

AsK₃S₄ Structure:

AB3C4_oP32_33_a_3a_4a-001

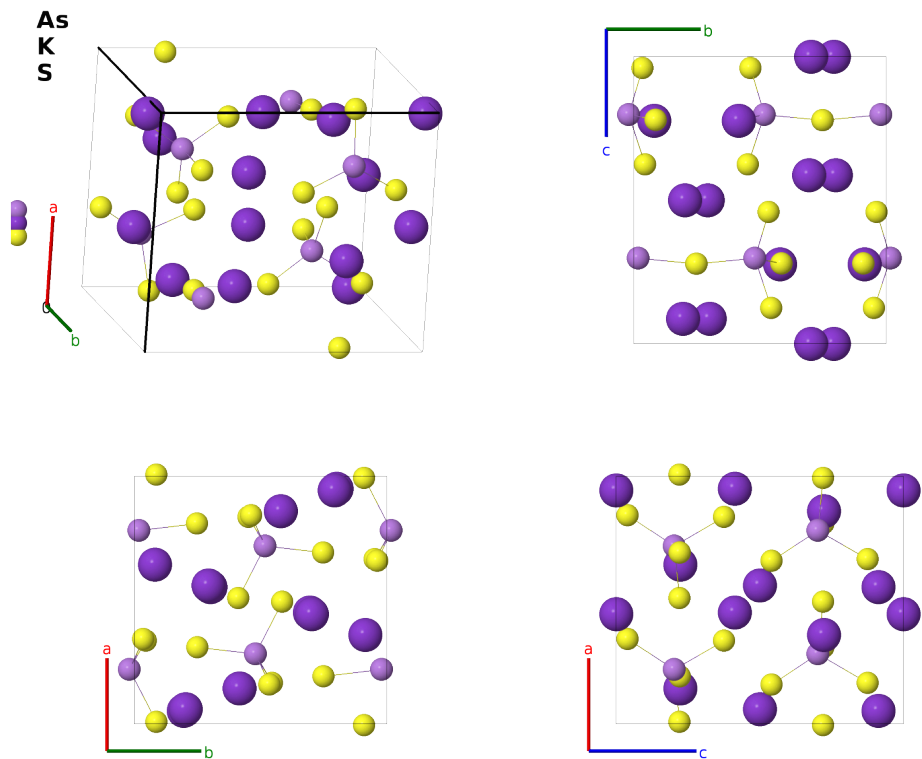
This structure previously used the label(s) **AB3C4_oP32_33_a_3a_4a**. Calls to these addresses will be redirected here.

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/H422>

https://aflow.org/prototype-encyclopedia/AB3C4_oP32_33_a_3a_4a-001



Prototype	AsK ₃ S ₄
AFLOW prototype label	AB3C4_oP32_33_a_3a_4a-001
ICSD	2314
CCDC	1592221
Pearson symbol	oP32
Space group number	33
Space group symbol	<i>Pna</i> 2 ₁
AFLOW prototype command	<pre>aflow --proto=AB3C4_oP32_33_a_3a_4a-001 --params=a, b/a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</pre>

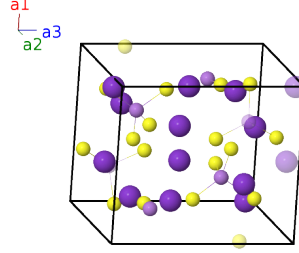
- Space group $Pna2_1$ #33 allows an arbitrary origin for the z -axis, which is set here by taking $z_2 = 1/4$.

Simple Orthorhombic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	$(4a)$		As I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		As I
$\mathbf{B}_3$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	$(4a)$		As I
$\mathbf{B}_4$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		As I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	$(4a)$		K I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		K I
$\mathbf{B}_7$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	$(4a)$		K I
$\mathbf{B}_8$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		K I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	$(4a)$		K II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		K II
$\mathbf{B}_{11}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	$(4a)$		K II
$\mathbf{B}_{12}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		K II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	$(4a)$		K III
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		K III
$\mathbf{B}_{15}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	$(4a)$		K III
$\mathbf{B}_{16}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		K III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	$(4a)$		S I
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		S I
$\mathbf{B}_{19}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	$(4a)$		S I
$\mathbf{B}_{20}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		S I
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	$(4a)$		S II
$\mathbf{B}_{22}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	$(4a)$		S II

$$\begin{aligned}
\mathbf{B}_{23} &= (x_6 + \tfrac{1}{2}) \mathbf{a}_1 - (y_6 - \tfrac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 = a(x_6 + \tfrac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \tfrac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{24} &= -(x_6 - \tfrac{1}{2}) \mathbf{a}_1 + (y_6 + \tfrac{1}{2}) \mathbf{a}_2 + (z_6 + \tfrac{1}{2}) \mathbf{a}_3 = -a(x_6 - \tfrac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \tfrac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \tfrac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (4a) & \text{S III} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \tfrac{1}{2}) \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \tfrac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{S III} \\
\mathbf{B}_{27} &= (x_7 + \tfrac{1}{2}) \mathbf{a}_1 - (y_7 - \tfrac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3 = a(x_7 + \tfrac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \tfrac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (4a) & \text{S III} \\
\mathbf{B}_{28} &= -(x_7 - \tfrac{1}{2}) \mathbf{a}_1 + (y_7 + \tfrac{1}{2}) \mathbf{a}_2 + (z_7 + \tfrac{1}{2}) \mathbf{a}_3 = -a(x_7 - \tfrac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \tfrac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \tfrac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{S III} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{S IV} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \tfrac{1}{2}) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \tfrac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{S IV} \\
\mathbf{B}_{31} &= (x_8 + \tfrac{1}{2}) \mathbf{a}_1 - (y_8 - \tfrac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3 = a(x_8 + \tfrac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \tfrac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{S IV} \\
\mathbf{B}_{32} &= -(x_8 - \tfrac{1}{2}) \mathbf{a}_1 + (y_8 + \tfrac{1}{2}) \mathbf{a}_2 + (z_8 + \tfrac{1}{2}) \mathbf{a}_3 = -a(x_8 - \tfrac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \tfrac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \tfrac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{S IV}
\end{aligned}$$

References

- [1] M. Palazzi, S. Jaulmes, and P. Laruelle, *Structure cristalline de K_3AsS_4* , Acta Crystallogr. Sect. B **30**, 2378–2381 (1974), doi:10.1107/S0567740874007151.

Found in

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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