Lu$_2$Co$_3$Si$_5$ Structure: A3B2C5_mC40_15_ef_f_3ef-001
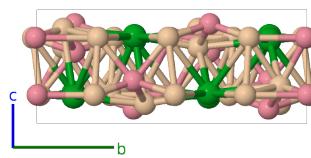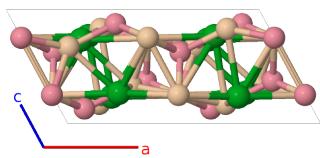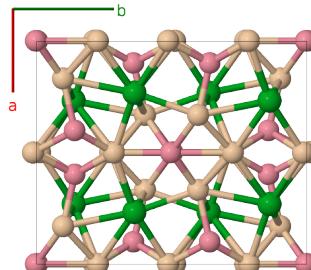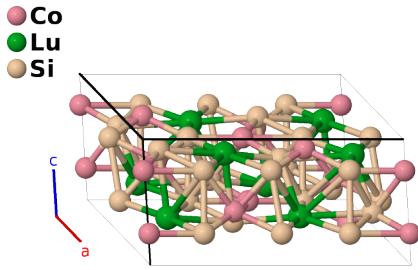
Prototype	Co$_3$Lu$_2$Si$_5$
AFLOW prototype label	A3B2C5_mC40_15_ef_f_3ef-001
ICSD	76349
Pearson symbol	mC40
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	aflow --proto=A3B2C5_mC40_15_ef_f_3ef-001 --params=$a, b/a, c/a, \beta, y_1, y_2, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure

Dy$_2$Co$_3$Si$_5$, Sc$_2$Co$_3$Si$_5$, Y$_2$Co$_3$Si$_5$

- This is a monoclinic distortion of the orthorhombic U$_2$Co$_3$Si$_5$ structure. (Chabot, 1985)

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
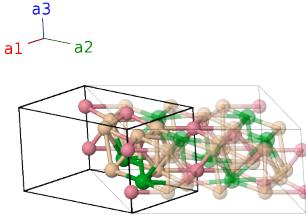
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$-y_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Co I
$\mathbf{B_2}$	$=$	$y_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Co I
$\mathbf{B_3}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_5}$	$=$	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si II
$\mathbf{B_6}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si II
$\mathbf{B_7}$	$=$	$-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si III
$\mathbf{B_8}$	$=$	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Si III
$\mathbf{B_9}$	$=$	$(x_5 - y_5)\,\mathbf{a_1} + (x_5 + y_5)\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Co II
$\mathbf{B_{10}}$	$=$	$-(x_5 + y_5)\,\mathbf{a_1} - (x_5 - y_5)\,\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Co II
$\mathbf{B_{11}}$	$=$	$-(x_5 - y_5)\,\mathbf{a_1} - (x_5 + y_5)\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Co II
$\mathbf{B_{12}}$	$=$	$(x_5 + y_5)\,\mathbf{a_1} + (x_5 - y_5)\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Co II
$\mathbf{B_{13}}$	$=$	$(x_6 - y_6)\,\mathbf{a_1} + (x_6 + y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	Lu I
$\mathbf{B_{14}}$	$=$	$-(x_6 + y_6)\,\mathbf{a_1} - (x_6 - y_6)\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Lu I
$\mathbf{B_{15}}$	$=$	$-(x_6 - y_6)\,\mathbf{a_1} - (x_6 + y_6)\,\mathbf{a_2} - z_6\,\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	Lu I
$\mathbf{B_{16}}$	$=$	$(x_6 + y_6)\,\mathbf{a_1} + (x_6 - y_6)\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$\left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Lu I
$\mathbf{B_{17}}$	$=$	$(x_7 - y_7)\,\mathbf{a_1} + (x_7 + y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si IV
$\mathbf{B_{18}}$	$=$	$-(x_7 + y_7)\,\mathbf{a_1} - (x_7 - y_7)\,\mathbf{a_2} - \left(z_7 - \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-\left(ax_7 + c\left(z_7 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si IV
$\mathbf{B_{19}}$	$=$	$-(x_7 - y_7)\,\mathbf{a_1} - (x_7 + y_7)\,\mathbf{a_2} - z_7\,\mathbf{a_3}$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si IV
$\mathbf{B_{20}}$	$=$	$(x_7 + y_7)\,\mathbf{a_1} + (x_7 - y_7)\,\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\,\mathbf{a_3}$	$=$	$\left(ax_7 + c\left(z_7 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si IV

References

[1] B. Chabot and E. Parthé, *Dy$_2$Co$_3$Si$_5$, Lu$_2$Co$_3$Si$_5$, Y$_2$Co$_3$Si$_5$ and Sc$_2$Co$_3$Si$_5$, with a Monoclinic Structural Deformation Variant of the Orthorhombic U$_2$Co$_3$Si$_5$ Structure Type*, J. Less-Common Met. **106**, 53–59 (1985), doi:10.1016/0022-5088(85)90365-0.