

Th ₇ S ₁₂	<i>hP20</i>	(176) <i>P6₃/m – h³a</i>
---------------------------------	-------------	--

Th₇S₁₂ [1], Strukturbericht notation D8_k; Th₇Se₁₂ [3]; Pd₁₂(Ga,As)₇ [2]
 Structural features: Infinite columns of base-linked ThS₆S₂ bicapped trigonal prisms (ThS₈ square antiprisms) share atoms to form a 3D-framework with WC-type columns (3 prisms in the triangular cross-section); additional Th in channels of hexagonal cross-section parallel to [001] (partial disorder). See Fig. IV.54.

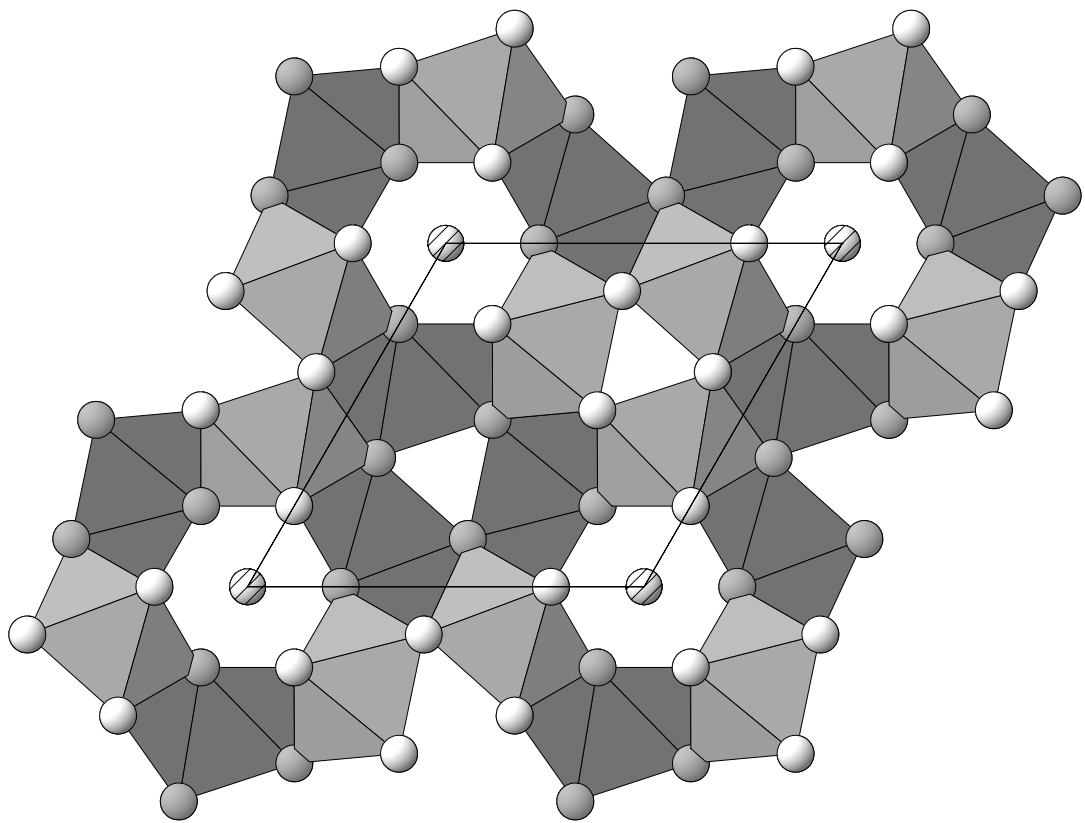


Fig. IV.54. **Th₇S₁₂**

Arrangement of ThS₈ square antiprisms and additional Th atoms (partly occupied site) viewed along [001]. Light and dark antiprisms are shifted by *c*/2.

Zachariasen W.H. (1949) [1]
 S₁₂Th₇
a = 1.1063, *c* = 0.3991 nm, *c/a* = 0.361, *V* = 0.4230 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	6 <i>h</i>	<i>m</i> ..	0.139	0.514	1/4		square pyramid Th ₅
S2	6 <i>h</i>	<i>m</i> ..	0.235	0.235	1/4		tetrahedron Th ₄
Th3	6 <i>h</i>	<i>m</i> ..	0.436	0.153	1/4		square antiprism S ₈
Th4	2 <i>a</i>	-6..	0	0	1/4	0.5	

Transformation from published data: origin shift 0 0 1/2
 Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Zachariasen W.H. (1949), Acta Crystallogr. 2, 288-291. [2] Députier S., Pivan J.Y., Guérin R. (1991), J. Less-Common Met. 171, 357-368. [3] D'Eye R.W.M. (1953), J. Chem. Soc. 1953, 1670-1672.