

U₂Co₃Si₅ Structure:

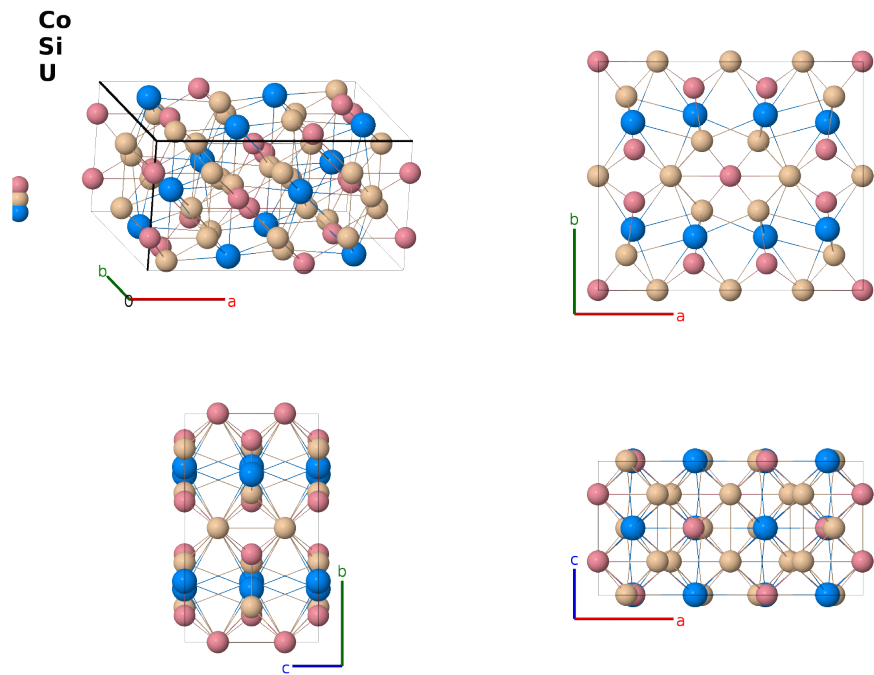
A3B5C2_oI40_72_aj_bfj_j-001

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<https://aflow.org/prototype-encyclopedia/LD1K>

https://aflow.org/prototype-encyclopedia/A3B5C2_oI40_72_aj_bfj_j-001



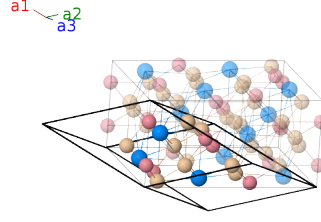
Prototype	Co ₃ Si ₅ U ₂
AFLOW prototype label	A3B5C2_oI40_72_aj_bfj_j-001
ICSD	20930
CCDC	1598655
Pearson symbol	oI40
Space group number	72
Space group symbol	<i>Ibam</i>
AFLOW prototype command	<code>aflow --proto=A3B5C2_oI40_72_aj_bfj_j-001</code> <code>--params=a, b/a, c/a, x₃, x₄, y₄, x₅, y₅, x₆, y₆</code>

Other compounds with this structure

Ce₂Co₃Si₅, Ce₂Pt₃Si₅, Ce₂Rh₃Ge₅, Ce₂Ru₃Ge₅, Dy₂Ni₃Si₅, Gd₂Ru₃Ge₅, Ho₂Ni₃Si₅, La₂Ru₃Ge₅, Li₂Ir₃Si₅, Lu₂Ir₃Si₅, Lu₂Ru₃Si₅, Nd₂Ru₃Ge₅, Pu₂Pt₃Si₅, Tb₂Ni₃Si₅, Tb₂Ru₃Ge₅, Y₂Ni₃Si₅

Body-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(4a)	Co I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(4a)	Co I
$\mathbf{B}_3$	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B}_4$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B}_5$	$= \frac{1}{4}\mathbf{a}_1 + (x_3 + \frac{1}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B}_6$	$= \frac{1}{4}\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B}_7$	$= \frac{3}{4}\mathbf{a}_1 - (x_3 - \frac{3}{4})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{3}{4}c\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B}_8$	$= \frac{3}{4}\mathbf{a}_1 + (x_3 + \frac{3}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{3}{4}c\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B}_9$	$= y_4\mathbf{a}_1 + x_4\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + by_4\hat{\mathbf{y}}$	(8j)	Co II
$\mathbf{B}_{10}$	$= -y_4\mathbf{a}_1 - x_4\mathbf{a}_2 - (x_4 + y_4)\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - by_4\hat{\mathbf{y}}$	(8j)	Co II
$\mathbf{B}_{11}$	$= (y_4 + \frac{1}{2})\mathbf{a}_1 - (x_4 - \frac{1}{2})\mathbf{a}_2 - (x_4 - y_4)\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} + by_4\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8j)	Co II
$\mathbf{B}_{12}$	$= -(y_4 - \frac{1}{2})\mathbf{a}_1 + (x_4 + \frac{1}{2})\mathbf{a}_2 + (x_4 - y_4)\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} - by_4\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8j)	Co II
$\mathbf{B}_{13}$	$= y_5\mathbf{a}_1 + x_5\mathbf{a}_2 + (x_5 + y_5)\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} + by_5\hat{\mathbf{y}}$	(8j)	Si III
$\mathbf{B}_{14}$	$= -y_5\mathbf{a}_1 - x_5\mathbf{a}_2 - (x_5 + y_5)\mathbf{a}_3$	$=$	$-ax_5\hat{\mathbf{x}} - by_5\hat{\mathbf{y}}$	(8j)	Si III
$\mathbf{B}_{15}$	$= (y_5 + \frac{1}{2})\mathbf{a}_1 - (x_5 - \frac{1}{2})\mathbf{a}_2 - (x_5 - y_5)\mathbf{a}_3$	$=$	$-ax_5\hat{\mathbf{x}} + by_5\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8j)	Si III
$\mathbf{B}_{16}$	$= -(y_5 - \frac{1}{2})\mathbf{a}_1 + (x_5 + \frac{1}{2})\mathbf{a}_2 + (x_5 - y_5)\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} - by_5\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8j)	Si III
$\mathbf{B}_{17}$	$= y_6\mathbf{a}_1 + x_6\mathbf{a}_2 + (x_6 + y_6)\mathbf{a}_3$	$=$	$ax_6\hat{\mathbf{x}} + by_6\hat{\mathbf{y}}$	(8j)	U I
$\mathbf{B}_{18}$	$= -y_6\mathbf{a}_1 - x_6\mathbf{a}_2 - (x_6 + y_6)\mathbf{a}_3$	$=$	$-ax_6\hat{\mathbf{x}} - by_6\hat{\mathbf{y}}$	(8j)	U I
$\mathbf{B}_{19}$	$= (y_6 + \frac{1}{2})\mathbf{a}_1 - (x_6 - \frac{1}{2})\mathbf{a}_2 - (x_6 - y_6)\mathbf{a}_3$	$=$	$-ax_6\hat{\mathbf{x}} + by_6\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8j)	U I
$\mathbf{B}_{20}$	$= -(y_6 - \frac{1}{2})\mathbf{a}_1 + (x_6 + \frac{1}{2})\mathbf{a}_2 + (x_6 - y_6)\mathbf{a}_3$	$=$	$ax_6\hat{\mathbf{x}} - by_6\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(8j)	U I

References

- [1] L. G. Aksel'rud, Y. P. Yarmolyuk, and E. I. Gladyshevskii, *Crystal structure of the compound $U_2Co_3Si_5$* , Sov. Phys. Crystallogr. **22**, 492–493 (1997).

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