

TaS ₂ [NH ₃]	<i>hP</i> 8	(186) <i>P</i> 6 ₃ <i>mc</i> – b ² a ²
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TaS₂·NH₃ [1]

Structural features: Directly superposed close-packed S layers; Ta and NH₃ in trigonal prismatic voids (stacking sequence AbA β AcA γ). TaS₆ trigonal prisms share edges to form infinite slabs; NH₃ in trigonal prismatic voids between the slabs.

Chianelli R.R. et al. (1975) [1]

H₃NS₂Ta

a = 0.332, *c* = 1.816 nm, *c/a* = 5.470, *V* = 0.1733 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ta1	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.087		trigonal prism S ₆
(NH ₃)2	2 <i>b</i>	3 <i>m.</i>	¹ / ₃	² / ₃	0.337		anticuboctahedron (NH ₃) ₆ S ₆
S3	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		non-coplanar triangle Ta ₃
S4	2 <i>a</i>	3 <i>m.</i>	0	0	0.174		non-coplanar triangle Ta ₃

Transformation from published data (*P*6₃*mc* *): origin shift ¹/₃ ²/₃ 0.663

Experimental: powder, diffractometer, X-rays, R_B = 0.208

Remarks: In [1] the origin of the cell is shifted by ¹/₃ ²/₃ 0 from the description in the International Tables for Crystallography. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In fig. 4 of [1] the Hermann-Mauguin symbol for the space group is misprinted as *P*6₃/*mmc* instead of *P*6₃*mc*.

References: [1] Chianelli R.R., Scanlon J.C., Whittingham M.S., Gamble F.R. (1975), *Inorg. Chem.* 14, 1691-1696.