Fluorapatite [$Ca_5F(PO_4)_3$, $H5_7$] Structure: A5BC12D3_hP42_176_fh_a_2hi_h-001

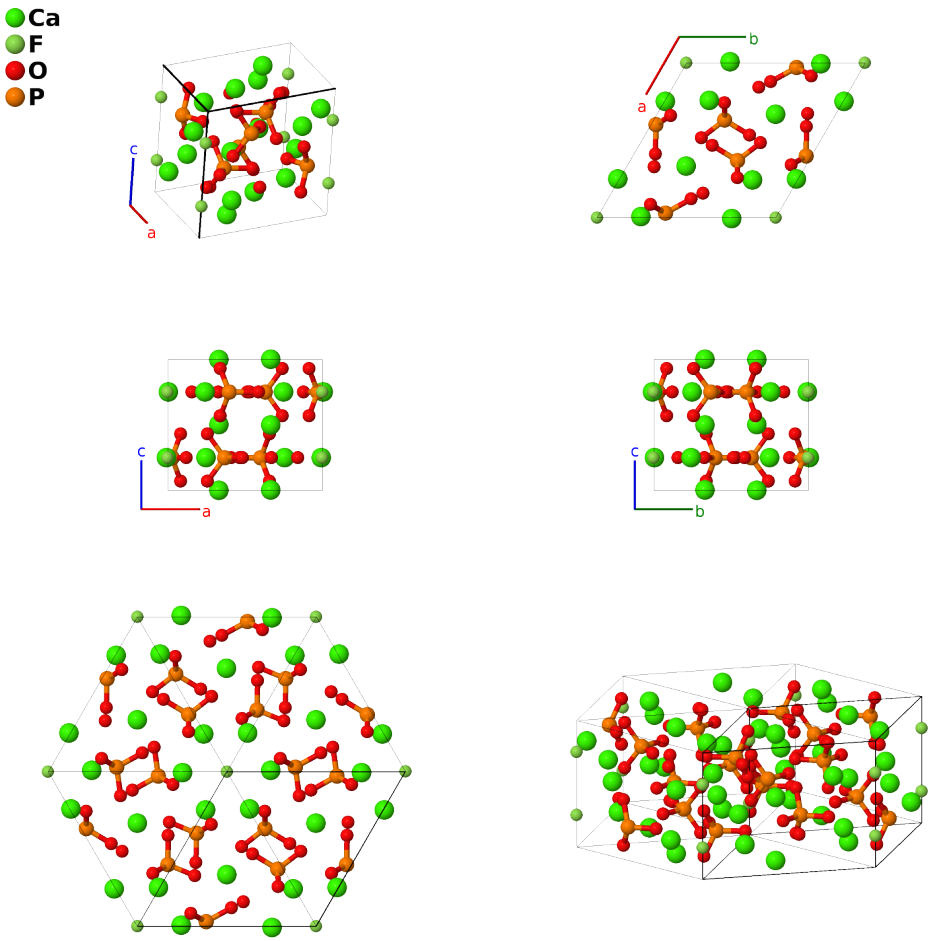
This structure originally had the label `A5BC12D3_hP42_176_fh_a_2hi_h`. Calls to that address will be redirected here.

Cite this page as: 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/p/KHCK

https://aflow.org/p/A5BC12D3_hP42_176_fh_a_2hi_h-001



Prototype	$Ca_5FO_{12}P$
AFLOW prototype label	A5BC12D3_hP42_176_fh_a_2hi_h-001
***Strukturbericht* designation**	$H5_7$
Mineral name	fluorapatite
ICSD	137670
Pearson symbol	hP42
Space group number	176
Space group symbol	$P6_3/m$

AFLOW prototype command `aflow --proto=A5BC12D3_hP42_176_fh_a_2hi_h-001 --params=`$a, c/a, z_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, z_7$

