Cr_3Si ($A15$) Structure: A3B_cP8_223_c_a-001

This structure originally had the label `A3B_cP8_223_c_a`. Calls to that address will be redirected here.

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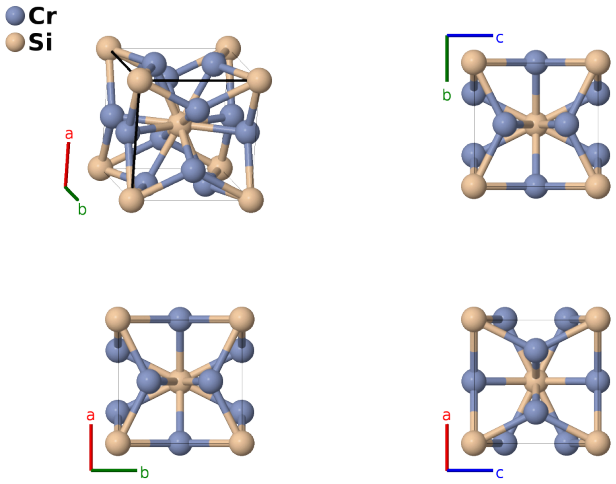
https://aflow.org/p/7MHE

https://aflow.org/p/A3B_cP8_223_c_a-001



Prototype	Cr_3Si
AFLOW prototype label	A3B_cP8_223_c_a-001
***Strukturbericht* designation**	$A15$
ICSD	53218
Pearson symbol	cP8
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	`aflow --proto=A3B_cP8_223_c_a-001 --params=`a

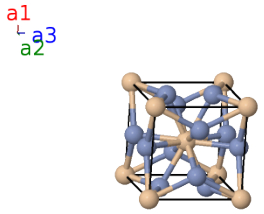
Other compounds with this structure

β-W, Cr_3Ga, Cr_3Ge, Cr_3Ir, Cr_3O, Cr_3Os, Cr_3Pt, Cr_3Rh, Cr_3Ru, Cr_3Si, Mo_3Al, Mo_3Be, Mo_3Ga, Mo_3Ge, Mo_3Ir, Mo_3O, Mo_3Os, Mo_3Pt, Mo_3Si, Mo_3Sn, Nb_3Al, Nb_3Au, Nb_3Bi, Nb_3Ga, Nb_3Ge, Nb_3In, Nb_3Ir, Nb_3Os, Nb_3Pb, Nb_3Pt, Nb_3Rh, Nb_3Sb, Nb_3Sn, Ta_3Au, Ta_3Sb, Ta_3Sn, Ti_3Au, Ti_3Hg, Ti_3Ir, Ti_3Sb, Tl_3Pt, V_3Al, α-UH_3, V_3As, V_3Au, V_3Cd, V_3Co, V_3Ga, V_3Ge, V_3Ir, V_3Ni, V_3Pb, V_3Pd, V_3Pt, V_3Rh, V_3Sb, V_3Si, V_3Sn, W_3O, W_3Si, Zr_3Au, Zr_3Hg, Zr_3Sn

- 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.