

NaTi₂P₃S₁₂

hP188

(184) *P6cc* – d¹⁵ba²**NaTi₂(PS₄)₃** [1]

Structural features: PS₄ tetrahedra and TiS₆ octahedra share edges to form a 3D-framework; part of Na in large channels parallel to [001] (partial disorder).

Cieren X. et al. (1996) [1]

NaP₃S₁₂Ti₂*a* = 1.9906, *c* = 1.1552 nm, *c/a* = 0.580, *V* = 3.9642 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Na1	12 <i>d</i>	1	0.019	0.083	0.041	0.1	
Na2	12 <i>d</i>	1	0.021	0.508	0.252	0.13	
S3	12 <i>d</i>	1	0.0336	0.2459	0.3175		non-colinear PTi
Ti4	12 <i>d</i>	1	0.0453	0.346	0.4476		octahedron S ₆
Na5	12 <i>d</i>	1	0.06	0.51	0.213	0.25	
S6	12 <i>d</i>	1	0.0659	0.36	0.0783		non-colinear PTi
Na7	12 <i>d</i>	1	0.088	0.038	0.143	0.09	
S8	12 <i>d</i>	1	0.1727	0.4167	0.3672		non-colinear PTi
P9	12 <i>d</i>	1	0.1835	0.5131	0.4472		tetrahedron S ₄
S10	12 <i>d</i>	1	0.2201	0.6016	0.3333		non-colinear PTi
P11	12 <i>d</i>	1	0.3018	0.0112	0.2008		tetrahedron S ₄
S12	12 <i>d</i>	1	0.3112	0.1004	0.1071		non-colinear PTi
S13	12 <i>d</i>	1	0.3949	0.0423	0.3056		single atom P
S14	12 <i>d</i>	1	0.4775	0.0752	0.0072		single atom P
S15	12 <i>d</i>	1	0.5534	0.2634	0.0773		non-colinear PTi
Ti16	4 <i>b</i>	3..	1/3	2/3	0.457		octahedron S ₆
Na17	2 <i>a</i>	6..	0	0	0.0	0.35	
Na18	2 <i>a</i>	6..	0	0	0.047	0.23	

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.543

Experimental: single crystal, diffractometer, X-rays, wR = 0.051

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

References: [1] Cieren X., Angenault J., Couturier J.C., Jaulmes S., Quarton M., Robert F. (1996), J. Solid State Chem. 121, 230-235.