$LiCo_6P_4$ Structure: A6BC4_hP11_187_jk_a_ck-001

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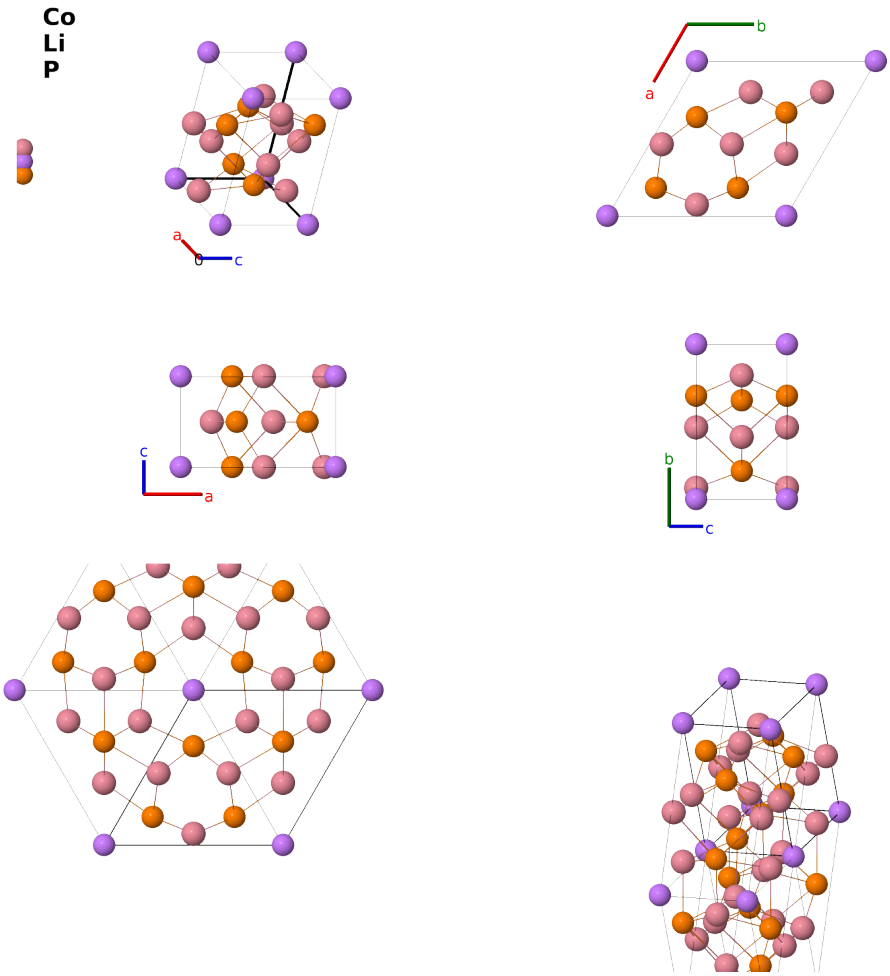
https://aflow.org/prototype-encyclopedia/NFL9

https://aflow.org/prototype-encyclopedia/A6BC4_hP11_187_jk_a_ck-001



Prototype	Co_6LiP_4
AFLOW prototype label	A6BC4_hP11_187_jk_a_ck-001
ICSD	69692
CCDC	1631543
Pearson symbol	hP11
Space group number	187
Space group symbol	$P\bar{6}m2$

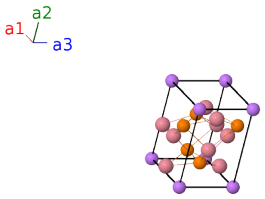
AFLOW prototype command `aflow --proto=A6BC4_hP11_187_jk_a_ck-001 --params=`$a, c/a, x_3, x_4, x_5$

Other compounds with this structure

$CeCo_6P_4$, $CeRh_6Ge_4$, $CeRh_6Ge_4$, $DyCo_6P_4$, $DyRh_6Ge_4$, $ErCo_6P_4$, $ErRh_6Ge_4$, $EuCo_6P_4$, $EuRh_6Ge_4$, $GdCo_6P_4$, $GdRh_6Ge_4$, $HoCo_6P_4$, $HoRh_6Ge_4$, $LaCo_6P_4$, $LaRh_6Ge_4$, $LuCo_6P_4$, $LuRh_6Ge_4$, $LuRh_6P_4$, $NdCo_6P_4$, $NdRh_6Ge_4$, $PrCo_6P_4$, $PrRh_6Ge_4$, $ScRh_6P_4$, $SmCo_6P_4$, $SmRh_6Ge_4$, $TbCo_6P_4$, $TbRh_6Ge_4$, $TmCo_6P_4$, $TmRh_6Ge_4$, YCo_6P_4, YRh_6Ge_4, YRh_6P_4, $YbCo_6P_4$, $YbRh_6Ge_4$

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Li I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(1c)	P I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}}$	(3j)	Co I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3j)	Co I
$\mathbf{B_5}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3j)	Co I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Co II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Co II
$\mathbf{B_8}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	Co II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	P II
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 + 2x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	P II
$\mathbf{B_{11}}$	=	$-2x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	P II

References

[1] R. Buschmann and H.-U. Schuster, *Darstellung und Kristallstruktur der Verbindung $LiCo_6P_4$*, Z. Naturforsch. B **46**, 699–701 (1991), doi:10.1515/znb-1991-0525.

Found in

[1] S. F. Matar, A. Al-Alam, N. Ouaini, and R. Pöttgen, *Ab initio investigations of the electronic structures and chemical bonding in $LiCo_6P_4$ and $Li_2Co_{12}P_7$*, J. Solid State Chem. **202**, 227–233 (2013), doi:10.1016/j.jssc.2013.03.032.

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