

Sr₂As₂O₇ Structure: A2B7C2_tP88_78_4a_14a_4a-001

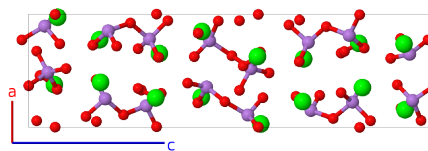
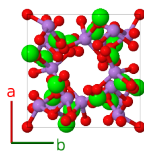
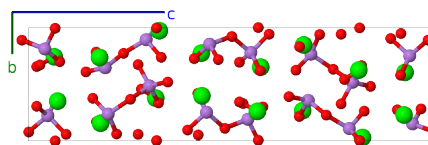
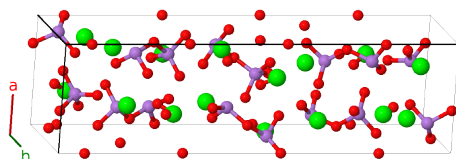
This structure originally had the label A2B7C2_tP88_78_4a_14a_4a. Calls to that address will be redirected here.

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<https://aflow.org/p/SCRS>

https://aflow.org/p/A2B7C2_tP88_78_4a_14a_4a-001

● As
● O
● Sr

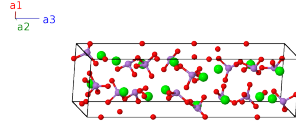


Prototype	As ₂ O ₇ Sr ₂
AFLOW prototype label	A2B7C2_tP88_78_4a_14a_4a-001
ICSD	190008
Pearson symbol	tP88
Space group number	78
Space group symbol	<i>P</i> 4 ₃
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- This structure may also be found in the enantiomorphic space group *P*4₁ #76.

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	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	As I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	As I
\mathbf{B}_3	$= -y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	As I
\mathbf{B}_4	$= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	As I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	As II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	As II
\mathbf{B}_7	$= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	As II
\mathbf{B}_8	$= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	As II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	As III
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	As III
\mathbf{B}_{11}	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	As III
\mathbf{B}_{12}	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	As III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	As IV
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	As IV
\mathbf{B}_{15}	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	As IV
\mathbf{B}_{16}	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	As IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{18}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{19}	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{20}	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{22}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{23}	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{24}	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{26}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{27}	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{28}	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{29}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{30}	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{31}	$= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + (z_8 + \frac{3}{4}) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{32}	$= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{33}	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4a)	O V
\mathbf{B}_{34}	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O V

$$\begin{aligned}
\mathbf{B}_{76} &= y_{19} \mathbf{a}_1 - x_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{4}\right) \mathbf{a}_3 &= ay_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{4}\right) \hat{\mathbf{z}} & (4a) & \text{Sr I} \\
\mathbf{B}_{77} &= x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (4a) & \text{Sr II} \\
\mathbf{B}_{78} &= -x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{Sr II} \\
\mathbf{B}_{79} &= -y_{20} \mathbf{a}_1 + x_{20} \mathbf{a}_2 + \left(z_{20} + \frac{3}{4}\right) \mathbf{a}_3 &= -ay_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{3}{4}\right) \hat{\mathbf{z}} & (4a) & \text{Sr II} \\
\mathbf{B}_{80} &= y_{20} \mathbf{a}_1 - x_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{4}\right) \mathbf{a}_3 &= ay_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{4}\right) \hat{\mathbf{z}} & (4a) & \text{Sr II} \\
\mathbf{B}_{81} &= x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3 &= ax_{21} \hat{\mathbf{x}} + ay_{21} \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}} & (4a) & \text{Sr III} \\
\mathbf{B}_{82} &= -x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 + \left(z_{21} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{21} \hat{\mathbf{x}} - ay_{21} \hat{\mathbf{y}} + c \left(z_{21} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{Sr III} \\
\mathbf{B}_{83} &= -y_{21} \mathbf{a}_1 + x_{21} \mathbf{a}_2 + \left(z_{21} + \frac{3}{4}\right) \mathbf{a}_3 &= -ay_{21} \hat{\mathbf{x}} + ax_{21} \hat{\mathbf{y}} + c \left(z_{21} + \frac{3}{4}\right) \hat{\mathbf{z}} & (4a) & \text{Sr III} \\
\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 $Sr_2As_2O_7$* , 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.