

CsPr₉NbBr₁₅N₆*hP*64(176) *P*6₃/*m* – i⁴h²ca**CsPr₉NbBr₁₅N₆** [1]

Structural features: Pr₉NbN₆ clusters (a central Nb atom surrounded by a N₆ trigonal prism and a Pr₆Pr₃ tricapped trigonal prism) in a Mg-type (h.c.p.) arrangement.

Lulei M., Corbett J.D. (1995) [1]

Br₁₅CsN₆NbPr₉*a* = 1.207, *c* = 1.3801 nm, *c/a* = 1.143, *V* = 1.7412 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	12 <i>i</i>	1	0.1849	0.557	0.149		tetrahedron NbPr ₃
Br2	12 <i>i</i>	1	0.25327	0.01634	0.09351		non-coplanar triangle Pr ₃
Pr3	12 <i>i</i>	1	0.27868	0.45803	0.0656		non-colinear N ₂
Br4	12 <i>i</i>	1	0.61454	0.1341	0.09136		non-coplanar triangle Pr ₃
Pr5	6 <i>h</i>	<i>m</i> ..	0.02158	0.43659	¹ / ₄		non-colinear N ₂
Br6	6 <i>h</i>	<i>m</i> ..	0.26303	0.32082	¹ / ₄		non-colinear Pr ₂
Nb7	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		trigonal prism N ₆
Cs8	2 <i>a</i>	-6..	0	0	¹ / ₄		tricapped trigonal prism Br ₉

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.029, T = 296 K

References: [1] Lulei M., Corbett J.D. (1995), Angew. Chem. Int. Ed. Engl. 34, 2262-2264 (Angew. Chem. 107, 2463-2465).