Cr_5B_3 ($D8_l$) Structure: A3B5_tI32_140_ah_cl-001

This structure previously used the label(s) `A3B5_tI32_140_ah_cl`. Calls to these addresses will be redirected here.

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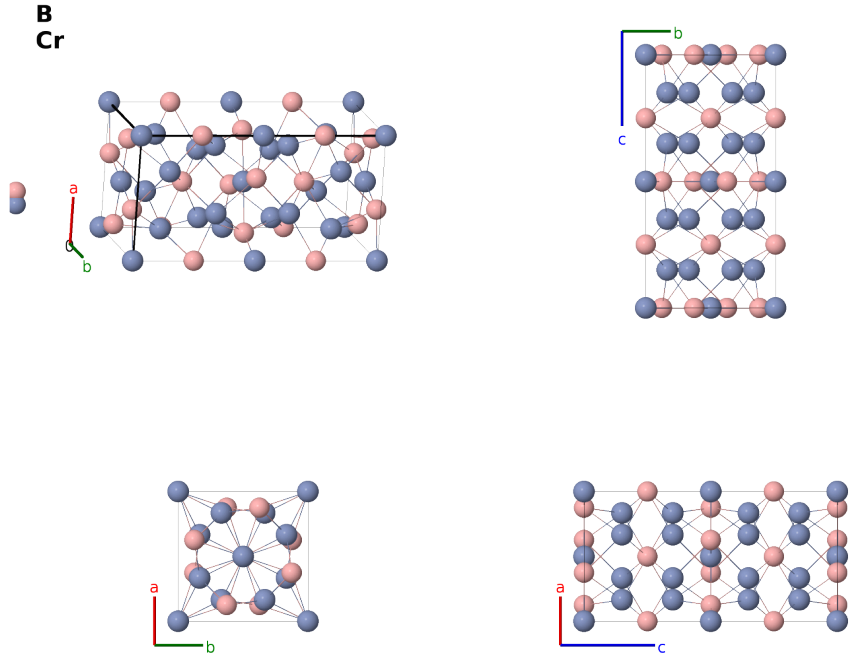
https://aflow.org/prototype-encyclopedia/AK18

https://aflow.org/prototype-encyclopedia/A3B5_tI32_140_ah_cl-001



Prototype	B_3Cr_5
AFLOW prototype label	A3B5_tI32_140_ah_cl-001
***Strukturbericht* designation**	$D8_l$
ICSD	27124
CCDC	1602452
Pearson symbol	tI32
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A3B5_tI32_140_ah_cl-001 --params=`$a, c/a, x_3, x_4, z_4$

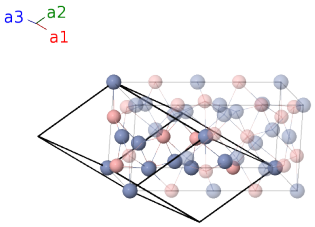
Other compounds with this structure

Ca_5Si_3, Eu_5Ge_3, $EuIrGe_2$, Fe_5PB_2, Fe_5SiB_2, Fe_4CoPB_2, Fe_4CoSiB_2, Fe_4MnPB_2, Fe_4MnSiB_2, Gd_5CoSi_2, Mo_5SiB_2, Nb_5Si_3, Pr_5Si_3, Sr_5In_3, Sr_5Si_3, Sr_5Sn_3, Ta_5Ge_3, Ta_5Si_3

- We have been unable to obtain a copy of (Bertaut, 1953), so we use the data found online from (Downs, 2003). Although Cr_5B_3 is universally regarded as the prototype for $D8_l$, it appears that no other determination of the internal parameters has ever been made. The values found in (Downs, 2003) seem to be reasonable choices, and agree with the ICSD entry.
- We originally transposed the decimal part of the value for c, using c = 10.46 rather than c = 10.64. This has now been corrected.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_3}$	=	0	=	0	(4c)	Cr I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Cr I
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	B II
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	B II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	B II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	B II
$\mathbf{B_9}$	=	$\left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + z_4\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Cr II
$\mathbf{B_{10}}$	=	$\left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - z_4\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Cr II
$\mathbf{B_{11}}$	=	$\left(x_4 + z_4\right)\,\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Cr II
$\mathbf{B_{12}}$	=	$-\left(x_4 - z_4\right)\,\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Cr II
$\mathbf{B_{13}}$	=	$\left(x_4 - z_4\right)\,\mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16l)	Cr II
$\mathbf{B_{14}}$	=	$-\left(x_4 + z_4\right)\,\mathbf{a}_1 + \left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16l)	Cr II

$$\mathbf{B_{15}} = \begin{array}{c}\left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \\ (x_4 - z_4)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3\end{array} = ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \quad (16l) \quad \text{Cr II}$$

$$\mathbf{B_{16}} = \begin{array}{c}-\left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \\ (x_4 + z_4)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3\end{array} = -ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}} \quad (16l) \quad \text{Cr II}$$

References

[1] F. Bertaut and P. Blum, *C. R. Acad. Sci.*, Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences **236**, 1055–1056 (1953).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043