

$\text{Cs}_3\text{B}_6\text{S}_4\text{BrH}_{12}$ *hP52*(186) $P6_3mc - dc^6ba$ **Cs₃(BH₂)₆S₄Br [1]**

Structural features: Adamantane-type S₄(BH₂)₆ units consisting of six B(S₂H₂) tetrahedra sharing S vertices (a central S₄B₆ cage with four 6-membered rings) in a Mg-type (h.c.p.) arrangement; infinite columns of face-linked BrCs₆ octahedra in channels parallel to [001].

Binder H. et al. (1991) [1]

 $\text{B}_6\text{BrCs}_3\text{H}_{12}\text{S}_4$ $a = 1.0473$, $c = 0.8716$ nm, $c/a = 0.832$, $V = 0.8279$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	12 <i>d</i>	1	0.1211	0.4104	0.0708		single atom B
S2	6 <i>c</i>	. <i>m</i> .	0.23106	0.76896	0.3422		non-coplanar triangle B ₃
B3	6 <i>c</i>	. <i>m</i> .	0.2349	0.765	0.1208		non-colinear H ₂
B4	6 <i>c</i>	. <i>m</i> .	0.4322	0.5678	0.4129		non-colinear H ₂
H5	6 <i>c</i>	. <i>m</i> .	0.5005	0.4995	0.3772		single atom B
H6	6 <i>c</i>	. <i>m</i> .	0.5751	0.4248	0.0372		single atom B
Cs7	6 <i>c</i>	. <i>m</i> .	0.84143	0.15857	0.2476		non-colinear H ₂
S8	2 <i>b</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0395		non-coplanar triangle B ₃
Br9	2 <i>a</i>	3. <i>m</i> .	0	0	0.0		octahedron Cs ₆

Transformation from published data: origin shift 0 0 0.0024

Experimental: single crystal, diffractometer, X-rays, $R = 0.025$, $T = 293$ K

References: [1] Binder H., Loos H., Dermentzis K., Borrmann H., Simon A. (1991), Chem. Ber. 124, 427-432.