CaB_6 ($D2_1$) Structure: A6B_cP7_221_e_b-001

This structure originally had the label `A6B_cP7_221_f_a`. Calls to that address will be redirected here.

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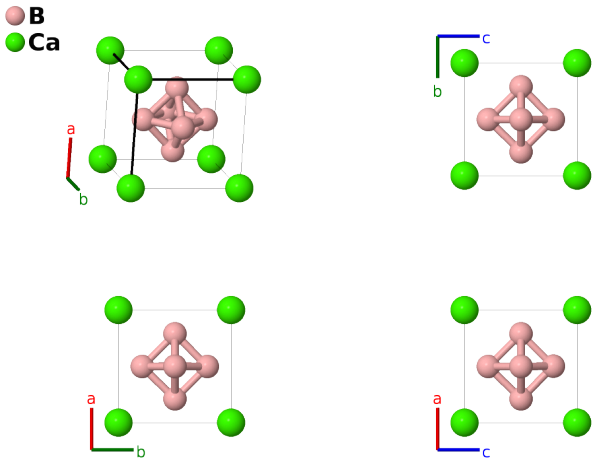
https://aflow.org/p/GKJM

https://aflow.org/p/A6B_cP7_221_e_b-001



Prototype	B_6Ca
AFLOW prototype label	A6B_cP7_221_e_b-001
***Strukturbericht* designation**	$D2_1$
ICSD	26753
Pearson symbol	cP7
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A6B_cP7_221_e_b-001 --params=`a, x_2

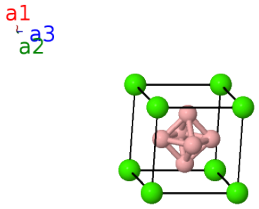
Other compounds with this structure

BaB_6, CeB_6, DyB_6, ErB_6, EuB_6, GdB_6, HoB_6, LaB_6, LuB_6, NaB_6, NdB_6, PrB_6, PuB_6, ScB_6, SiB_6, SmB_6, SrB_6, TbB_6, ThB_6, TmB_6, YB_6, YbB_6, (Ca, Sm)B_6, (Ce, La)B_6

- The internal parameter is chosen to match the intraoctalhedral boron-boron distance of 1.755Å found in (Yahia, 1990). The ICSD entry is from (Pauling, 1934).

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Ca I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}}$	(6e)	B I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1$	=	$-ax_2\,\hat{\mathbf{x}}$	(6e)	B I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{y}}$	(6e)	B I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{y}}$	(6e)	B I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{z}}$	(6e)	B I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{z}}$	(6e)	B I

References

[1] Z. Yahia, S. Turrell, G. Turrell, and J. P. Mercurio, *Infrared and Raman spectra of hexaborides: force-field calculations, and isotopic effects*, J. Mol. Struct. **224**, 303–312 (1990), doi:10.1016/0022-2860(90)87025-S.

[2] L. Pauling and S. Weinbaum, *The Structure of Calcium Boride, CaB_6*, Z. Krystallogr. **87**, 181–182 (1934), doi:10.1524/zkri.1934.87.1.181.