons, $T = 295$ K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Yamaura K., Huang Q., Takayama Muromachi E. (2001), Phys. Rev. B: Condens. Matter 64, 184428: 1-7. [2] Babu T.G.N., Greaves C. (1991), J. Solid State Chem. 95, 417-423.