

$\text{Mo}_{15}\text{In}_{3.7}\text{S}_{19}$ $hP84$ $(176) P6_3/m - i^4h^4f^2e$ **In_{3.7}Mo₁₅S₁₉** [1]

Structural features: Mo₆S₈ units (a Mo₆ octahedron surrounded by a S₈ cube) and Mo₉S₁₁ units (two fused Mo₆S₈ units) in an α -Nd type (d.h.c.p.) arrangement; In between the units (partial disorder). Mo₆ and Mo₉ clusters.

Salloum D. et al. (2004) [1]

 $\text{In}_{3.72}\text{Mo}_{15}\text{S}_{19}$ $a = 0.94293$, $c = 1.89529$ nm, $c/a = 2.010$, $V = 1.4594$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mo1	12i	1	0.17061	0.01447	0.05802		tricapped trigonal prism S ₅ Mo ₄
S2	12i	1	0.2842	0.31892	0.0511		4-vertex polyhedron Mo ₄
S3	12i	1	0.38451	0.01369	0.13839		4-vertex polyhedron Mo ₄
Mo4	12i	1	0.49706	0.31788	0.13228		tricapped trigonal prism S ₅ Mo ₄
In5	6h	$m..$	0.0456	0.20114	$\frac{1}{4}$	0.342	bicapped square antiprism S ₆ In ₃ Mo
In6	6h	$m..$	0.24211	0.5452	$\frac{1}{4}$	0.233	
S7	6h	$m..$	0.35466	0.31266	$\frac{1}{4}$		trigonal bipyramid Mo ₄ In
Mo8	6h	$m..$	0.50463	0.15885	$\frac{1}{4}$		icosahedron S ₄ Mo ₆ In ₂
In9	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.10772		
S10	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.53472		tetrahedron Mo ₃ In
S11	4e	3..	0	0	0.15742		trigonal prism Mo ₃ In ₃

Experimental: single crystal, diffractometer, X-rays, $R = 0.027$, $T = 293$ K

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

References: [1] Salloum D., Gougeon P., Roisnel T., Potel M. (2004), J. Alloys Compd. 383, 57-62.