

$\text{Ti}_{0.6}\text{S}$	$hP24$	$(186) P6_3mc - b^8a^4$
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TiS_{1.67} 12H [1]

Structural features: Close-packed S layers in h_2chc_2 stacking; Ti occupies all octahedral voids in every second interlayer and part of the octahedral sites in all others.

Tronc E., Huber M. (1973) [1]

STi_{0.60}

$a = 0.343$, $c = 3.438$ nm, $c/a = 10.023$, $V = 0.3503$ nm³, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.04167		octahedron Ti ₆
Ti2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.16667	0.20	octahedron S ₆
Ti3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.25		octahedron S ₆
Ti4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.33333	0.20	octahedron S ₆
S5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.45833		trigonal prism Ti ₆
Ti6	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.58333		octahedron S ₆
S7	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.70833		trigonal prism Ti ₆
S8	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.875		octahedron Ti ₆
Ti9	$2a$	$3m.$	0	0	0.0	0.20	octahedron S ₆
S10	$2a$	$3m.$	0	0	0.125		octahedron Ti ₆
S11	$2a$	$3m.$	0	0	0.29167		trigonal prism Ti ₆
Ti12	$2a$	$3m.$	0	0	0.41667		octahedron S ₆

Transformation from published data: origin shift 0 0 0.58333

Experimental: single crystal, oscillation and Weissenberg photographs, X-rays, $R = 0.110$

Remarks: Zhdanov notation $(123)_2$; idealized coordinates. In [1] the x -coordinate of the Ti positions with $z_6 = 6z$, $10z$ is misprinted as $\frac{1}{3}$ instead of $\frac{2}{3}$.

References: [1] Tronc E., Huber M. (1973), J. Phys. Chem. Solids 34, 2045-2058.