

Nb₈P₅ Structure:

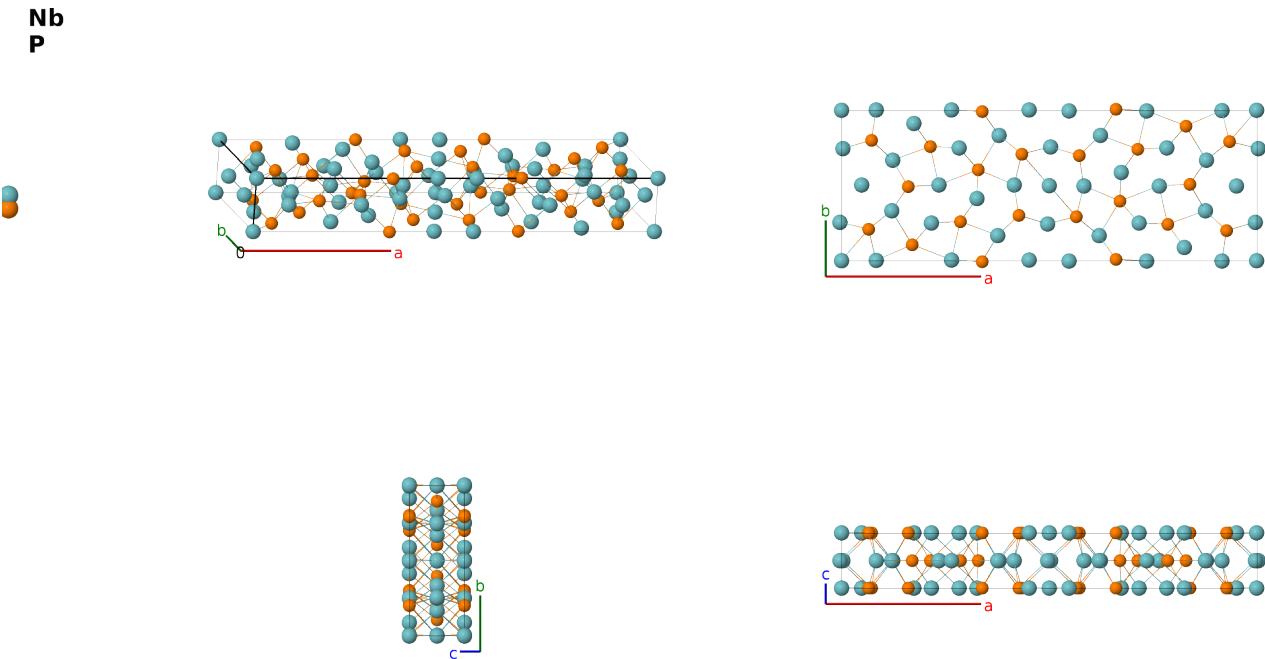
A17B10_oP54_55_a3g5h_3g2h-001

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/BWRM>

https://aflow.org/prototype-encyclopedia/A17B10_oP54_55_a3g5h_3g2h-001



Prototype	Nb ₈ P ₅
AFLOW prototype label	A17B10_oP54_55_a3g5h_3g2h-001
ICSD	15054
CCDC	1595837
Pearson symbol	oP54
Space group number	55
Space group symbol	<i>Pbam</i>
AFLOW prototype command	<pre>aflow --proto=A17B10_oP54_55_a3g5h_3g2h-001 --params=a,b/a,c/a,x₂,y₂,x₃,y₃,x₄,y₄,x₅,y₅,x₆,y₆,x₇,y₇,x₈,y₈,x₉,y₉,x₁₀,y₁₀,x₁₁, y₁₁,x₁₂,y₁₂,x₁₃,y₁₃,x₁₄,y₁₄</pre>

Other compounds with this structure

Zr₈As₅

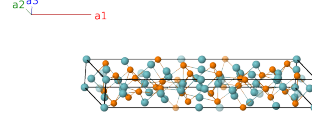
- The Nb-IV (4g) site is only occupied 50% of the time.

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
$\mathbf{B}_1$	$=$	0	$=$	0	Nb I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2a) Nb I
$\mathbf{B}_3$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g) Nb II
$\mathbf{B}_4$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g) Nb II
$\mathbf{B}_5$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Nb II
$\mathbf{B}_6$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Nb II
$\mathbf{B}_7$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g) Nb III
$\mathbf{B}_8$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g) Nb III
$\mathbf{B}_9$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Nb III
$\mathbf{B}_{10}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Nb III
$\mathbf{B}_{11}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g) Nb IV
$\mathbf{B}_{12}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g) Nb IV
$\mathbf{B}_{13}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Nb IV
$\mathbf{B}_{14}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Nb IV
$\mathbf{B}_{15}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(4g) P I
$\mathbf{B}_{16}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(4g) P I
$\mathbf{B}_{17}$	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) P I
$\mathbf{B}_{18}$	$=$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) P I
$\mathbf{B}_{19}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}}$	(4g) P II
$\mathbf{B}_{20}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}}$	(4g) P II
$\mathbf{B}_{21}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) P II
$\mathbf{B}_{22}$	$=$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) P II
$\mathbf{B}_{23}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}}$	(4g) P III
$\mathbf{B}_{24}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}}$	(4g) P III
$\mathbf{B}_{25}$	$=$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) P III
$\mathbf{B}_{26}$	$=$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) P III
$\mathbf{B}_{27}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Nb V
$\mathbf{B}_{28}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Nb V
$\mathbf{B}_{29}$	$=$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Nb V
$\mathbf{B}_{30}$	$=$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Nb V

$\mathbf{B}_{31}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VI
$\mathbf{B}_{32}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VI
$\mathbf{B}_{33}$	$=$	$-\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VI
$\mathbf{B}_{34}$	$=$	$\left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VI
$\mathbf{B}_{35}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VII
$\mathbf{B}_{36}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VII
$\mathbf{B}_{37}$	$=$	$-\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VII
$\mathbf{B}_{38}$	$=$	$\left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VII
$\mathbf{B}_{39}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VIII
$\mathbf{B}_{40}$	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VIII
$\mathbf{B}_{41}$	$=$	$-\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VIII
$\mathbf{B}_{42}$	$=$	$\left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb VIII
$\mathbf{B}_{43}$	$=$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb IX
$\mathbf{B}_{44}$	$=$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb IX
$\mathbf{B}_{45}$	$=$	$-\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb IX
$\mathbf{B}_{46}$	$=$	$\left(x_{12} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_{12} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Nb IX
$\mathbf{B}_{47}$	$=$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P IV
$\mathbf{B}_{48}$	$=$	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P IV
$\mathbf{B}_{49}$	$=$	$-\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P IV
$\mathbf{B}_{50}$	$=$	$\left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P IV
$\mathbf{B}_{51}$	$=$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P V
$\mathbf{B}_{52}$	$=$	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P V
$\mathbf{B}_{53}$	$=$	$-\left(x_{14} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_{14} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P V
$\mathbf{B}_{54}$	$=$	$\left(x_{14} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{14} - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_{14} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	P V

References

- [1] S. Anugul, C.-O. Pontchour, and S. Rundqvist, *The Crystal Structure of Nb₈P₅*, Acta Chem. Scand. **27**, 26–34 (1973), doi:10.3891/acta.chem.scand.27-0026.

First cited in

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.