

$\text{I}_5\text{N}[\text{NH}_3]$ $hP14$ $(186) P6_3mc - cb^3a$ **$\text{I}[\text{NI}_4]\cdot\text{NH}_3$ [1]**

Structural features: NI_4 tetrahedra in a Mg-type (h.c.p.) arrangement are loosely interconnected via additional I to form infinite slabs; NH_3 coordinated to the free I vertices.

Plewa M., Tebbe K.F. (1981) [1]

 $\text{H}_3\text{I}_5\text{N}_2$ $a = 0.8425$, $c = 0.8765$ nm, $c/a = 1.040$, $V = 0.5388$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	6c	.m.	0.19254	0.80746	0.3536		single atom N
I2	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0119		colinear N(NH_3)
N3	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2666		tetrahedron I ₄
(NH_3)4	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7436		single atom I
I5	2a	3m.	0	0	0.0		non-coplanar triangle I ₃

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.1464

Experimental: single crystal, diffractometer, X-rays, $R = 0.047$

Remarks: The authors state that the NH_3 molecules are displaced from the ideal position; refinement considering splitting of site (NH_3)4 into Wyckoff position 6c gave the same R factor. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Plewa M., Tebbe K.F. (1981), Z. Anorg. Allg. Chem. 477, 7-20.