$Mo_{15}In_3Se_{19}$	*hP*78	(176) $P6_3/m$ – $i^4h^3f^2e$

$In_3Mo_{15}Se_{19}$ [1]
Structural features: Mo_6Se_8 units (a Mo_6 octahedron surrounded by a Se_8 cube) and Mo_9Se_{11} units (two fused Mo_6Se_8 units) in an α-Nd type (d.h.c.p.) arrangement; In (partial disorder) between the units. Mo_6 and Mo_9 clusters.

Grüttner A. et al. (1979) [1]
$In_{2.87}Mo_{15}Se_{19}$
a = 0.9804, c = 1.949 nm, c/a = 1.988, V = 1.6224 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Mo1	12*i*	1	0.1647	0.0142	0.0571		tricapped trigonal prism Se_5Mo_4
Se2	12*i*	1	0.2858	0.3198	0.0509		4-vertex polyhedron Mo_4
Se3	12*i*	1	0.3794	0.0091	0.1393		pentagonal pyramid Mo_4In_2
Mo4	12*i*	1	0.5035	0.3185	0.1334		tricapped trigonal prism Se_5Mo_4
In5	6*h*	*m*..	0.0458	0.2127	$^1/_4$	0.29	tricapped trigonal prism Se_6MoIn_2
Se6	6*h*	*m*..	0.3543	0.3136	$^1/_4$		octahedron Mo_4In_2
Mo7	6*h*	*m*..	0.5127	0.1692	$^1/_4$		pseudo Frank-Kasper Se_4Mo_6In
In8	4*f*	3..	$^1/_3$	$^2/_3$	0.1288		monocapped trigonal prism Se_7
Se9	4*f*	3..	$^1/_3$	$^2/_3$	0.5297		non-coplanar triangle Mo_3
Se10	4*e*	3..	0	0	0.1617		trigonal prism Mo_3In_3

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.090

Remarks: Refinements on single crystals of different compositions $In_xMo_{15}Se_{19}$, $0 < x < 3$, are reported in [2] (atom coordinates not published).

References: [1] Grüttner A., Yvon K., Chevrel R., Potel M., Sergent M., Seeber B. (1979), Acta Crystallogr. B 35, 285-292. [2] Salloum D., Gautier R., Gougeon P., Potel M. (2004), J. Solid State Chem. 177, 1672-1680.