$Ag_3(PO_4)$ ($H2_1$) Structure: A3B4C_cP16_218_c_e_a-001

This structure originally had the label `A3B4C_cP16_218_c_e_a`. Calls to that address will be redirected here.

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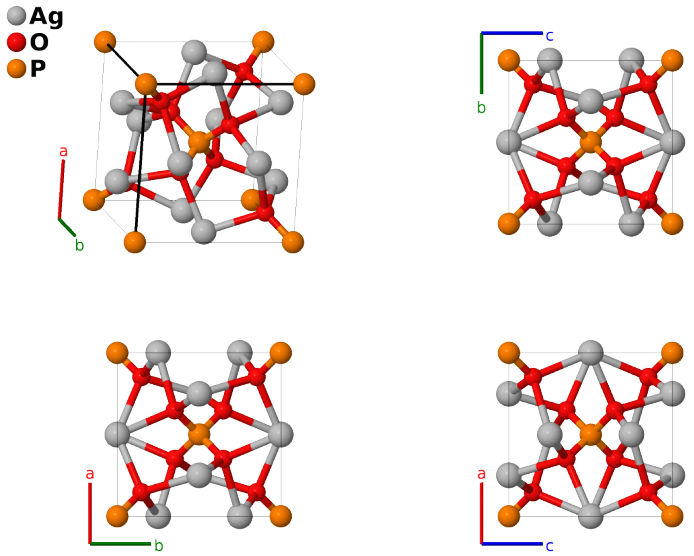
https://aflow.org/p/X143

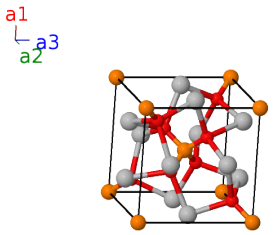
https://aflow.org/p/A3B4C_cP16_218_c_e_a-001



Prototype	Ag_3O_4P
AFLOW prototype label	A3B4C_cP16_218_c_e_a-001
***Strukturbericht* designation**	$H2_1$
ICSD	14000
Pearson symbol	cP16
Space group number	218
Space group symbol	$P\bar{4}3n$
AFLOW prototype command	`aflow --proto=A3B4C_cP16_218_c_e_a-001 --params=`a, x_3

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	P I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(6c)	Ag I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(6c)	Ag I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Ag I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Ag I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6c)	Ag I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6c)	Ag I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{13}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{14}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{15}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{16}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	O I

References

[1] R. Masse, I. Tordjman, and A. Durif, *Affinement de la structure cristalline du monophosphate d'argent Ag_3PO_4. Existence d'dune forme haute témperature*, Z. Krystallogr. **144**, 76–81 (1976), doi:10.1524/zkri.1976.144.16.76.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.