Zr_6CoAs_2: A2BC6_hP9_189_c_b_fg-002

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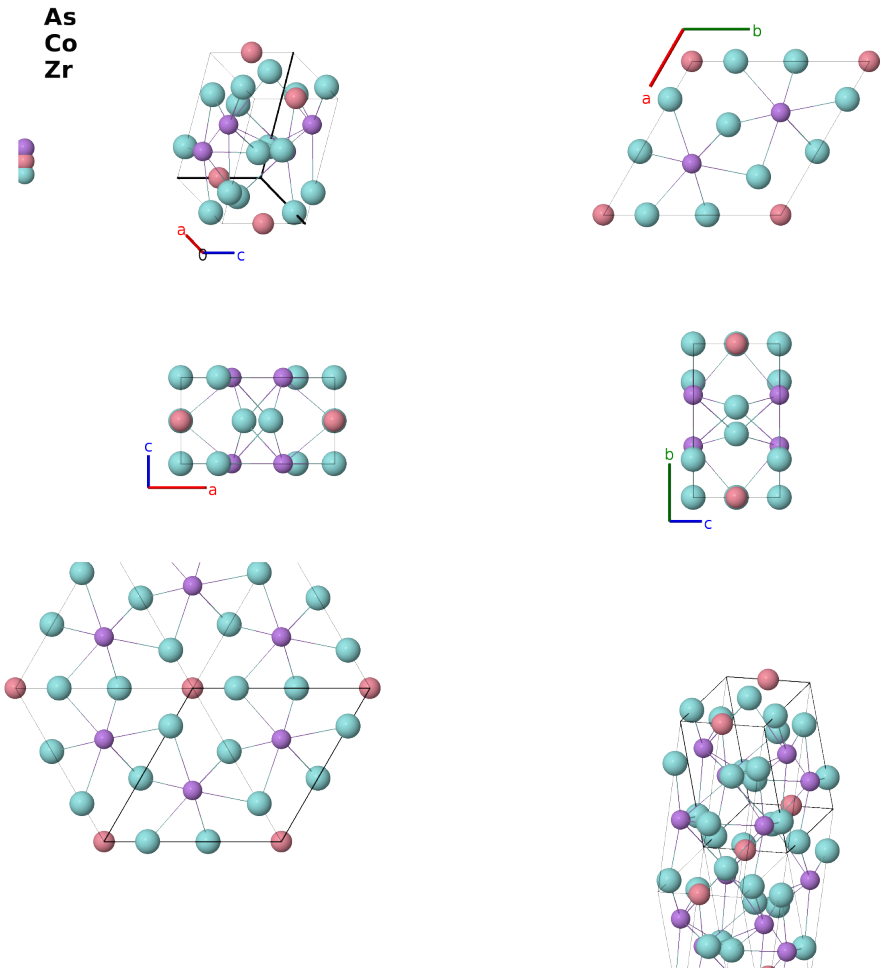
https://aflow.org/prototype-encyclopedia/6CW0

https://aflow.org/prototype-encyclopedia/A2BC6_hP9_189_c_b_fg-002



Prototype	As_2CoZr_3
AFLOW prototype label	A2BC6_hP9_189_c_b_fg-002
ICSD	83932
CCDC	1643955
Pearson symbol	hP9
Space group number	189
Space group symbol	$P\bar{6}2m$

AFLOW prototype command `aflow --proto=A2BC6_hP9_189_c_b_fg-002 --params=`$a, c/a, x_3, x_4$

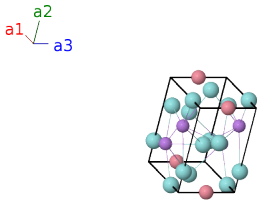
Other compounds with this structure

Dy_6FeSb_2, Dy_6RuTe_2, Er_6CoSb_2, Er_6MnBi_2, Gd_6FeBi_2, Hf_6GeSb_2, Ho_6FeBi_2, Ho_6FeSb_2, Ho_6MnTe_2, Ho_6RhBi_2, Lu_6FeSb_2, Sc_6CoTe_2, Sc_6FeSb_2, Sc_6FeTe_2, Sc_6MnTe_2, Sc_6NiTe_2, Sc_6OsTe_2, Sc_6RhTe_2, Tb_6FeBi_2, Tb_6FeSb_2, Ti_6BSi_2, Tm_6FeSb_2, Y_6FeSb_2, Zr_6CoAl_2, Zr_6CuBi_2, Zr_6GeSb_2

- This is a ternary form of Barringerite (Fe_2P).
- We represent the quaternary form of this structure, with each of the four Wyckoff positions filled by a different atomic species, by the $Tb_3Mn_3Ga_2Si$ structure.
- (Kleinke, 1997) either incorrectly labels the zirconium (3g) and (3f) sites or misstates the coordinates. The distances given in the paper are consistent with the coordinates given, so we assume the sites were mislabeled.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Co I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	As I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	As I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Zr I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Zr I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3f)	Zr I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr II

References

[1] H. Kleinke, *Zr_6CoAs_2, the first zirconium cobalt arsenide: a new ordered variant of the Fe2P type*, J. Alloys Compd. **252**, L29–L31 (1997), doi:10.1016/S0925-8388(96)03120-9.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 83932 (Zr_6CoAl_2).

First cited in

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