

$\text{Tb}_3\text{Ni}_3\text{Al}_3\text{H}_{1.63}$	$hP11$	(189) $P\text{-}62m - \text{gfdca}$
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TbNiAlH_{0.54} [1]

Structural features: Filled-up derivative of ZrNiAl with H in trigonal bipyramidal (Tb_3Ni_2) voids.

Brinks H.W. et al. (2002) [1]

$\text{Al}_3\text{D}_{1.63}\text{Ni}_3\text{Tb}_3$

$a = 0.70931$, $c = 0.39174$ nm, $c/a = 0.552$, $V = 0.1707$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	$3g$	$m2m$	0.2372	0	$\frac{1}{2}$		octahedron Ni_4Al_2
Tb2	$3f$	$m2m$	0.5878	0	0		non-colinear D_2
Ni3	$2d$	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		colinear D_2
D4	$2c$	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0	0.815	trigonal bipyramid Ni_2Tb_3
Ni5	$1a$	$-62m$	0	0	0		tricapped trigonal prism Al_6Tb_3

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$

Experimental: powder, diffractometer, neutrons, $R_p = 0.040$, $T = 293$ K

References: [1] Brinks H.W., Yartys V.A., Hauback B.C., Fjellvag H. (2002), J. Alloys Compd. 330/332, 169-174.