

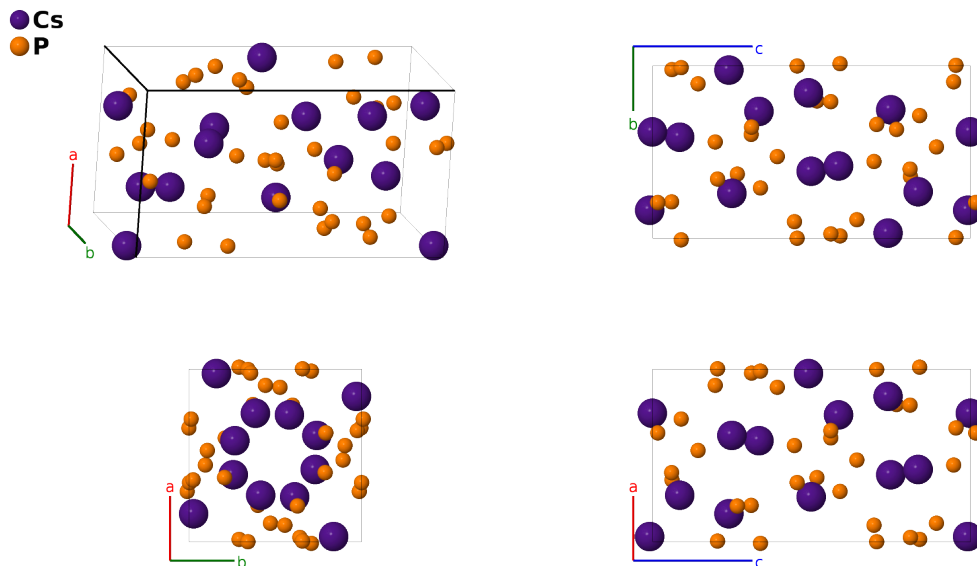
Cs₃P₇ Structure: A3B7_tP40_76_3a_7a-001

This structure originally had the label A3B7_tP40_76_3a_7a. Calls to that address will be redirected here.

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

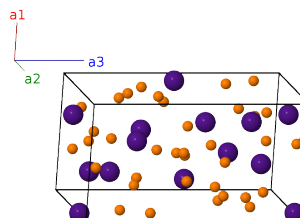
https://aflow.org/p/A3B7_tP40_76_3a_7a-001



Prototype	Cs ₃ P ₇
AFLOW prototype label	A3B7_tP40_76_3a_7a-001
ICSD	62259
Pearson symbol	tP40
Space group number	76
Space group symbol	$P4_1$
AFLOW prototype command	aflow --proto=A3B7_tP40_76_3a_7a-001 --params=a, c/a, x ₁ , y ₁ , z ₁ , x ₂ , y ₂ , z ₂ , x ₃ , y ₃ , z ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= a \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$



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)	Cs 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)	Cs I
\mathbf{B}_3	$= -y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	Cs I
\mathbf{B}_4	$= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	Cs 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)	Cs 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)	Cs II
\mathbf{B}_7	$= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	Cs II
\mathbf{B}_8	$= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	Cs 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)	Cs 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)	Cs III
\mathbf{B}_{11}	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	Cs III
\mathbf{B}_{12}	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	Cs 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)	P I
\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)	P I
\mathbf{B}_{15}	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	P I
\mathbf{B}_{16}	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	P I
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	P II
\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)	P II
\mathbf{B}_{19}	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	P II
\mathbf{B}_{20}	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	P II
\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)	P III
\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)	P III
\mathbf{B}_{23}	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	P III
\mathbf{B}_{24}	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	P III
\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)	P IV
\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)	P IV
\mathbf{B}_{27}	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	P IV
\mathbf{B}_{28}	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	P IV
\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)	P V
\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)	P V
\mathbf{B}_{31}	$= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + (z_8 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	P V
\mathbf{B}_{32}	$= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	P V
\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)	P VI
\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)	P VI
\mathbf{B}_{35}	$= -y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + (z_9 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{4}) \hat{\mathbf{z}}$	(4a)	P VI
\mathbf{B}_{36}	$= y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + (z_9 + \frac{3}{4}) \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{3}{4}) \hat{\mathbf{z}}$	(4a)	P VI
\mathbf{B}_{37}	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4a)	P VII
\mathbf{B}_{38}	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	P VII

$$\mathbf{B}_{39} = -y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{4}\right) \mathbf{a}_3 = -ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}} \quad (4a) \quad \text{P VII}$$

$$\mathbf{B}_{40} = y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{3}{4}\right) \mathbf{a}_3 = ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{3}{4}\right) \hat{\mathbf{z}} \quad (4a) \quad \text{P VII}$$

References

- [1] T. Meyer, W. Höhle, and H. G. von Schnering, *Tricäsiumheptaphosphid Cs₃P₇: Darstellung, Struktur und Eigenschaften*, *Z. Anorganische und Allgemeine Chemie* **552**, 69–80 (1987), doi:10.1002/zaac.19875520907.

Found in

- [1] R. J. D. Tilley, *Crystals and Crystal Structures* (Wiley, Chichester, England, 2006), chap. 5, p. 102.