

GdBrH<sub>0.69</sub>*hP*14(186)  $P6_3mc - b^5a^2$ **GdBrH<sub>0.69</sub>** [1]

Structural features: Close-packed Gd and Br layers in hc<sub>3</sub> stacking (-Br-Br-Gd-Gd-); H in octahedral and tetrahedral voids between Gd layers (partial disorder).

Mattausch H.J. et al. (1985) [1]

BrGdH<sub>0.69</sub>
 $a = 0.38707$ ,  $c = 1.9463$  nm,  $c/a = 5.028$ ,  $V = 0.2525$  nm<sup>3</sup>,  $Z = 4$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.02468	0.46	tetrahedron Gd <sub>4</sub>
Gd2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.14336		10-vertex polyhedron H <sub>7</sub> Br <sub>3</sub>
Br3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.40308		non-coplanar triangle Gd <sub>3</sub>
H4	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.57168	0.46	octahedron H <sub>6</sub>
Br5	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.74028		non-coplanar triangle Gd <sub>3</sub>
Gd6	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		10-vertex polyhedron H <sub>7</sub> Br <sub>3</sub>
H7	2 <i>a</i>	3 <i>m.</i>	0	0	0.11868	0.46	tetrahedron Gd <sub>4</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.67832

Experimental: single crystal, diffractometer, X-rays, R = 0.048

Remarks: Homogeneity range GdBrH<sub>x</sub>, 0.7 < x < 0.9. We assigned an approximate value to the occupancy of the H sites based on the nominal composition.

References: [1] Mattausch H.J., Schramm W., Eger R., Simon A. (1985), Z. Anorg. Allg. Chem. 530, 43-59.