

Skutterudite (CoAs₃, *D*0₂) Structure: A3B_cI32_204_g_c-001

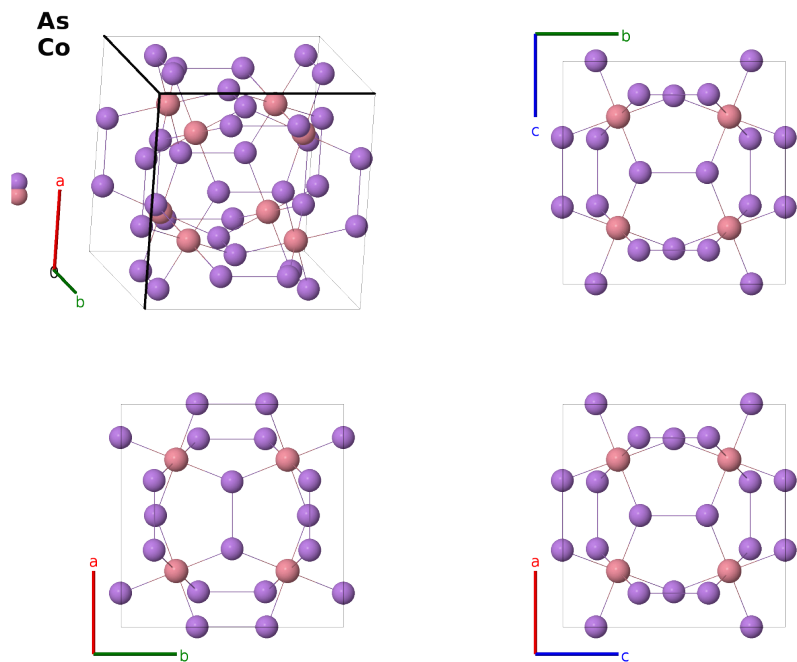
This structure previously used the label(s) **A3B_cI32_204_g_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/9U6F>

https://aflow.org/prototype-encyclopedia/A3B_cI32_204_g_c-001



Prototype	As ₃ Co
AFLOW prototype label	A3B_cI32_204_g_c-001
<i>Strukturbericht</i> designation	<i>D</i> 0 ₂
Mineral name	skutterudite
ICSD	9188
CCDC	1594218
Pearson symbol	cI32
Space group number	204
Space group symbol	<i>Im</i> $\bar{3}$
AFLOW prototype command	<code>aflow --proto=A3B_cI32_204_g_c-001</code> <code>--params=<i>a</i>, <i>y</i>₂, <i>z</i>₂</code>

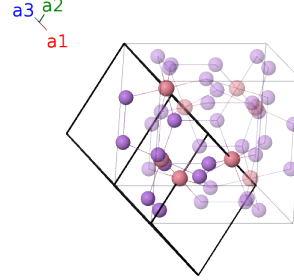
Other compounds with this structure

(Fe, Ni)As₃, IrAs₃, RhAs₃, CoP₃, IrP₃, NiP₃, PdP₃, CoSb₃, IrSb₃, RhSb₃

- Useful skutterudites have iron and nickel alloyed with cobalt.
 - We have corrected the lattice constant for this structure.
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Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	Co I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	Co I
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	Co I
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(8c)	Co I
$\mathbf{B}_5$	$= (y_2 + z_2)\mathbf{a}_1 + z_2\mathbf{a}_2 + y_2\mathbf{a}_3$	$=$	$ay_2\hat{\mathbf{y}} + az_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_6$	$= -(y_2 - z_2)\mathbf{a}_1 + z_2\mathbf{a}_2 - y_2\mathbf{a}_3$	$=$	$-ay_2\hat{\mathbf{y}} + az_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_7$	$= (y_2 - z_2)\mathbf{a}_1 - z_2\mathbf{a}_2 + y_2\mathbf{a}_3$	$=$	$ay_2\hat{\mathbf{y}} - az_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_8$	$= -(y_2 + z_2)\mathbf{a}_1 - z_2\mathbf{a}_2 - y_2\mathbf{a}_3$	$=$	$-ay_2\hat{\mathbf{y}} - az_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_9$	$= y_2\mathbf{a}_1 + (y_2 + z_2)\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$az_2\hat{\mathbf{x}} + ay_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_{10}$	$= -y_2\mathbf{a}_1 - (y_2 - z_2)\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$az_2\hat{\mathbf{x}} - ay_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_{11}$	$= y_2\mathbf{a}_1 + (y_2 - z_2)\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$-az_2\hat{\mathbf{x}} + ay_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_{12}$	$= -y_2\mathbf{a}_1 - (y_2 + z_2)\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$-az_2\hat{\mathbf{x}} - ay_2\hat{\mathbf{z}}$	(24g)	As I
$\mathbf{B}_{13}$	$= z_2\mathbf{a}_1 + y_2\mathbf{a}_2 + (y_2 + z_2)\mathbf{a}_3$	$=$	$ay_2\hat{\mathbf{x}} + az_2\hat{\mathbf{y}}$	(24g)	As I
$\mathbf{B}_{14}$	$= z_2\mathbf{a}_1 - y_2\mathbf{a}_2 - (y_2 - z_2)\mathbf{a}_3$	$=$	$-ay_2\hat{\mathbf{x}} + az_2\hat{\mathbf{y}}$	(24g)	As I
$\mathbf{B}_{15}$	$= -z_2\mathbf{a}_1 + y_2\mathbf{a}_2 + (y_2 - z_2)\mathbf{a}_3$	$=$	$ay_2\hat{\mathbf{x}} - az_2\hat{\mathbf{y}}$	(24g)	As I
$\mathbf{B}_{16}$	$= -z_2\mathbf{a}_1 - y_2\mathbf{a}_2 - (y_2 + z_2)\mathbf{a}_3$	$=$	$-ay_2\hat{\mathbf{x}} - az_2\hat{\mathbf{y}}$	(24g)	As I

References

- [1] N. Mandel and J. Donohue, *The refinement of the crystal structure of skutterudite, CoAs₃*, Acta Crystallogr. Sect. B **27**, 2288–2289 (1971), doi:10.1107/S0567740871005727.

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