

$\text{Li}_{10}\text{BrN}_3$	$hP14$	$(187) P\text{-}6m2 - k_j^3 f_a$
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$\text{Li}_{10}\text{N}_3\text{Br}$ [1]

Structural features: NLi_7 pentagonal bipyramids share vertices to form a 3D-framework; Br in trigonal prismatic voids.

Marx R. (1995) [1]

$\text{BrLi}_{10}\text{N}_3$

$a = 0.7413$, $c = 0.38657$ nm, $c/a = 0.521$, $V = 0.1840$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	$3k$	$mm2$	0.16767	0.83233	$\frac{1}{2}$		non-colinear N_2
N2	$3j$	$mm2$	0.15887	0.84113	0		pentagonal bipyramid Li_7
Li3	$3j$	$mm2$	0.44507	0.55493	0		non-colinear N_2
Li4	$3j$	$mm2$	0.83427	0.16573	0		non-coplanar triangle N_2Li
Br5	$1f$	$-6m2$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		trigonal prism Li_6
Li6	$1a$	$-6m2$	0	0	0		coplanar hexagon N_3Li_3

Transformation from published data: origin shift $\frac{1}{3} \frac{2}{3} 0$

Experimental: powder, diffractometer, neutrons, $R_B = 0.036$

Remarks: In table II of [1] the z -coordinate of former Li1 is misprinted as 0 instead of $\frac{1}{2}$ and the Wyckoff position of the same site as $3j$ instead of $3k$ (from the drawing in fig. 3).

References: [1] Marx R. (1995), Z. Naturforsch. B 50, 1061-1066.