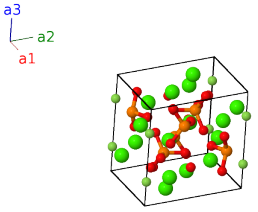
Other compounds with this structure

$Ca_5OH(PO_4)_3$ (hydroxylapatite), $Ca_5Cl(PO_4)_3$ (chlorapatite), $Ca_5F(SiO_4)_3$, $Eu_5F(SiO_4)_3$, $CaDy_4(SiO_4)_3O$, $CaEr_4(SiO_4)_3O$, $CaNd_4(SiO_4)_3O$, $CaGd_4(SiO_4)_3O$, $CaSm_4(SiO_4)_3O$, $CaY_4(SiO_4)_3O$, $CaYb_4(SiO_4)_3O$

- Apatite can be formed with most M^{+2} metallic ions replacing the calcium, and many ions (AsO_3. CO_3, Si_3, *etc.*) replacing the phosphate. While these structures are related to the prototype, they may have slight changes in crystal structure. The phosphate apatites are the main source of phosphorus on Earth. (Hughes, 2002)
- When OH or Cl replaces F, that ion is displaced from the (1a) position to the (4e) position, with $z = 0.1979$ for OH and 0.4323 for Cl. The substitute ion fills half of the (4f) sites.
- In the calcium-rare earth oxides, the extra oxygen atom is on the (2a) site, one of the rare-earth atoms is mixed with calcium on the (4f) site, and the remainder of the rare-earths replace silicon on that (6h) site.
- Other apatite configurations are discussed on the lead apatite page.
- There is no ICSD or CCDC entry for (Hughes, 2002). Fortunately (Hazrah, 2022) study a large number of apatites from a variety of sources. Their ICSD entry 137670 closely matches the structure found by (Hughes, 2002).

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

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

$\mathbf{B_{16}}$	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_4+y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4-y_4)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{17}}$	$y_4\,\mathbf{a}_1 - (x_4-y_4)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_4+2y_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{18}}$	$(x_4-y_4)\;\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_4-y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{19}}$	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_5+y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5-y_5)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{20}}$	$-y_5\,\mathbf{a}_1 + (x_5-y_5)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_5-2y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{21}}$	$-(x_5-y_5)\;\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_5-y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{22}}$	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5+y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5-y_5)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{23}}$	$y_5\,\mathbf{a}_1 - (x_5-y_5)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_5+2y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{24}}$	$(x_5-y_5)\;\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_5-y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{25}}$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{26}}$	$-y_6\,\mathbf{a}_1 + (x_6-y_6)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6-2y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{27}}$	$-(x_6-y_6)\;\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{28}}$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{29}}$	$y_6\,\mathbf{a}_1 - (x_6-y_6)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_6+2y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{30}}$	$(x_6-y_6)\;\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_{31}}$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{32}}$	$-y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{33}}$	$-(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{34}}$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\;\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{35}}$	$y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\;\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{36}}$	$(x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\;\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{37}}$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{38}}$	$y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{39}}$	$(x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{40}}$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7-\frac{1}{2}\right)\;\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} - c\left(z_7-\frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{41}}$	$-y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 - \left(z_7-\frac{1}{2}\right)\;\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - c\left(z_7-\frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III
$\mathbf{B_{42}}$	$-(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 - \left(z_7-\frac{1}{2}\right)\;\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - c\left(z_7-\frac{1}{2}\right)\;\hat{\mathbf{z}}$	(12i)	O III

References

[1] J. M. Hughes and J. Rakovan, *The Crystal Structure of Apatite, $Ca_5(PO_4)_3(F,OH,Cl)$*, Reviews in Mineralogy and Geochemistry **48**, 1–12 (2002), doi:10.2138/rmg.2002.48.1.

[2] K. S. H. and S. M. Antao, *Apatite, $Ca_{10}(PO_4)_6(OH,F,Cl)_2$: Structural Variations, Natural Solid Solutions, Intergrowths, and Zoning*, Minerals **12**, 527 (2022), doi:10.3390/min12050527.