

Cs_{1.7}Yb₆F_{19.7}

hP56

(186) $P6_3mc - c^8b^2a^2$ **Cs_{3.4}Yb₁₂F_{39.4}** [1]

Structural features: Units of three edge-linked YbF₇ pentagonal bipyramids (in part converted into octahedra) share vertices to form a 3D-framework; Cs in channels parallel to [001].

Aleonard S. et al. (1985) [1]

Cs_{1.70}F_{19.70}Yb₆ $a = 0.8, c = 1.707 \text{ nm}, c/a = 2.134, V = 0.9461 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	6c	.m.	0.1645	0.8355	0.1277		non-coplanar triangle Yb ₂ F
F2	6c	.m.	0.1697	0.8303	0.3738		non-coplanar triangle Yb ₂ F
F3	6c	.m.	0.4824	0.5176	0.2536		non-colinear Yb ₂
Yb4	6c	.m.	0.4884	0.5116	0.1312		pentagonal bipyramid F ₇
Yb5	6c	.m.	0.4939	0.5061	0.3817		pentagonal bipyramid F ₇
F6	6c	.m.	0.4983	0.5017	0.0082		non-colinear Yb ₂
F7	6c	.m.	0.778	0.222	0.3743		non-colinear Yb ₂
F8	6c	.m.	0.7869	0.2131	0.1298		non-colinear Yb ₂
F9	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1044		non-coplanar triangle Yb ₃
F10	2b	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.4131	0.7	non-coplanar hexagon Yb ₃ F ₃
Cs11	2a	3m.	0	0	0.0	0.89	octahedron F ₆
Cs12	2a	3m.	0	0	0.2603	0.81	trigonal prism F ₆

Transformation from published data: origin shift 0 0 0.3711

Experimental: single crystal, diffractometer, neutrons, wR = 0.050

Remarks: Homogeneity range Cs_{4-x}Yb₁₂F_{40-x}, 0 < x < 1. We assigned an approximate value to the *a*-parameter (omitted in [1]). Two alternative models with compositions CsYb₄F₁₃ and CsYb₃F₁₀, respectively, were tested and rejected (R = 0.059 and 0.054, respectively).

References: [1] Aleonard S., Lambert B., Pannetier J., Gorius M.F., Roux M.T. (1985), J. Solid State Chem. 58, 226-232.