

CsMo₁₅In_{2.2}S₁₉*hP*82(176) *P*6₃/*m* – i⁴h³f³e**CsIn_{2.2}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; Ca and In between the units (partial disorder). Mo₆ and Mo₉ clusters.

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

Cs_{1.06}In_{2.29}Mo₁₅S₁₉*a* = 0.95446, *c* = 1.88625 nm, *c/a* = 1.976, *V* = 1.4881 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mo1	12 <i>i</i>	1	0.16885	0.01367	0.05799		tricapped trigonal prism S ₅ Mo ₄
S2	12 <i>i</i>	1	0.28284	0.31397	0.05149		4-vertex polyhedron Mo ₄
S3	12 <i>i</i>	1	0.38528	0.02243	0.13728		4-vertex polyhedron Mo ₄
Mo4	12 <i>i</i>	1	0.50023	0.31962	0.13123		tricapped trigonal prism S ₅ Mo ₄
In5	6 <i>h</i>	<i>m</i> ..	0.05159	0.2138	¹ / ₄	0.449	tricapped trigonal prism S ₆ MoIn ₂
S6	6 <i>h</i>	<i>m</i> ..	0.35974	0.3165	¹ / ₄		trigonal bipyramid Mo ₄ In
Mo7	6 <i>h</i>	<i>m</i> ..	0.50459	0.16219	¹ / ₄		pseudo Frank-Kasper S ₄ Mo ₆ In
In8	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.11241	0.471	
Cs9	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.15112	0.529	
S10	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.53267		tetrahedron Mo ₃ In
S11	4 <i>e</i>	3..	0	0	0.15823		trigonal prism Mo ₃ In ₃

Experimental: single crystal, diffractometer, X-rays, *R* = 0.031, *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.