

Cs₃P₇ Structure: A3B7_tP40_76_3a_7a-001

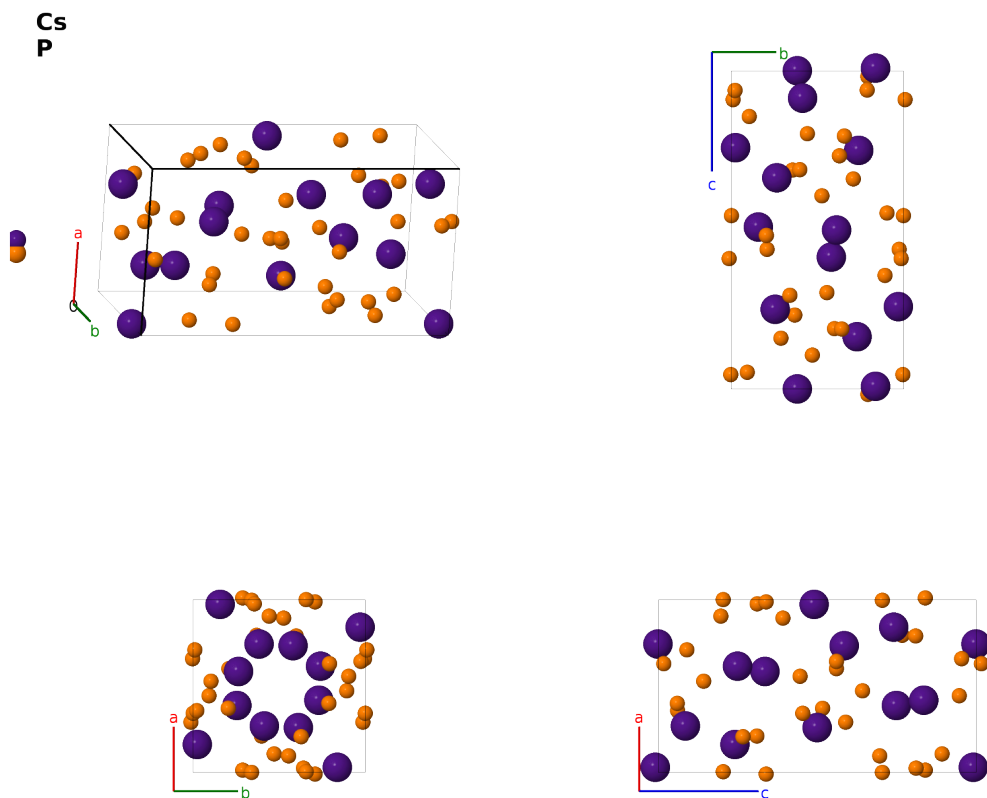
This structure previously used the label(s) **A3B7_tP40_76_3a_7a**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A3B7_tP40_76_3a_7a-001



Prototype	Cs ₃ P ₇
AFLOW prototype label	A3B7_tP40_76_3a_7a-001
ICSD	62259
CCDC	1625523
Pearson symbol	tP40
Space group number	76
Space group symbol	$P4_1$

$\mathbf{B}_{26}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B}_{27}$	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B}_{28}$	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(z_7 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{30}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	P V
$\mathbf{B}_{31}$	$= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	P V
$\mathbf{B}_{32}$	$= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(z_8 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{34}$	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	P VI
$\mathbf{B}_{35}$	$= -y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	P VI
$\mathbf{B}_{36}$	$= y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + \left(z_9 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{38}$	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	P VII
$\mathbf{B}_{39}$	$= -y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	P VII
$\mathbf{B}_{40}$	$= y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \left(z_{10} + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{3}{4}\right) \hat{\mathbf{z}}$	(4a)	P VII

References

- [1] T. Meyer, W. Hönlé, and H. G. von Schnering, *Tricäsiumheptaphosphid Cs_3P_7 : 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.

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