

$\text{Pb}_5[\text{SiO}_4]_{1.5}[\text{SO}_4]_{1.5}\text{Cl}_{0.57}[\text{OH}]_{0.43}$	<i>hP48</i>	(176) $P6_3/m - i^2h^3fb$
--	-------------	---------------------------

Pb₅Si_{1.5}S_{1.5}O₁₂(OH)_{0.43}Cl_{0.57} [1], mattheddleite, apatite family

Structural features: Infinite columns of base-linked PbO₆O₃ tricapped trigonal prisms share atoms with (Si,S)O₄ tetrahedra to form a 3D-framework; infinite columns of face-linked (Cl,OH)Pb₆ octahedra parallel to [001] (split Pb site).

Steele I.M. et al. (2000) [1]

Cl_{0.57}H_{0.43}O_{12.43}Pb₅S_{1.50}Si_{1.50}

$a = 1.00056$, $c = 0.7496$ nm, $c/a = 0.749$, $V = 0.6499$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Pb1	12i	1	0.2507	0.2511	0.2136	0.5	
O2	12i	1	0.357	0.082	0.082		single atom S
O3	6h	<i>m</i> ..	0.155	0.487	¹ / ₄		single atom S
M4	6h	<i>m</i> ..	0.4058	0.0244	¹ / ₄		tetrahedron O ₄
O5	6h	<i>m</i> ..	0.589	0.109	¹ / ₄		single atom S
Pb6	4f	3..	¹ / ₃	² / ₃	0.0057		tricapped trigonal prism O ₉
M7	2b	-3..	0	0	0		octahedron Pb ₆

M4 = 0.5S + 0.5Si; M7 = 0.57Cl + 0.43OH

Transformation from published data: *y,x,-z*

Experimental: single crystal, diffractometer, X-rays, wR = 0.017

Remarks: Natural specimen from Leadhills, Scotland. 84.7 wt.% PbO, 8.11 wt.% SiO₂, 5.24 wt.% SO₃, and 1.05 wt.% Cl found by electron microprobe analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Steele I.M., Pluth J.J., Livingstone A. (2000), Mineral. Mag. 64, 915-921.