Ba_3FeN_3	*hP*14	(176) $P6_3/m - h^2c$

Ba_3FeN_3 [1]
Structural features: Single FeN_3 trigonal units in Ba_6Ba_3 tricapped trigonal prisms, which share atoms to form a 3D-framework. Filled-up derivative of UCl_3 with N in octahedral (Ba_5Fe) voids.

Höln P. et al. (1991) [1]
Ba_3FeN_3
$a = 0.8014$, $c = 0.5608$ nm, $c/a = 0.700$, $V = 0.3119$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
N1	6*h*	*m*..	0.1294	0.4405	$^1/_4$		single atom Fe
Ba2	6*h*	*m*..	0.3583	0.2714	$^1/_4$		square pyramid N_5
Fe3	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		coplanar triangle N_3

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.041
References: [1] Höln P., Kniep R., Rabenau A. (1991), Z. Kristallogr. 196, 153-158.