

$\text{Mo}_{15}\text{In}_{0.7}\text{S}_{19}$ $hP74$ $(176) P6_3/m - i^4h^3fe$ **In_{0.7}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]

 $\text{In}_{0.71}\text{Mo}_{15}\text{S}_{19}$ $a = 0.92947$, $c = 1.89844$ nm, $c/a = 2.042$, $V = 1.4204$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12i	1	0.01358	0.38274	0.14078		4-vertex polyhedron Mo ₄
Mo2	12i	1	0.01565	0.17544	0.0609		tricapped trigonal prism S ₅ Mo ₄
Mo3	12i	1	0.31597	0.49199	0.12962		tricapped trigonal prism S ₅ Mo ₄
S4	12i	1	0.31773	0.28633	0.04883		4-vertex polyhedron Mo ₄
Mo5	6h	$m..$	0.15849	0.50506	$\frac{1}{4}$		pseudo Frank-Kasper S ₄ Mo ₆ In
In6	6h	$m..$	0.205	0.047	$\frac{1}{4}$	0.236	tricapped trigonal prism S ₆ MoIn ₂
S7	6h	$m..$	0.3081	0.3491	$\frac{1}{4}$		octahedron Mo ₄ In ₂
S8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.03193		non-coplanar triangle Mo ₃
S9	4e	3..	0	0	0.15863		trigonal prism Mo ₃ In ₃

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.051$, $T = 293$ KRemarks: Homogeneity range $\text{In}_x\text{Mo}_{15}\text{S}_{19}$, $0 < x < 3.7$.

References: [1] Salloum D., Gautier R., Gougeon P., Potel M. (2004), J. Solid State Chem. 177, 1672-1680.