

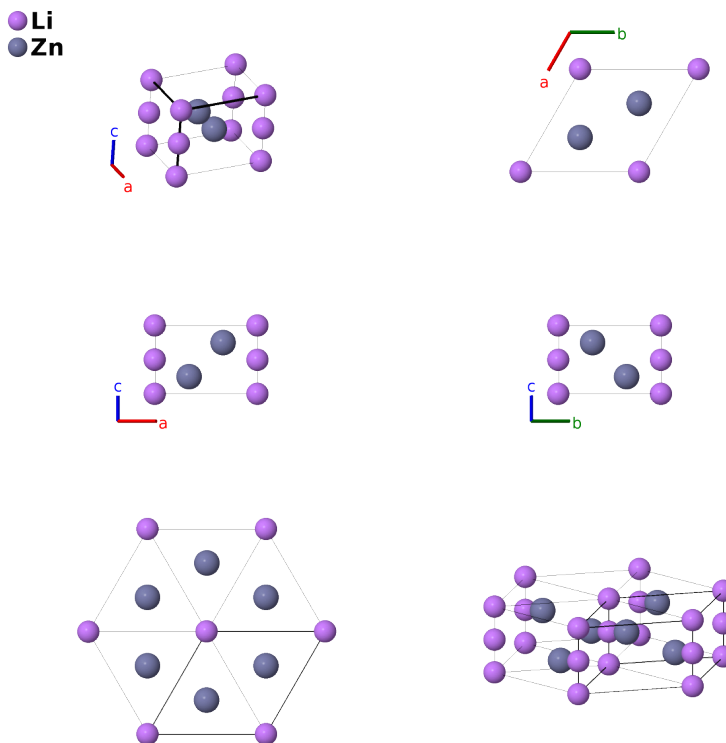
LiZn₂ (C_k) Structure: AB_hP4_194_a_c-003

This structure originally had the label AB_hP4_194_a_c. Calls to that address will be redirected here.

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<https://afLOW.org/p/CY59>

https://afLOW.org/p/AB_hP4_194_a_c-003

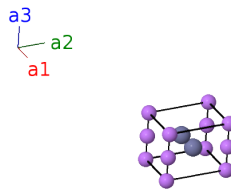


Prototype	LiZn ₂
AFLOW prototype label	AB_hP4_194_a_c-003
<i>Strukturbericht</i> designation	C_k
ICSD	104793
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>afLOW --proto=AB_hP4_194_a_c-003 --params=a, c/a</code>

- The actual stoichiometry of this compounds is Li_{0.8}Zn₂, so each (2a) site is only filled 40% of the time. This means that the short (1.26Å) distance between the lithium atoms shown here is illusionary.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(2a) Li I
\mathbf{B}_2	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a) Li I
\mathbf{B}_3	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c) Zn I
\mathbf{B}_4	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c) Zn I

References

- [1] E. Zintl and A. Schneider, *Röntgenanalyse der Lithium-Zink-Legierungen (15. Mitteilung über Metalle und Legierungen)*, Z. Elektrochem. **41**, 764–767 (1935), doi:10.1002/bbpc.19350411103.

Found in

- [1] C. J. Smithells, *Metals Reference Book* (Butterworths Scientific, London, 1955), second edn.