CrB ($B33$) Structure: AB_oC8_63_c_c-001

This structure originally had the label `AB_oC8_63_c_c`. Calls to that address will be redirected here.

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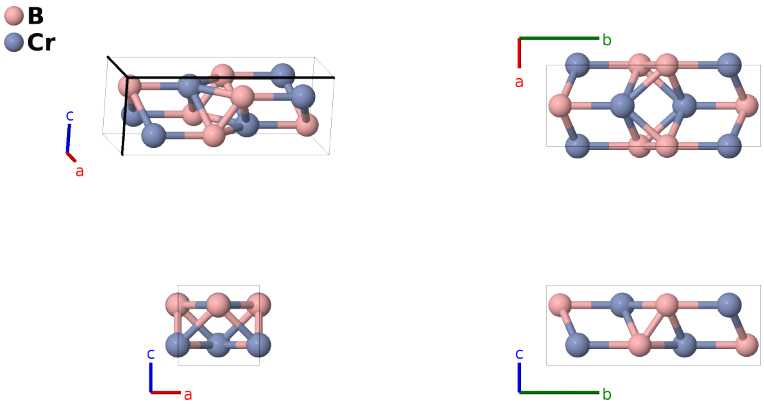
https://aflow.org/p/QWV1

https://aflow.org/p/AB_oC8_63_c_c-001



Prototype	BCr
AFLOW prototype label	AB_oC8_63_c_c-001
***Strukturbericht* designation**	$B33$
ICSD	44250
Pearson symbol	oC8
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=AB_oC8_63_c_c-001 --params=`$a, b/a, c/a, y_1, y_2$

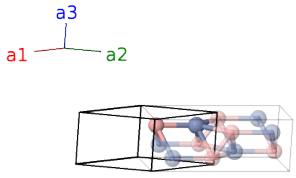
Other compounds with this structure

AgCa, AlHf, AlTh, AlY, AlZr, AuGd, BNb, BNi, BTa, BV, BaPb, CaGe, CaSi, CaSn, CeNi, CePt, CeRh, CoTh, DyGa, DyGe, ErNi, GaGd, GaPr, GdGe, GeHo, GeNi, GePr, HfNi, HfPt, HoNi, ITl, IrTh, LaNi, LaPt, LaRh, LuNi, NdNi, NdRh, NiPr, NiPu, NiSm, NiTb, NiTm, NiZr, PrRh, PtTh, PtZr, RhTh, RuTh, SiSr, SiY, (Ge, Si)Ho

- (Gottfried, 1938) originally gave the $B33$ *Strukturbericht* designation to thallium iodide, TiI. Later, (Smithells, 1955) gave CrB structure the new designation B_f. These structures are identical, and we follow (Parthé, 1993) in using $B33$ to designate both structures.
- Removing either the Cr or B atoms transforms this into the α-U (A20) structure.
- β-SnS and CrB ($B33$) have the same AFLOW label, AB_oC8_63_c_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Cr I

References

[1] S. Okada, T. Atoda, and I. Higashi, *Structural investigation of Cr_2B_3, Cr_3B_4, and CrB by single-crystal diffractometry*, J. Solid State Chem. **68**, 61–67 (1987), doi:10.1016/0022-4596(87)90285-4.

[2] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).

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[4] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

Found in

[1] P. Villars, *CrB Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.