$Ba_4Pr_7Si_{12}BN_3(N_{0.96}O_{0.04})_{24}$	*hP*51	(174) *P*-6 – $l^2k^5j^7dba$

$Ba_4Pr_7Si_{12}N_{23}O(BN_3)$ [1]
Structural features: $Si(N,O)_4$ tetrahedra share vertices to form a 3D-framework; BN_3 trigonal units (perpendicular to [001]) alternate with Pr atoms at the centers of 6-rings along [001], Ba and remaining Pr in channels parallel to [001].

Orth M. et al. (2001) [1]
$BBa_4N_{26.04}O_{0.96}Pr_7Si_{12}$
a = 1.2257, c = 0.54483 nm, c/a = 0.445, V = 0.7089 nm^3, Z = 1

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
M1	6*l*	1	0.2773	0.4067	0.2437		non-colinear Si_2
M2	6*l*	1	0.4029	0.1685	0.2419		non-colinear Si_2
M3	3*k*	*m*..	0.0434	0.282	$^1/_2$		non-colinear Si_2
Si4	3*k*	*m*..	0.1992	0.323	$^1/_2$		tetrahedron N_4
M5	3*k*	*m*..	0.2143	0.1849	$^1/_2$		non-colinear Si_2
Si6	3*k*	*m*..	0.3121	0.1188	$^1/_2$		tetrahedron N_4
Ba7	3*k*	*m*..	0.56991	0.08287	$^1/_2$		8-vertex polyhedron N_8
N8	3*j*	*m*..	0.0183	0.1281	0		single atom B
Pr9	3*j*	*m*..	0.03693	0.32628	0		tetrahedron N_4
M10	3*j*	*m*..	0.1887	0.5489	0		non-colinear Si_2
Pr11	3*j*	*m*..	0.25298	0.22269	0		trigonal prism N_6
Si12	3*j*	*m*..	0.3076	0.5075	0		tetrahedron N_4
Si13	3*j*	*m*..	0.5063	0.2337	0		tetrahedron N_4
M14	3*j*	*m*..	0.6086	0.1775	0		non-colinear Si_2
Ba15	1*d*	-6..	$^1/_3$	$^2/_3$	$^1/_2$		18-vertex polyhedron $N_{12}Si_6$
Pr16	1*b*	-6..	0	0	$^1/_2$		trigonal bipyramid N_3B_2
B17	1*a*	-6..	0	0	0		coplanar triangle N_3

M1 = 0.96N + 0.04O; M2 = 0.96N + 0.04O; M3 = 0.96N + 0.04O; M5 = 0.96N + 0.04O; M10 = 0.96N + 0.04O; M14 = 0.96N + 0.04O
Experimental: single crystal, diffractometer, X-rays, R = 0.013, T = 292 K

Remarks: We assigned an approximate value to the N/O ratio of sites M based on the nominal composition.

References: [1] Orth M., Hoffmann R.D., Pöttgen R., Schnick W. (2001), Chem. Eur. J. 7, 2791-2797.