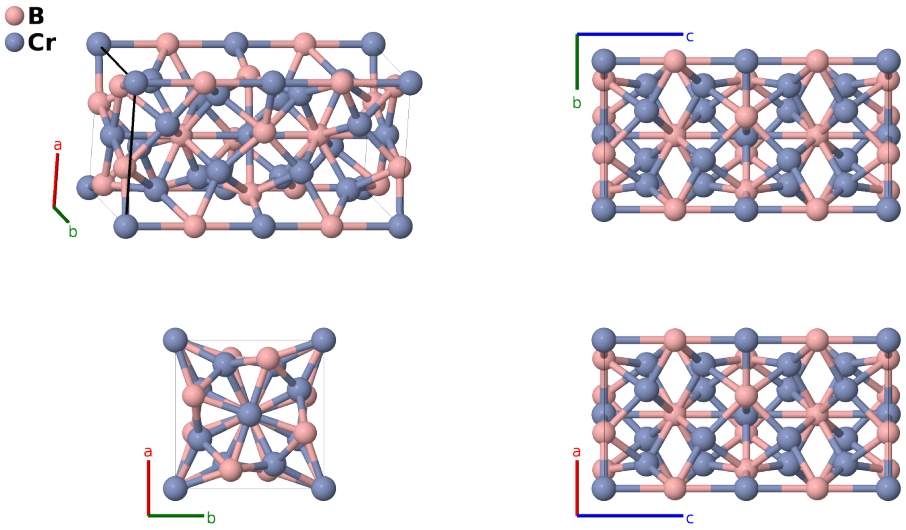
Cr_5B_3 ($D8_l$) Structure: A3B5_tI32_140_ah_cl-001

This structure originally had the label `A3B5_tI32_140_ah_cl`. Calls to that address will be redirected here.

Cite this page as: 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

https://aflow.org/p/AK18

https://aflow.org/p/A3B5_tI32_140_ah_cl-001



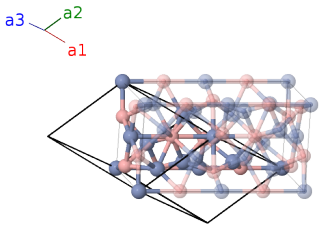
Prototype	B_3Cr_5
AFLOW prototype label	A3B5_tI32_140_ah_cl-001
***Strukturbericht* designation**	$D8_l$
ICSD	27124
Pearson symbol	tI32
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A3B5_tI32_140_ah_cl-001 --params=`$a, c/a, x_3, x_4, z_4$

Other compounds with this structure
Eu_5Ge_3, Pr_5Si_3, Ta_5Ge_3, Nb_5Si_3, Ta_5Si_3, $EuIrGe_2$, Fe_5PB_2, Fe_5SiB_2, Fe4CoPB$_2$, Fe4MnPB$_2$, Fe4CoSiB$_2$, Fe4MnSiB$_2$, Mo_5SiB_2, Sr_5In_3, Gd_5CoSi_2, Ca_5Si_3, Sr_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.

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

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).