Skutterudite ($CoAs_3$, $D0_2$) Structure: A3B_cI32_204_g_c-001

This structure originally had the label `A3B_cI32_204_g_c`. Calls to that address will be redirected here.

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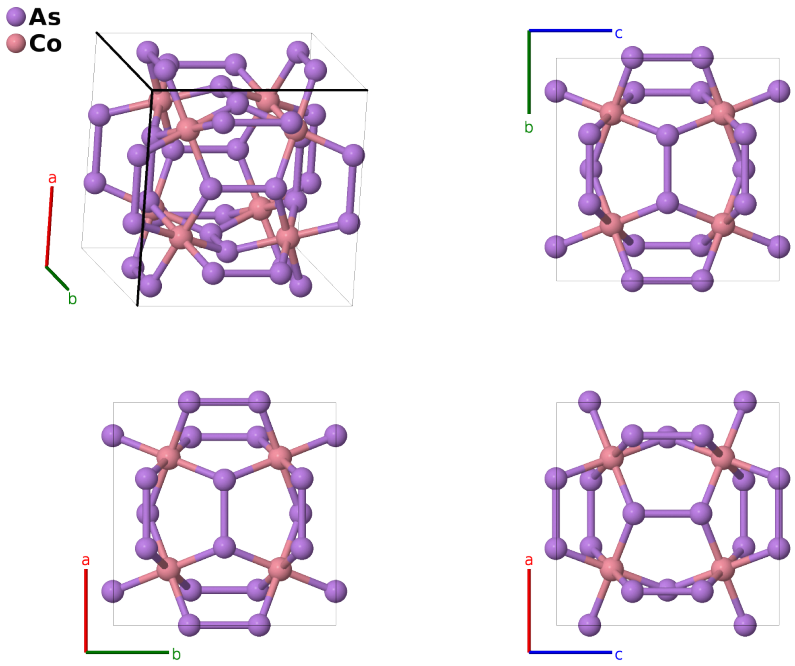
https://aflow.org/p/9U6F

https://aflow.org/p/A3B_cI32_204_g_c-001



Prototype	As_3Co
AFLOW prototype label	A3B_cI32_204_g_c-001
***Strukturbericht* designation**	$D0_2$
Mineral name	skutterudite
ICSD	9188
Pearson symbol	cI32
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	`aflow --proto=A3B_cI32_204_g_c-001 --params=`a, y_2, z_2

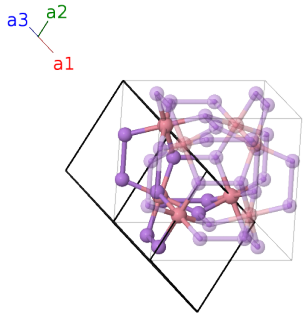
Other compounds with this structure
(Fe, Ni)As_3, $IrAs_3$, $RhAs_3$, CoP_3, IrP_3, NiP_3, PdP_3, $CoSb_3$, $IrSb_3$, $RhSb_3$

- Useful skutterudites have iron and nickel alloyed with cobalt.

- We have corrected the lattice constant for this structure.

Body-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}
$$



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, $CoAs_3$*, Acta Crystallogr. Sect. B **27**, 2288–2289 (1971), doi:10.1107/S0567740871005727.