

LiCo <sub>6</sub> P <sub>4</sub>	<i>hP</i> 11	(187) <i>P</i> -6 <i>m</i> 2 – k <sup>2</sup> jca
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**LiCo<sub>6</sub>P<sub>4</sub>** [1]; UCr<sub>6</sub>P<sub>4</sub> α [2]

Structural features: Infinite columns of base-linked P(Li<sub>2</sub>Co<sub>4</sub>)Co<sub>2</sub> bicapped and PCo<sub>6</sub>Co<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework (a framework formed by propeller-like columns with single prism columns shifted by *c*/2 in channels). See Fig. IV.13.

Buschmann R., Schuster H.U. (1991) [1]

Co<sub>6</sub>LiP<sub>4</sub>

*a* = 0.6584, *c* = 0.3338 nm, *c/a* = 0.507, *V* = 0.1253 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	3 <i>k</i>	<i>mm</i> 2	0.2002	0.7998	1/2		cuboctahedron P <sub>4</sub> Co <sub>6</sub> Li <sub>2</sub>
P2	3 <i>k</i>	<i>mm</i> 2	0.8192	0.1808	1/2		8-vertex polyhedron Co <sub>6</sub> Li <sub>2</sub>
Co3	3 <i>j</i>	<i>mm</i> 2	0.5365	0.4635	0		11-vertex polyhedron P <sub>5</sub> Co <sub>6</sub>
P4	1 <i>c</i>	-6 <i>m</i> 2	1/3	2/3	0		tricapped trigonal prism Co <sub>9</sub>
Li5	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		23-vertex polyhedron P <sub>9</sub> Co <sub>12</sub> Li <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, *R* = 0.035

Remarks: Preliminary data for α-UCr<sub>6</sub>P<sub>4</sub> in [3].

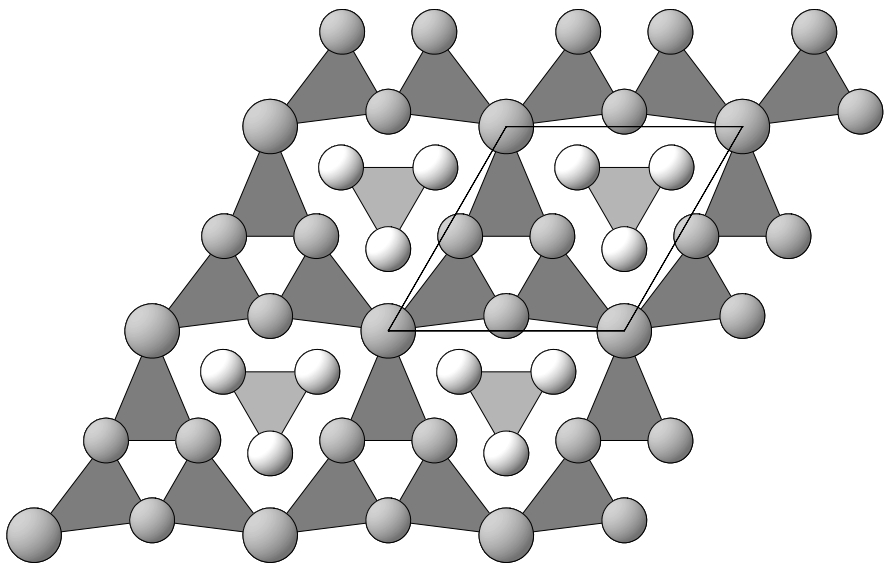


Fig. IV.13. **LiCo<sub>6</sub>P<sub>4</sub>**

Arrangement of P(Li<sub>2</sub>Co<sub>4</sub>) and PCo<sub>6</sub> trigonal prisms (Li atoms large, Co atoms small) viewed along [001]. Light and dark prisms are shifted by *c*/2.

References: [1] Buschmann R., Schuster H.U. (1991), *Z. Naturforsch. B* 46, 699-701. [2] Jeitschko W., Brink R. (1992), *Z. Naturforsch. B* 47, 192-196. [3] Brink R., Jeitschko W. (1986), *Z. Kristallogr.* 174, 27.