

$\text{Hg}_3\text{AsS}_4\text{Cl}$ $hP18$ $(186) P6_3mc - c^2b^2a$ **Hg₃AsS₄Cl** [1]

Structural features: AsS_3 ψ -tetrahedra and approximately planar HgS_3 trigonal units share vertices to form infinite slabs; single Cl between the slabs.

Beck J. et al. (2000) [1]

 $\text{AsClHg}_3\text{S}_4$ $a = 0.7431$, $c = 0.9003$ nm, $c/a = 1.212$, $V = 0.4305$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	6c	.m.	0.1486	0.8514	0.1368		non-coplanar triangle AsHg ₂
Hg2	6c	.m.	0.5041	0.49589	0.0227		non-coplanar triangle S ₃
S3	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.384		non-coplanar triangle Hg ₃
Cl4	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.8033		trigonal prism Hg ₆
As5	2a	3m.	0	0	0.0		non-coplanar triangle S ₃

Transformation from published data: origin shift 0 0 0.7246

Experimental: single crystal, diffractometer, X-rays, R = 0.037, T = 293 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Beck J., Hedderich S., Köllisch K. (2000), Inorg. Chem. 39, 5847-5850.