

CsB[CF₃]₃[OH]*hP*90(176) *P*6₃/*m* – i⁵h⁴fb**Cs[(CF₃)₃BOH] [1]**

Structural features: B(CF₃)₃OH tetrahedral units (a B(C₃[OH]) tetrahedron with three F bonded to each C).

Brauer D.J. et al. (1999) [1]

BC₃CsF₉HO*a* = 1.1365, *c* = 1.236 nm, *c/a* = 1.088, *V* = 1.3826 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>i</i>	1	0.0109	0.3568	0.0513		single atom C
F2	12 <i>i</i>	1	0.2183	0.3461	0.166		single atom C
F3	12 <i>i</i>	1	0.3207	0.1377	0.1291		single atom C
C4	12 <i>i</i>	1	0.3756	0.0606	0.142		tetrahedron F ₃ B
F5	12 <i>i</i>	1	0.5101	0.1469	0.1335		single atom C
B6	6 <i>h</i>	<i>m</i> ..	0.0312	0.3675	¹ / ₄		tetrahedron OC ₃
F7	6 <i>h</i>	<i>m</i> ..	0.0714	0.1701	¹ / ₄		single atom C
O8	6 <i>h</i>	<i>m</i> ..	0.1169	0.5137	¹ / ₄		single atom B
C9	6 <i>h</i>	<i>m</i> ..	0.1332	0.3062	¹ / ₄		tetrahedron F ₃ B
Cs10	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.06329		icosahedron F ₉ O ₃
Cs11	2 <i>b</i>	-3..	0	0	0		icosahedron F ₁₂
H12	6 <i>h</i>	<i>m</i> ..	0.073	0.5465	¹ / ₄		

Experimental: single crystal, diffractometer, X-rays, *R* = 0.037, *T* = 294 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Brauer D.J., Bürger H., Chebude Y., Pawelke G. (1999), Eur. J. Inorg. Chem. 1999, 247-253.