High-pressure cI16 Li Structure: A_cI16_220_c-001

This structure previously used the label(s) `A_cI16_220_c`. Calls to these addresses will be redirected here.

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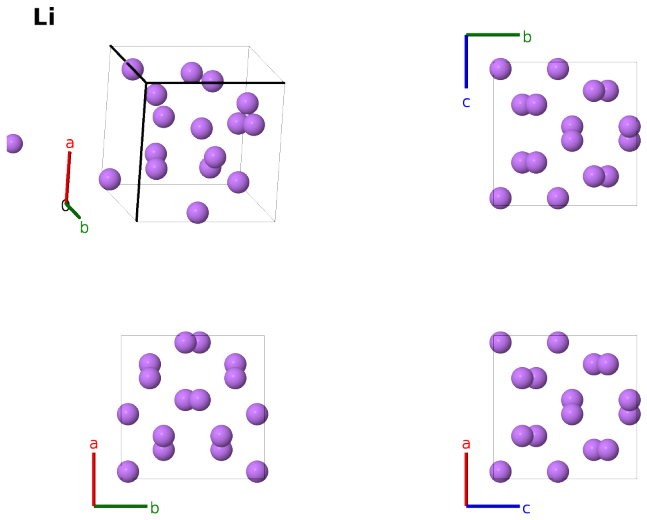
https://aflow.org/prototype-encyclopedia/BTF5

https://aflow.org/prototype-encyclopedia/A_cI16_220_c-001



Prototype	Li
AFLOW prototype label	A_cI16_220_c-001
ICSD	109012
CCDC	1666644
Pearson symbol	cI16
Space group number	220
Space group symbol	$I\bar{4}3d$
AFLOW prototype command	`aflow --proto=A_cI16_220_c-001 --params=`a, x_1

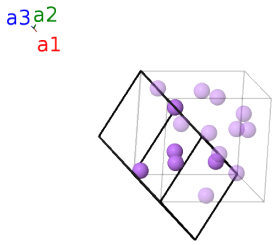
Other compounds with this structure
Na (under pressure)

- This is a high-pressure phase of lithium. We use the data from (Hanfland, 2000) at 38.9 GPa. When $x_1 = 0$ this becomes a body-centered cubic ($A2$) system.

- We have used the fact that all vectors of the form $(\pm a/2\hat{x} \pm a/2\hat{y} \pm a/2\hat{z})$ are primitive vectors of the body-centered cubic lattice to simplify the positions of some atoms in both lattice and Cartesian coordinates.
- The ICSD entry was recorded at 45 GPa.

Body-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$2x_1\,\mathbf{a}_1 + 2x_1\,\mathbf{a}_2 + 2x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_3}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_4}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_5}$	=	$\left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - 2x_1\,\mathbf{a}_3$	=	$-a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_7}$	=	$-2x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Li I
$\mathbf{B_8}$	=	$-2x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Li I

References

[1] M. Hanfland, K. Syassen, N. E. Christensen, and D. L. Novikov, *New high-pressure phases of lithium*, Nature **408**, 174–178 (2000), doi:10.1038/35041515.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017