

Fe₃N ϵ [2], siderazot; Fe₃C ϵ [4]; Ni₃N [3]; ReO₃ hp [5]

Structural features: Close-packed Fe layers in h stacking; N in octahedral voids. NFe₆ octahedra share vertices to form a 3D-framework. See Fig. IV.35.

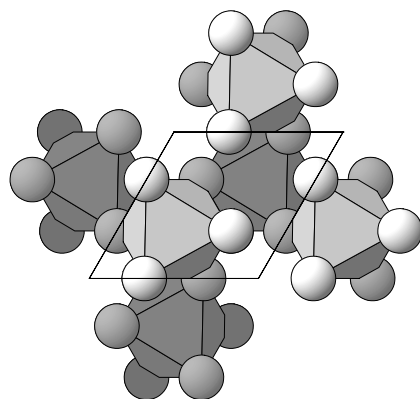


Fig. IV.35. **Fe₃N** ϵ

Arrangement of NFe₆ octahedra viewed along [001]. Light and dark octahedra are shifted by $c/2$.

Jacobs H. et al. (1995) [1]

Fe₃N

$a = 0.46982$, $c = 0.43789$ nm, $c/a = 0.932$, $V = 0.0837$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	6g	.2.	0.3249	0	0		non-colinear N ₂
N2	2c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron Fe ₆

Experimental: powder, diffractometer, neutrons, $R_B = 0.041$, $T = 295$ K

Remarks: Partial disorder of N was found in [7] (refinement on the same diffraction data). The description in space group (149) *P*312 in [6] does not take into consideration all symmetry elements of the proposed structure (stated by the author).

References: [1] Jacobs H., Rechenbach D., Zachwieja U. (1995), J. Alloys Compd. 227, 10-17. [2] Hendricks S.B., Kosting P.R. (1930), Z. Kristallogr. 74, 511-533. [3] Juza R., Sachsze W. (1943), Z. Anorg. Allg. Chem. 251, 201-212. [4] Nagakura S. (1959), J. Phys. Soc. Jpn. 14, 186-195. [5] Dyuzheva T.I., Bendeliani N.A., Kabalkina S.S. (1987), J. Less-Common Met. 133, 313-317. [6] Jack K.H. (1952), Acta Crystallogr. 5, 404-411. [7] Leineweber A., Jacobs H., Hüning F., Lueken H., Schilder H., Kockelmann W. (1999), J. Alloys Compd. 288, 79-87.