Ta_3SeI_7	*hP*22	(186) $P6_3mc$ – c^3ba

Ta_3SeI_7 [1]
Structural features: Ta_3SeI_7 units consisting of three edge-sharing $Ta(SeI_5)$ octahedra (a Ta_3 triangular cluster capped by a Se atom common to the three octahedra) share edges to form infinite slabs. See Fig. IV.25.

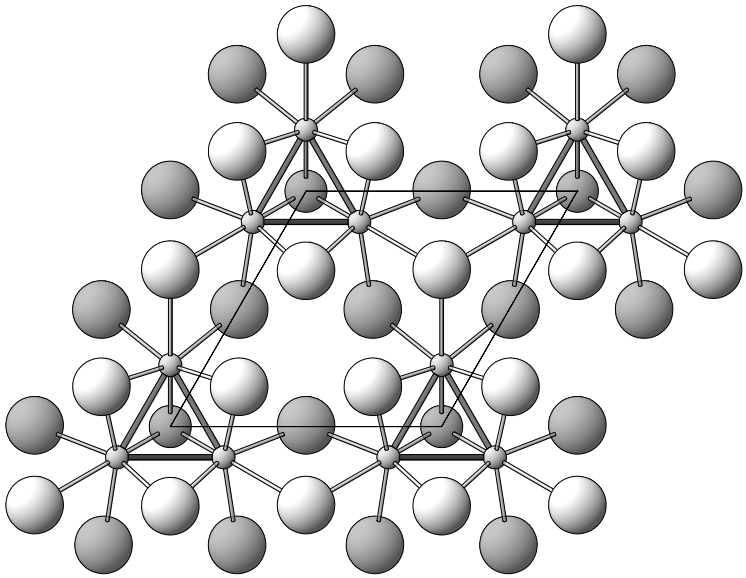

Fig. IV.25. **Ta_3SeI_7**

Arrangement of Ta_3SeI_7 units (Ta atoms small, Se atoms medium, I atoms large) in one slab viewed along [001].

Smith M.D., Miller G.J. (1996) [1]
I_7SeTa_3
$a = 0.7541$, $c = 1.359$ nm, $c/a = 1.802$, $V = 0.6693$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Ta1	6*c*	.*m*.	0.1307	0.8693	0.1382		8-vertex polyhedron SeI_5Ta_2
I2	6*c*	.*m*.	0.5027	0.4973	0.0246		non-colinear Ta_2
I3	6*c*	.*m*.	0.8309	0.1691	0.2738		non-colinear Ta_2
I4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2439		non-coplanar triangle Ta_3
Se5	2*a*	3*m*.	0	0	0.0		non-coplanar triangle Ta_3

Transformation from published data: *-x*,*-y*,*-z*; origin shift 0 0 0.6118
Experimental: single crystal, diffractometer, X-rays, wR = 0.046, T = 296 K

References: [1] Smith M.D., Miller G.J. (1996), J. Am. Chem. Soc. 118, 12238-12239.