

# BaAs<sub>2</sub> Structure:

## A2B\_mP18\_7\_6a\_3a-001

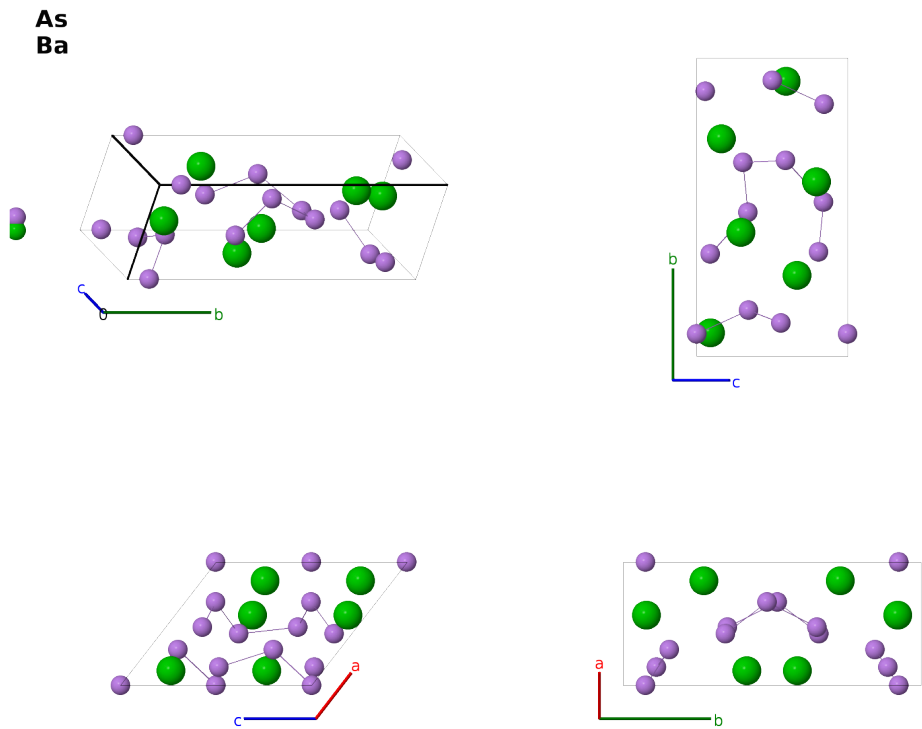
This structure previously used the label(s) **A2B\_mP18\_7\_6a\_3a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/34FL>

[https://aflow.org/prototype-encyclopedia/A2B\\_mP18\\_7\\_6a\\_3a-001](https://aflow.org/prototype-encyclopedia/A2B_mP18_7_6a_3a-001)



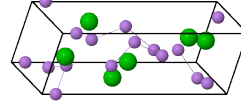
|                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | As <sub>2</sub> Ba                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| AFLOW prototype label   | A2B_mP18_7_6a_3a-001                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| ICSD                    | 414139                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| CCDC                    | 1728899                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| Pearson symbol          | mP18                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| Space group number      | 7                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| Space group symbol      | <i>Pc</i>                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| AFLOW prototype command | <pre>aflow --proto=A2B_mP18_7_6a_3a-001 --params=a,b/a,c/a,β,x<sub>1</sub>,y<sub>1</sub>,z<sub>1</sub>,x<sub>2</sub>,y<sub>2</sub>,z<sub>2</sub>,x<sub>3</sub>,y<sub>3</sub>,z<sub>3</sub>,x<sub>4</sub>,y<sub>4</sub>,z<sub>4</sub>,x<sub>5</sub>,y<sub>5</sub>,z<sub>5</sub>,x<sub>6</sub>,y<sub>6</sub>,z<sub>6</sub>,x<sub>7</sub>, y<sub>7</sub>,z<sub>7</sub>,x<sub>8</sub>,y<sub>8</sub>,z<sub>8</sub>,x<sub>9</sub>,y<sub>9</sub>,z<sub>9</sub></pre> |

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## Simple Monoclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
 \end{aligned}$$

$\mathbf{a}_3$   $\mathbf{a}_1$   $\mathbf{a}_2$




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## Basis vectors

|                   | Lattice<br>coordinates                                                   |   | Cartesian<br>coordinates                                                                                                               | Wyckoff<br>position | Atom<br>type |
|-------------------|--------------------------------------------------------------------------|---|----------------------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$                 | = | $(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | As I         |
| $\mathbf{B}_2$    | $x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | As I         |
| $\mathbf{B}_3$    | $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$                 | = | $(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | As II        |
| $\mathbf{B}_4$    | $x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | As II        |
| $\mathbf{B}_5$    | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                 | = | $(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | As III       |
| $\mathbf{B}_6$    | $x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | As III       |
| $\mathbf{B}_7$    | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$                 | = | $(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | As IV        |
| $\mathbf{B}_8$    | $x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | As IV        |
| $\mathbf{B}_9$    | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$                 | = | $(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | As V         |
| $\mathbf{B}_{10}$ | $x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | As V         |
| $\mathbf{B}_{11}$ | $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$                 | = | $(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | As VI        |
| $\mathbf{B}_{12}$ | $x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | As VI        |
| $\mathbf{B}_{13}$ | $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$                 | = | $(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | Ba I         |
| $\mathbf{B}_{14}$ | $x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | Ba I         |
| $\mathbf{B}_{15}$ | $x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$                 | = | $(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | Ba II        |
| $\mathbf{B}_{16}$ | $x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | Ba II        |
| $\mathbf{B}_{17}$ | $x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$                 | = | $(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$                                 | (2a)                | Ba III       |
| $\mathbf{B}_{18}$ | $x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$ | = | $(ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (2a)                | Ba III       |

## References

- [1] F. Emmerling, D. Petri, and C. Röhr, *Neue Arsenide mit  $As^-$ -Ketten und -Ringene:  $BaAs_2$  und  $A^I Ba_2As_5$  ( $A^I = K, Rb$ )*, Z. Anorganische und Allgemeine Chemie **630**, 2490–2501 (2004), doi:10.1002/zaac.200400257.

## Found in

- [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