Nb_8P_5 Structure: A17B10_oP54_55_a3g5h_3g2h-001

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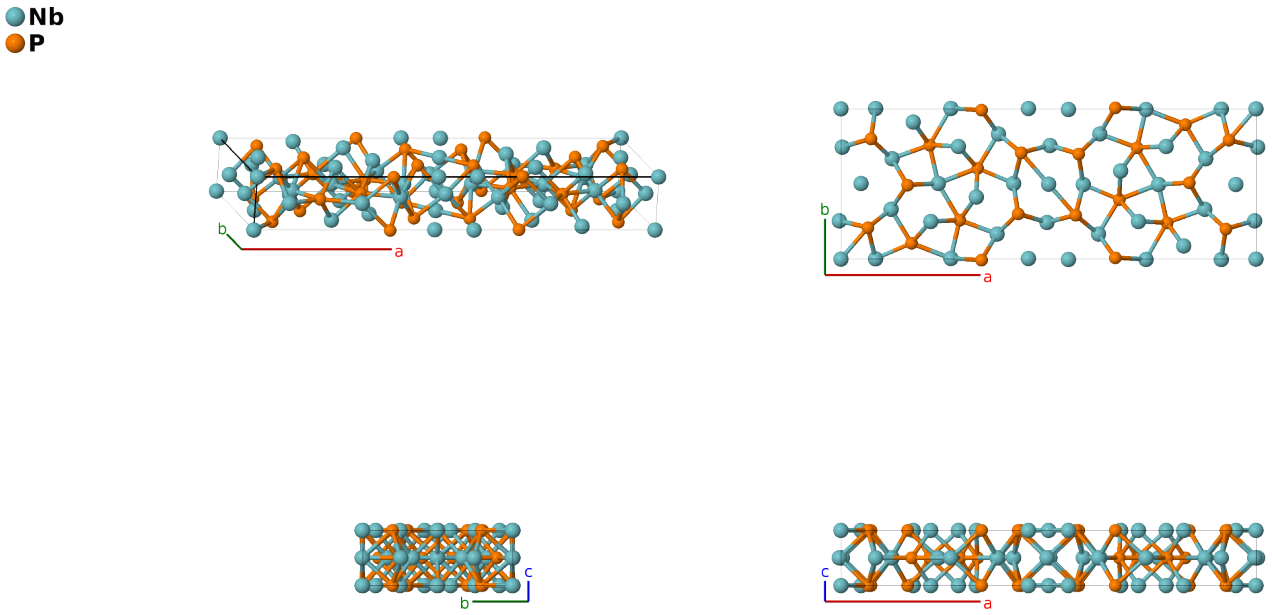
https://aflow.org/p/A17B10_oP54_55_a3g5h_3g2h-001



Prototype	Nb_8P_5
AFLOW prototype label	A17B10_oP54_55_a3g5h_3g2h-001
ICSD	15054
Pearson symbol	oP54
Space group number	55
Space group symbol	*Pbam*
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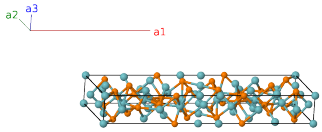
Other compounds with this structure
Zr_8As_5

- 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	(2a)	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
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Nb II
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(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
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Nb III
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{13}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Nb IV
$\mathbf{B_{14}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{17}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	P I
$\mathbf{B_{18}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{21}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	P II
$\mathbf{B_{22}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{25}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	P III
$\mathbf{B_{26}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{29}}$	=	$-\left(x_8 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Nb V
$\mathbf{B_{30}}$	=	$\left(x_8 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_8 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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 Nb_8P_5*, Acta Chem. Scand. **27**, 26–34 (1973), doi:10.3891/acta.chem.scand.27-0026.