

I₅N[NH₃]*hP*18(186) *P6₃mc* – *c*²*b*²*a***I[NL₄]·NH₃ [1]**

Structural features: NI₄ tetrahedra in a Mg-type (h.c.p.) arrangement are loosely interconnected via additional I to form infinite slabs; NH₃ (split site) coordinated to the free I vertices.

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

H₃I₅N₂*a* = 0.8425, *c* = 0.8765 nm, *c/a* = 1.04, *V* = 0.5388 nm³, *Z* = 2

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|---------------------|------------|--------------|-----------------------------|-----------------------------|----------|-------|--------------------------------------|
| I1 | 6 <i>c</i> | . <i>m</i> . | 0.19254 | 0.80746 | 0.3536 | | single atom N |
| (NH ₃)2 | 6 <i>c</i> | . <i>m</i> . | 0.64 | 0.36 | 0.2476 | 0.333 | |
| I3 | 2 <i>b</i> | 3 <i>m</i> . | ¹ / ₃ | ² / ₃ | 0.0119 | | |
| N4 | 2 <i>b</i> | 3 <i>m</i> . | ¹ / ₃ | ² / ₃ | 0.2666 | | tetrahedron I ₄ |
| I5 | 2 <i>a</i> | 3 <i>m</i> . | 0 | 0 | 0.0 | | non-coplanar triangle I ₃ |

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.1464Experimental: single crystal, diffractometer, X-rays, *R* = 0.047

Remarks: Refinement with site (NH₃)2 in Wyckoff position 2*b* gave the same *R* factor. Short interatomic distances for partly occupied site(s). 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.