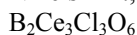


 $hP28$ $(176) P6_3/m - ih^2f$ **Ce₃(BO₃)₂Cl₃** [1]

Structural features: Ce(O₆Cl₄) polyhedra (an O₄ square on one side, an O₂Cl₃ pentagon capped by an additional Cl on the other side) share atoms to form a 3D-framework; B in trigonal (O₃) voids. Single BO₃ trigonal units.

Nikelski T., Schleid T. (2003) [1]

 $a = 0.92008$, $c = 0.58079$ nm, $c/a = 0.631$, $V = 0.4258$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.5359	0.1708	0.0018		single atom B
Cl2	6h	$m..$	0.0366	0.2396	$\frac{1}{4}$		tetrahedron Ce ₂ O ₂
Ce3	6h	$m..$	0.38622	0.33527	$\frac{1}{4}$		non-coplanar square O ₄
B4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0143		non-coplanar triangle O ₃

Transformation from published data: $y, x, -z$

Experimental: single crystal, diffractometer, X-rays, R = 0.018

References: [1] Nikelski T., Schleid T. (2003), Z. Anorg. Allg. Chem. 629, 2200-2205.