CeCr$_2$Si$_2$C Structure:
ABC2D2_tP6_123_b_a_e_h-001

https://aflow.org/p/G8WV

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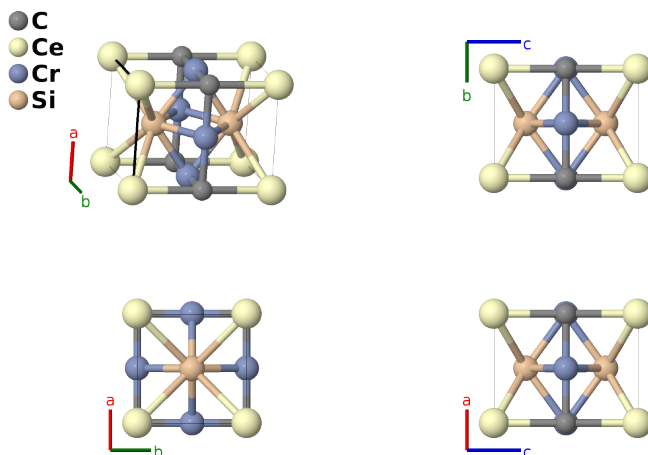
Prototype	CCeCr$_2$Si$_2$
AFLOW prototype label	ABC2D2_tP6_123_b_a_e_h-001
ICSD	90281
Pearson symbol	tP6
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	aflow --proto=ABC2D2_tP6_123_b_a_e_h-001 --params=$a, c/a, z_4$

Other compounds with this structure

BaTi$_2$As$_2$O, BaTi$_2$Ti$_2$O, DyCr$_2$Si$_2$C, GdCr$_2$Si$_2$C, HoCr$_2$Si$_2$C, LaCr$_2$Si$_2$C, NdCr$_2$Si$_2$C, PrCr$_2$Si$_2$C, SmCr$_2$Si$_2$C, TbCr$_2$Si$_2$C, YCr$_2$Si$_2$C
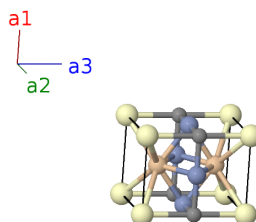

- (Pohlkamp, 2001) refer to this as a "filled ThCr$_2$Si$_2$ structure."

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ce I
$\mathbf{B_2}$	=	$\frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	C I
$\mathbf{B_3}$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Cr I
$\mathbf{B_4}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	Cr I
$\mathbf{B_5}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2h)	Si I
$\mathbf{B_6}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2h)	Si I

References

[1] C. Tang, S. Fan, and M. Zhu, *Structure and magnetic properties of CeCr$_2$Si$_2$C*, J. Alloys Compd. **299**, 1–4 (2000), doi:10.1016/S0925-8388(99)00631-3.

Found in

[1] M. W. Pohlkamp and W. Jeitschko, *Preparation, Properties, and Crystal Structure of Quaternary Silicide Carbides RCr$_2$Si$_2$C (R = Y, La-Nd, Sm, Gd-Ho)*, Z. Naturforsch. B **56**, 1143–1148 (2001), doi:10.1515/znb-2001-1108.