

Ca₇Ge Structure:

A7B_cF32_225_ad_b-001

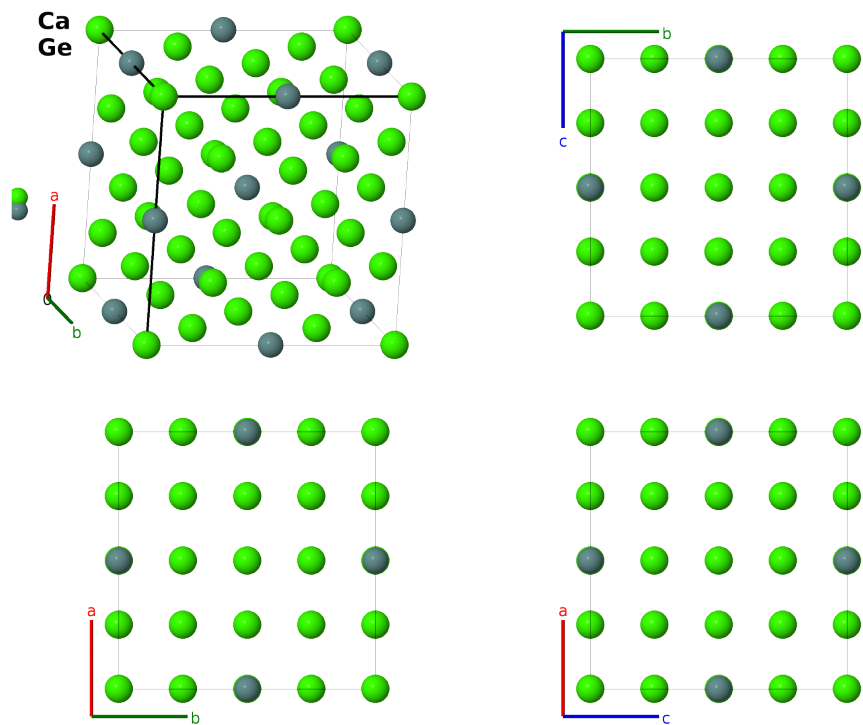
This structure previously used the label(s) **A7B_cF32.225.bd.a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/CAN8>

https://aflow.org/prototype-encyclopedia/A7B_cF32.225_ad_b-001



Prototype	Ca ₇ Ge
AFLOW prototype label	A7B_cF32_225_ad_b-001
ICSD	43321
CCDC	1612834
Pearson symbol	cF32
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A7B_cF32_225_ad_b-001</code> <code>--params=a</code>

Other compounds with this structure

CuPt₇, DyPd₇, LiPd₇, LiPt₇, SbPt₇, MoZn₇

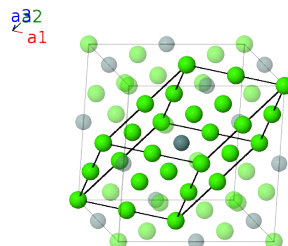
- The AFLOW prototype label protocol shifts the origin by (a/2,a/2,a/2) which places the Ca I atom on the (4a) site rather than the Ge I atom specified by (Helleis, 1963)

Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Ca I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(4b) Ge I
$\mathbf{B}_3$	=	$\frac{1}{2}\mathbf{a}_1$	=	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Ca II
$\mathbf{B}_4$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Ca II
$\mathbf{B}_5$	=	$\frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Ca II
$\mathbf{B}_6$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Ca II
$\mathbf{B}_7$	=	$\frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(24d) Ca II
$\mathbf{B}_8$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d) Ca II

References

- [1] O. Helleis, H. Kandler, E. Leicht, W. Quiring, and E. Wölfel, *Die Kristallstrukturen der intermetallischen Phasen Ca₃₃Ge, Ca₇Ge, Ca₃Pb und Ca₅Pb₃*, Z. Anorganische und Allgemeine Chemie **320**, 86–100 (1963), doi:10.1002/zaac.19633200113.

Found in

- [1] P. Villars, *Ca₇Ge Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

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