

Li₂CN₂ Structure:

AB2C2_tI10_139_a_d_e-002

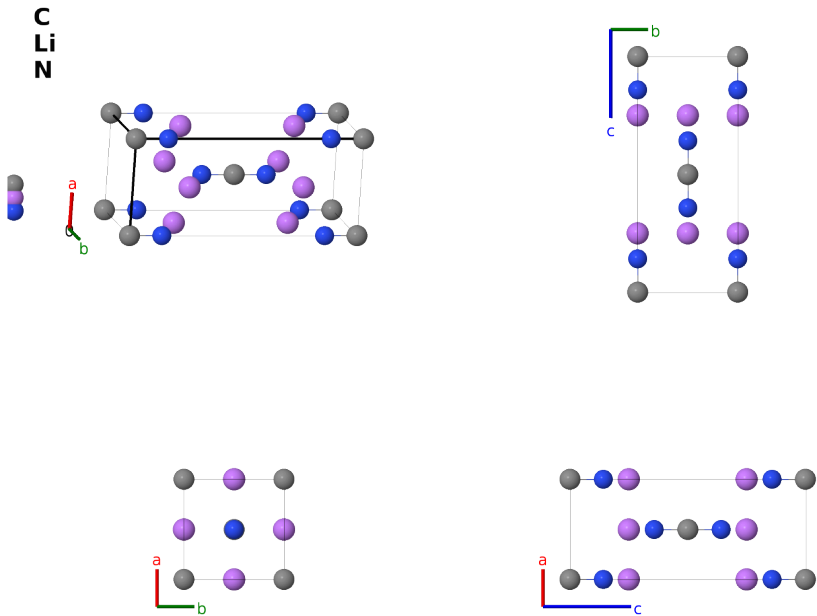
This structure previously used the label(s) **AB2C2.tI10_139_a_d_e.Li2CN2**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/5K3T>

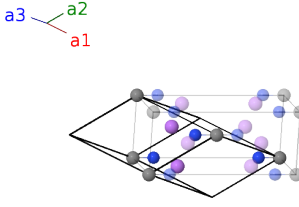
https://aflow.org/prototype-encyclopedia/AB2C2_tI10_139_a_d_e-002



Prototype	CLi ₂ N ₂
AFLOW prototype label	AB2C2.tI10_139_a_d_e-002
ICSD	200369
CCDC	1206769
Pearson symbol	tI10
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=AB2C2_tI10_139_a_d_e-002 --params=a,c/a,z₃</code>

- This structure has the same AFLOW prototype label, AB2C2_tI10_139_a_d_e, as autunite, $\text{Ca}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 10\frac{1}{2}\text{H}_2\text{O}$ ($H5_9$). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Tetragonal primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) C I
$\mathbf{B}_2$	$=$	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d) Li I
$\mathbf{B}_3$	$=$	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d) Li I
$\mathbf{B}_4$	$=$	$z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e) N I
$\mathbf{B}_5$	$=$	$-z_3 \mathbf{a}_1 - z_3 \mathbf{a}_2$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e) N I

References

- [1] M. G. Down, M. J. Haley, P. Hubberstey, R. J. Pulham, and A. E. Thunder, *Solutions of lithium salts in liquid lithium: preparation and X-ray crystal structure of the dilithium salt of carbodi-imide (cyanamide)*, Dalton Trans. **1978**, 1407–1411 (1978), doi:10.1039/DT9780001407.

Found in

- [1] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

First cited in

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