

Cr₃Si (A15) Structure: A3B_cP8_223_c_a-001

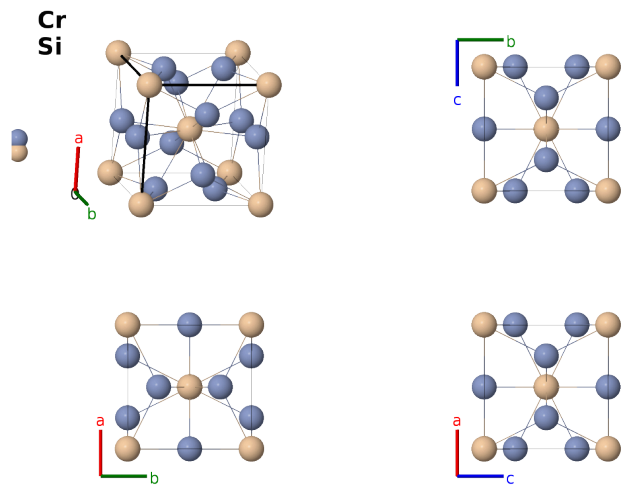
This structure previously used the label(s) **A3B_cP8_223_c_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/7MHE>

https://aflow.org/prototype-encyclopedia/A3B_cP8_223_c_a-001



Prototype	Cr ₃ Si
AFLOW prototype label	A3B_cP8_223_c_a-001
<i>Strukturbericht</i> designation	A15
ICSD	53218
CCDC	1617915
Pearson symbol	cP8
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A3B_cP8_223_c_a-001</code> <code>--params=a</code>

Other compounds with this structure

β -W, Cr₃Ga, Cr₃Ge, Cr₃Ir, Cr₃O, Cr₃Os, Cr₃Pt, Cr₃Rh, Cr₃Ru, Cr₃Si, Mo₃Al, Mo₃Be, Mo₃Ga, Mo₃Ge, Mo₃Ir, Mo₃O, Mo₃Os, Mo₃Pt, Mo₃Si, Mo₃Sn, Nb₃Al, Nb₃Au, Nb₃Bi, Nb₃Ga, Nb₃Ge, Nb₃In, Nb₃Ir, Nb₃Os, Nb₃Pb, Nb₃Pt, Nb₃Rh, Nb₃Sb, Nb₃Sn, Ta₃Au, Ta₃Sb, Ta₃Sn, Ti₃Au, Ti₃Hg, Ti₃Ir, Ti₃Sb, Ti₃Pt, V₃Al, α -UH₃, V₃As, V₃Au, V₃Cd, V₃Co, V₃Ga, V₃Ge, V₃Ir, V₃Ni, V₃Pb, V₃Pd, V₃Pt, V₃Rh, V₃Sb, V₃Si, V₃Sn, W₃O, W₃Si, Zr₃Au, Zr₃Hg, Zr₃Sn

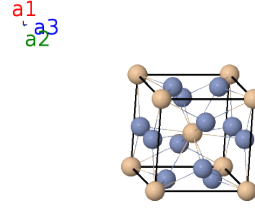
- The “A” Strukturbericht designation comes from the fact that this is also the structure of β -W.

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
$\mathbf{B}_1$	=	0	=	0	(2a) Si I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a) Si I
$\mathbf{B}_3$	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c) Cr I
$\mathbf{B}_4$	=	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c) Cr I
$\mathbf{B}_5$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(6c) Cr I
$\mathbf{B}_6$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(6c) Cr I
$\mathbf{B}_7$	=	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6c) Cr I
$\mathbf{B}_8$	=	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6c) Cr I

References

- [1] W. Jauch, A. J. Schultz, and G. Heger, *Single-crystal time-of-flight neutron diffraction of Cr_3Si and MnF_2 comparison with monochromatic-beam techniques*, J. Appl. Crystallogr. **20**, 117–119 (1987), doi:10.1107/S002188988708703X.

Found in

- [1] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

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- M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017