

CsNb₆I₁₁*hP36*(182) *P6₃22 – i²gfb***CsNb₆I₁₁** [1]

Structural features: Nb₆I₁₄ units (a Nb₆ octahedron surrounded by an I₈ cube and an I₆ octahedron) share vertices of the I₆ octahedron to form a 3D-framework.

Imoto H., Corbett J.D. (1980) [1]

CsI₁₁Nb₆*a* = 1.1007, *c* = 1.1894 nm, *c/a* = 1.081, *V* = 1.2479 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	12 <i>i</i>	1	0.3704	0.022	0.342		non-coplanar triangle Nb ₃
Nb2	12 <i>i</i>	1	0.5157	0.1915	0.151		tricapped trigonal prism Nb ₄ I ₅
I3	6 <i>g</i>	.2.	0.2813	0	0		non-colinear Nb ₂
I4	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0477		non-coplanar triangle Nb ₃
Cs5	2 <i>b</i>	3.2	0	0	¹ / ₄		icosahedron I ₁₂

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.047, T = 293 K

References: [1] Imoto H., Corbett J.D. (1980), Inorg. Chem. 19, 1241-1245.