

Sr₂As₂O₇ Structure:

A2B7C2_tP88_78_4a_14a_4a-001

This structure previously used the label(s) **A2B7C2_tP88_78_4a_14a_4a**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B7C2_tP88_78_4a_14a_4a-001

Prototype	As ₂ O ₇ Sr ₂
AFLOW prototype label	A2B7C2_tP88_78_4a_14a_4a-001
ICSD	190008
CCDC	972785
Pearson symbol	tP88
Space group number	78
Space group symbol	<i>P</i> 4 ₃
AFLOW prototype command	<pre>aflow --proto=A2B7C2_tP88_78_4a_14a_4a-001 --params=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, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃, x₁₄, y₁₄, z₁₄, x₁₅, y₁₅, z₁₅, x₁₆, y₁₆, z₁₆, x₁₇, y₁₇, z₁₇, x₁₈, y₁₈, z₁₈, x₁₉, y₁₉, z₁₉, x₂₀, y₂₀, z₂₀, x₂₁, y₂₁, z₂₁, x₂₂, y₂₂, z₂₂</pre>

- This structure may also be found in the enantiomorphic space group *P*4₁ #76.

Simple Tetragonal primitive vectors

a₁

a₂

a₃

$\hat{x}$

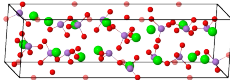
$\hat{y}$

$\hat{z}$

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	=	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{x} + ay_1 \hat{y} + cz_1 \hat{z}$	(4a) As I

$$\begin{aligned}
\mathbf{B}_{84} &= y_{21} \mathbf{a}_1 - x_{21} \mathbf{a}_2 + \left(z_{21} + \frac{1}{4}\right) \mathbf{a}_3 &= ay_{21} \hat{\mathbf{x}} - ax_{21} \hat{\mathbf{y}} + c \left(z_{21} + \frac{1}{4}\right) \hat{\mathbf{z}} &(4a) &\text{Sr III} \\
\mathbf{B}_{85} &= x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= ax_{22} \hat{\mathbf{x}} + ay_{22} \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}} &(4a) &\text{Sr IV} \\
\mathbf{B}_{86} &= -x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + \left(z_{22} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{22} \hat{\mathbf{x}} - ay_{22} \hat{\mathbf{y}} + c \left(z_{22} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\text{Sr IV} \\
\mathbf{B}_{87} &= -y_{22} \mathbf{a}_1 + x_{22} \mathbf{a}_2 + \left(z_{22} + \frac{3}{4}\right) \mathbf{a}_3 &= -ay_{22} \hat{\mathbf{x}} + ax_{22} \hat{\mathbf{y}} + c \left(z_{22} + \frac{3}{4}\right) \hat{\mathbf{z}} &(4a) &\text{Sr IV} \\
\mathbf{B}_{88} &= y_{22} \mathbf{a}_1 - x_{22} \mathbf{a}_2 + \left(z_{22} + \frac{1}{4}\right) \mathbf{a}_3 &= ay_{22} \hat{\mathbf{x}} - ax_{22} \hat{\mathbf{y}} + c \left(z_{22} + \frac{1}{4}\right) \hat{\mathbf{z}} &(4a) &\text{Sr IV}
\end{aligned}$$

References

- [1] A. Mbarek and F. Edhokkar, *The $P4_3$ enantiomorph of $\text{Sr}_2\text{As}_2\text{O}_7$* , Acta Crystallogr. Sect. E **69**, i84 (2013), doi:10.1107/S1600536813031619.

Found in

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

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As
O
Sr

