

$\text{Yb}_9\text{In}_{3.67}\text{S}_{18}$ $hP62$ $(176) P6_3/m - h^{10}c$ **$\text{Yb}_{18}\text{In}_{7.33}\text{S}_{36}$** [1]

Structural features: Double infinite chains of edge-linked $(\text{Yb},\text{In})\text{S}_6$ octahedra (partial vacancies ignored) and single columns of base-linked YbS_6S monocapped trigonal prisms share atoms to form a 3D-framework; additional In in channels parallel to $[001]$. Ordering variant of $\text{KTm}_{11.67}\text{S}_{18}$, $\text{In}[\text{Yb}_3(\text{Yb},\text{In})_{8.67}]\text{S}_{18}$.

Lemoine P. et al. (1989) [1]

 $\text{In}_{3.66}\text{S}_{18}\text{Yb}_9$ $a = 2.0688$, $c = 0.3861$ nm, $c/a = 0.187$, $V = 1.4311$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Yb1	$6h$	$m..$	0.0165	0.3453	$\frac{1}{4}$		monocapped trigonal prism S_7
S2	$6h$	$m..$	0.0234	0.5812	$\frac{1}{4}$		square pyramid Yb_5
S3	$6h$	$m..$	0.0322	0.169	$\frac{1}{4}$		non-coplanar triangle Yb_3
S4	$6h$	$m..$	0.1514	0.5071	$\frac{1}{4}$		non-coplanar triangle Yb_3
M5	$6h$	$m..$	0.2259	0.4351	$\frac{1}{4}$		octahedron S_6
M6	$6h$	$m..$	0.2336	0.1078	$\frac{1}{4}$	0.889	octahedron S_6
S7	$6h$	$m..$	0.2361	0.3137	$\frac{1}{4}$		square pyramid Yb_5
S8	$6h$	$m..$	0.3546	0.2356	$\frac{1}{4}$		square pyramid Yb_5
S9	$6h$	$m..$	0.5169	0.2052	$\frac{1}{4}$		non-coplanar triangle Yb_3
M10	$6h$	$m..$	0.5485	0.099	$\frac{1}{4}$		octahedron S_6
In11	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism S_9

 $\text{M5} = 0.667\text{Yb} + 0.333\text{In}$; $\text{M6} = 0.75\text{Yb} + 0.25\text{In}$; $\text{M10} = 0.667\text{Yb} + 0.333\text{In}$ Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.053$, $T = 293$ K

References: [1] Lemoine P., Tomas A., Carré D., Guittard M., Likforman A. (1989), Acta Crystallogr. C 45, 1858-1861.