# $BaGe_2As_2$ Structure: A2BC2_tP20_105_f_bc_2d-001

This structure originally had the label `A2BC2_tP20_105_f_ac_2e`. Calls to that address will be redirected here.

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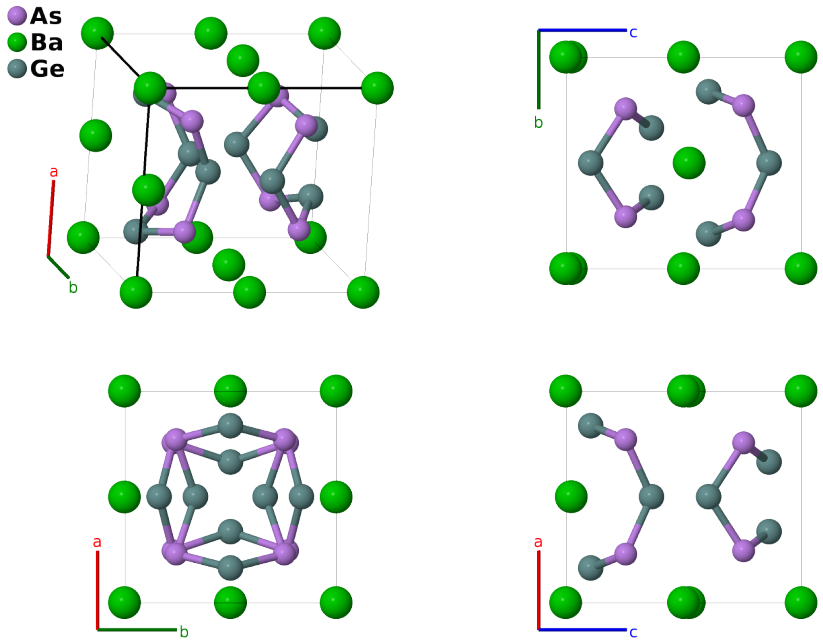
https://aflow.org/p/W96U

https://aflow.org/p/A2BC2_tP20_105_f_bc_2d-001




| | |
|---|---|
| **Prototype** | $As_2BaGe_2$ |
| **AFLOW prototype label** | A2BC2_tP20_105_f_bc_2d-001 |
| **ICSD** | 26417 |
| **Pearson symbol** | tP20 |
| **Space group number** | 105 |
| **Space group symbol** | $P4_2mc$ |
| **AFLOW prototype command** | `aflow --proto=A2BC2_tP20_105_f_bc_2d-001 --params=`$a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$ |

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**Other compounds with this structure**
$BaGe_2P_2$

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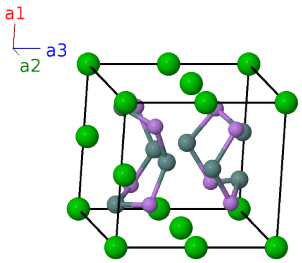
- Our previous listing of this structure (Hicks, 2017) misplaced the $z$ coordinates of the Ba II and Ge II atoms by $c/2$. We have corrected this here.
- Space group $P4_2mc$ #105 allows an arbitary placement of the origin of the $z$-axis. Here we use this freedom to set $z_1 = 0$ for the Ba-I atoms.

## Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (2b) | Ba I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4d) | Ge I |
| $\mathbf{B_8}$ | = | $-x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{11}}$ | = | $x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4d) | Ge II |
| $\mathbf{B_{12}}$ | = | $-x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{15}}$ | = | $-y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8f) | As I |
| $\mathbf{B_{16}}$ | = | $y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{19}}$ | = | $-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8f) | As I |
| $\mathbf{B_{20}}$ | = | $y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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.

**Found in**

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