

$\text{Ti}_{0.62}\text{S}$	$hP8$	$(186) P6_3mc - b^3a$
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$\text{Ti}_{2+x}\text{S}_4$ [2]

Structural features: Close-packed S layers in hc stacking; Ti in octahedral voids. Ignoring vacancies, units of two face-linked TiS_6 octahedra share edges to form a 3D-framework.

Norrby L.J., Franzen H.F. (1970) [1]

$\text{STi}_{0.61}$

$a = 0.34198$, $c = 1.1444$ nm, $c/a = 3.346$, $V = 0.1159$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.12539		octahedron S_6
Ti2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.3909	0.227	octahedron S_6
S3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.7525		trigonal prism Ti_6
S4	$2a$	$3m.$	0	0	0.0		octahedron Ti_6

Transformation from published data: origin shift 0 0 0.62461

Experimental: single crystal, diffractometer, X-rays, $R = 0.026$

References: [1] Norrby L.J., Franzen H.F. (1970), J. Solid State Chem. 2, 36-41. [2] Wadsley A.D. (1957), Acta Crystallogr. 10, 715-716.