

Tb₂CBBrH_{0.83}*hP*12(186) *P*6₃*mc* – b⁴a²**Tb₂BrCH_{0.83}** [1]

Structural features: Infinite slabs of edge-linked CTb₆ octahedra and close-packed Br layers (partial stacking disorder) alternate along [001]; H in trigonal voids in Tb layers.

Ruck M., Simon A. (1992) [1]

BrCD_{0.40}Tb₂*a* = 0.37395, *c* = 1.4331 nm, *c/a* = 3.832, *V* = 0.1736 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Tb1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.155		non-coplanar triangle C ₃
D2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.342	0.395	tetrahedron Tb ₃ Br
Br3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.506	0.46	4-vertex polyhedron Br ₃ D
Tb4	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.834		non-coplanar triangle D ₃
Br5	2 <i>a</i>	3 <i>m.</i>	0	0	0.0	0.54	non-coplanar triangle Br ₃
C6	2 <i>a</i>	3 <i>m.</i>	0	0	0.225		non-coplanar triangle Tb ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.275Experimental: powder, diffractometer, neutrons, R_B = 0.160Remarks: Composition Tb₂BrCH_{0.83} from chemical analysis; part of H not located.

References: [1] Ruck M., Simon A. (1992), Z. Anorg. Allg. Chem. 617, 7-18.