

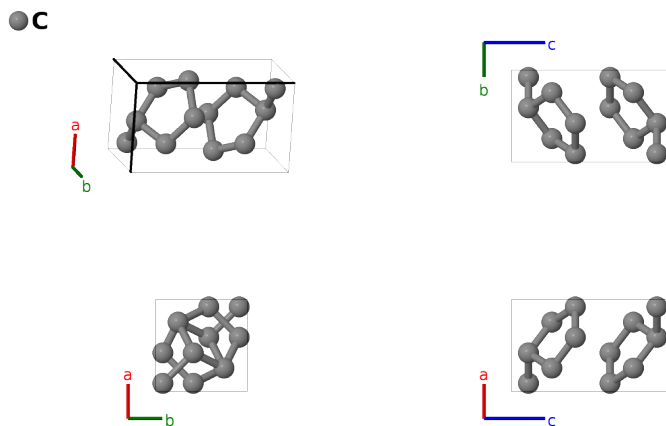
C (T12 Group IV) Structure: A_tP12_138_bi-001

This structure originally had the label `A_tP12_138_bi`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/HZJ9>

https://aflow.org/p/A_tP12_138_bi-001



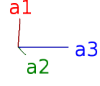
Prototype	C
AFLOW prototype label	A_tP12_138_bi-001
ICSD	None
Pearson symbol	tP12
Space group number	138
Space group symbol	$P4_2/ncm$
AFLOW prototype command	<code>aflow --proto=A_tP12_138_bi-001 --params=a, c/a, x₂, z₂</code>

Other compounds with this structure

Ge, Si

- This is a tetragonal allotrope of the diamond structure found computationally in C, Si, and Ge. The authors state “the T12 polymorph naturally accounts for the experimental d spacings and Raman spectra of synthesized metastable Ge and Si-XIII phases with long-puzzling unknown structures, respectively.”

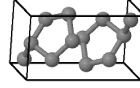
Simple Tetragonal primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4b)	C I
\mathbf{B}_2	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	C I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4b)	C I
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	C I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_7	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_8	$= x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_9	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_{10}	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_{11}	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8i)	C II
\mathbf{B}_{12}	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8i)	C II

References

- [1] Z. Zhao, F. Tian, X. Dong, Q. Li, Q. Wang, H. Wang, X. Zhong, B. Xu, D. Yu, J. He, H.-T. Wang, Y. Ma, and Y. Tian, *Tetragonal Allotrope of Group 14 Elements*, *J. Am. Chem. Soc.* **134**, 12362–12365 (2012), doi:10.1021/ja304380p.