

BaGe₂As₂ Structure:

A2BC2_tP20_105_f_bc_2d-001

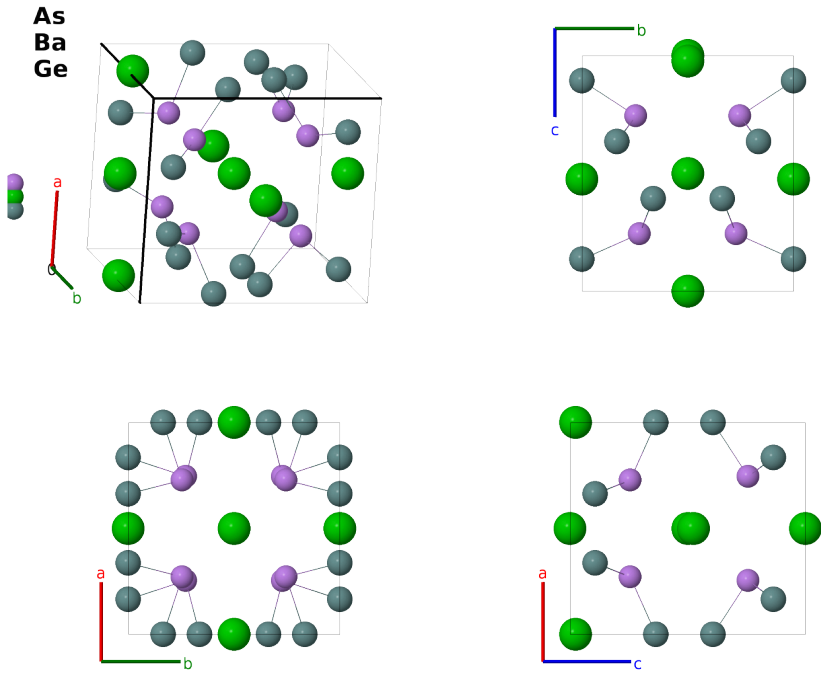
This structure previously used the label(s) **A2BC2.tP20_105_f.ac.2e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/W96U>

https://aflow.org/prototype-encyclopedia/A2BC2_tP20_105_f_bc_2d-001



Prototype	As ₂ BaGe ₂
AFLOW prototype label	A2BC2_tP20_105_f_bc_2d-001
ICSD	26417
CCDC	1601825
Pearson symbol	tP20
Space group number	105
Space group symbol	<i>P</i> 4 ₂ <i>m</i> <i>c</i>
AFLOW prototype command	<code>aflow --proto=A2BC2_tP20_105_f_bc_2d-001</code> <code>--params=a, c/a, z₁, z₂, x₃, z₃, x₄, z₄, x₅, y₅, z₅</code>

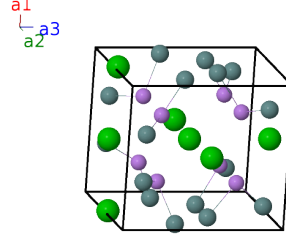
Other compounds with this structure

BaGe₂P₂

- Our previous listing of this structure (Hicks, 2017) misplaced the z coordinates of the Ba II and Ge II atoms by $c/2$. We have corrected this here.
- Space group $P4_2mc$ #105 allows an arbitrary placement of the origin of the z -axis. Here we use this freedom to set $z_1 = 0$ for the Ba-I atoms.

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(4d)	Ge I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(4d)	Ge I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ge I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ge I
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(4d)	Ge II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(4d)	Ge II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ge II
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ge II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{15}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{16}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{19}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	As I
$\mathbf{B}_{20}$	$= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	As I

References

- [1] B. Eisenmann and H. Schäfer, *Zintlphasen mit binären Anionen: Zur Kenntnis von BaGe_2P_2 und BaGe_2As_2 / Zintl Phases with Binary Anions: BaGe_2P_2 and BaGe_2As_2* , Z. Naturforsch. B **36**, 415–419 (1981), doi:10.1515/znb-1981-0403.

- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

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- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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