

$\text{Na}_2(\text{Na}_{0.33}\text{Pb}_{0.67})_3[\text{SO}_4]_3\text{Cl}$	<i>hP42</i>	(176) $P6_3/m - ih^4fb$
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Na₃Pb₂(SO₄)₃Cl [1], caracolite, apatite family; Ca₂Pb₃(AsO₄)₃Cl [2], hedyphane

Structural features: Infinite columns of base-linked NaO₆O₃ tricapped trigonal prisms share atoms with SO₄ tetrahedra to form a 3D-framework; infinite columns of face-linked Cl(Pb,Na)₆ octahedra in channels parallel to [001].

Schneider W. (1967) [1]

ClNa₃O₁₂Pb₂S₃

$a = 0.981$, $c = 0.714$ nm, $c/a = 0.728$, $V = 0.5951$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.085	0.356	0.071		single atom S
S2	6 <i>h</i>	<i>m</i> ..	0.031	0.412	$\frac{1}{4}$		tetrahedron O ₄
O3	6 <i>h</i>	<i>m</i> ..	0.119	0.579	$\frac{1}{4}$		single atom S
M4	6 <i>h</i>	<i>m</i> ..	0.2553	0.2456	$\frac{1}{4}$		non-coplanar triangle O ₃
O5	6 <i>h</i>	<i>m</i> ..	0.495	0.12	$\frac{1}{4}$		single atom S
Na6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.009		tricapped trigonal prism O ₉
Cl7	2 <i>b</i>	-3..	0	0	0		icosahedron Pb ₆ O ₆

$M4 = 0.667\text{Pb} + 0.333\text{Na}$

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

Experimental: single crystal, precession photographs, X-rays, $R = 0.110$

Remarks: Natural specimen from Caracoles, Chile, and synthetic crystals gave identical results. Contrary to earlier reports based on optical measurements, no deviation from hexagonal symmetry was detected for any of the crystals investigated in [1]. A fully ordered structure is reported for Ca₂Pb₃(AsO₄)₃Cl [2].

References: [1] Schneider W. (1967), Neues Jahrb. Mineral., Monatsh. 1967, 284-289. [2] Rouse R.C., Dunn P.J., Peacor A.R. (1984), Am. Mineral. 69, 920-927.