Lead Apatite [$Pb_{10}(PO_4)_6O$] Structure: A14B3C5_hP44_176_e2hi_h_fh-001

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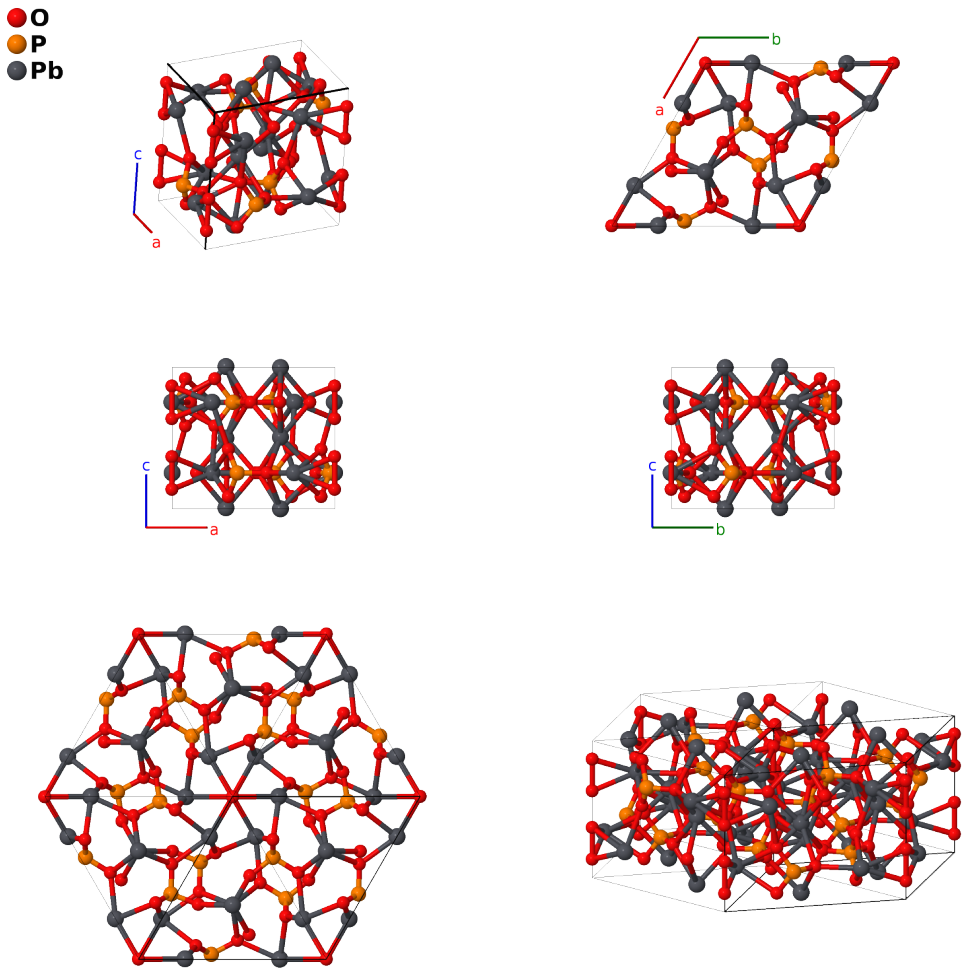
https://aflow.org/p/4302

https://aflow.org/p/A14B3C5_hP44_176_e2hi_h_fh-001



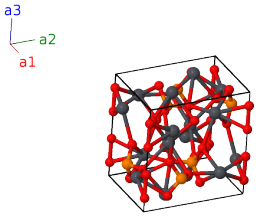
Prototype	$O_{25}P_6Pb_{10}$
AFLOW prototype label	A14B3C5_hP44_176_e2hi_h_fh-001
ICSD	9870
Pearson symbol	hP44
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	`aflow --proto=A14B3C5_hP44_176_e2hi_h_fh-001 --params=`$a, c/a, z_1, z_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, z_7$

Other compounds with this structure
$Pb_3(PO_4O)_2$, $Sr_5(PO_4O)_3(OH)_{1-x}$

- The apatites have similar structures differing in the details.
- In this structure $[Pb_{10}(PO_4)_6O]$ only 1/4 of the O-I (4e) sites are occupied.
- In $Pb_3(PO_4O)_2$ (Hata, 1980) the (4e) site is not occupied, and only 3/4 of the Pb-I (4f) sites are filled.
- In fluorapatite ($Ca_5(PO_4)_3F$, $H5_7$) calcium replaces the lead atoms and the partially filled O-I (4e) site is replace by filled fluorine (2a) (0,0,1/4).

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_4}$	=	$-\left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4f)	Pb I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Pb I
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(4f)	Pb I
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Pb I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{10}}$	=	$-y_3\,\mathbf{a}_1+(x_3-y_3)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{11}}$	=	$-(x_3-y_3)\,\mathbf{a}_1-x_3\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1-(x_3-y_3)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{14}}$	=	$(x_3-y_3)\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{16}}$	=	$-y_4\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{17}}$	=	$-(x_4-y_4)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{19}}$	=	$y_4\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{20}}$	=	$(x_4-y_4)\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O III
$\mathbf{B_{21}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	P I

$\mathbf{B_{22}}$	$= -y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{23}}$	$= -(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{24}}$	$= -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{25}}$	$= y_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{26}}$	$= (x_5 - y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{27}}$	$= x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Pb II
$\mathbf{B_{28}}$	$= -y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Pb II
$\mathbf{B_{29}}$	$= -(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Pb II
$\mathbf{B_{30}}$	$= -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Pb II
$\mathbf{B_{31}}$	$= y_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Pb II
$\mathbf{B_{32}}$	$= (x_6 - y_6)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Pb II
$\mathbf{B_{33}}$	$= x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{34}}$	$= -y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{35}}$	$= -(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{36}}$	$= -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{37}}$	$= y_7\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7 + 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{38}}$	$= (x_7 - y_7)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{39}}$	$= -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{40}}$	$= y_7\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7 + 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{41}}$	$= (x_7 - y_7)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{42}}$	$= x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{43}}$	$= -y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{44}}$	$= -(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV

References

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[2] M. Hata, F. Marumo, S.-I. Iwai, and H. Aoki, *Structure of a lead apatite $Pb_9(PO_4)_6$*, Acta Crystallogr. Sect. B **36**, 2128–2130 (1980), doi:10.1107/S0567740880008096.

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