

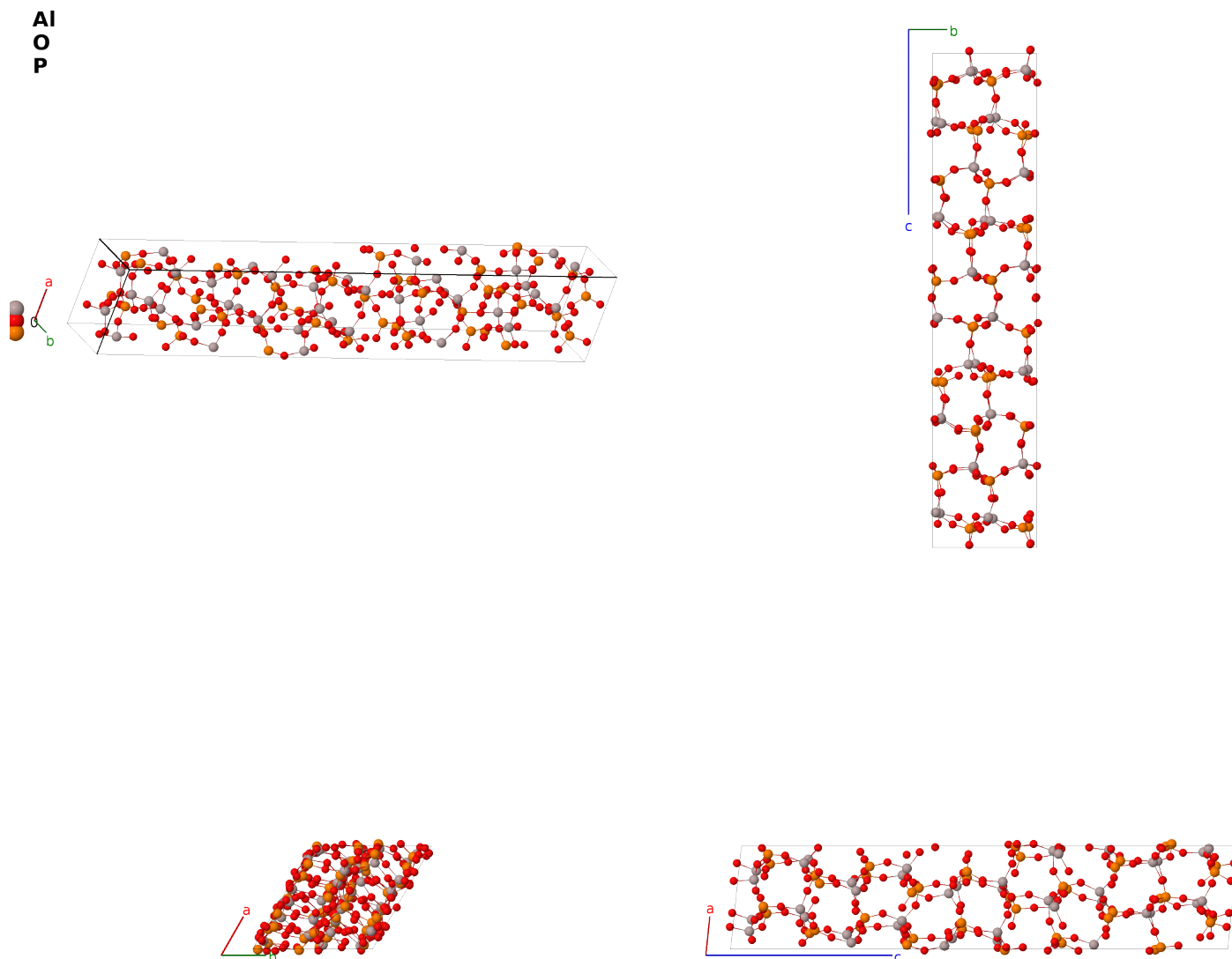
Triclinic tridymite (295K) AlPO_4 Structure: AB4C_aP240_1_40a_160a_40a-001

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/FWJQ>

https://aflow.org/prototype-encyclopedia/AB4C_aP240_1_40a_160a_40a-001



Prototype	AlO ₄ P
AFLOW prototype label	AB4C_aP240_1_40a_160a_40a-001
ICSD	280307
CCDC	1721023
Pearson symbol	aP240
Space group number	1
Space group symbol	<i>P</i> 1
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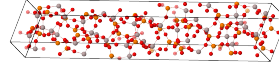
-
- The tridymite form of AlPO₄ is related to the tridymite forms of SiO₂. Like SiO₂ it undergoes a series of temperature driven phase transitions (Graetsch, 2002):
 - The high temperature form is hexagonal, space group *P*6₃*mc* #186 at temperatures above $\approx 590\text{K}$
 - The first intermediate form is monoclinic, space group *P*2₁ #4 at temperatures above $\approx 460\text{K}$

- The second intermediate form, $P2_1(\alpha/\beta)$, is incommensurate but averages to a structure similar to the previous one
- This is followed by an orthorhombic form, space group $P2_12_12_1$ #19, for which we have no data.
- Near room temperature we find another monoclinic structure, space group Pc #7
- The low temperature structure is triclinic, space group $P1$ #1 (this structure), also measured at room temperature.
- The astute reader will recognize that we are very vague about these phase transitions, as we have found no definitive phase diagram.
- For more information on related structures see our silica and aluminum phosphate page.
- Data for this structure was given in the $F1$ setting of space group #1. This gives a conventional unit cell which is four times larger than the primitive cell and is very close to an orthorhombic cell. We used AFLOW to convert this to the standard $P1$ setting, which produces a cell equivalent to the primitive unit cell in the $F1$ setting.

Triclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= a \hat{\mathbf{x}} \\
\mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
c_x &= c \cos \beta \\
c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}$$

$\hat{\mathbf{x}}$
 $\hat{\mathbf{y}}$
 $\hat{\mathbf{z}}$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(1a)	Al I
$\mathbf{B}_2$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(1a)	Al II
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(1a)	Al III
$\mathbf{B}_4$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(1a)	Al IV
$\mathbf{B}_5$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(1a)	Al V
$\mathbf{B}_6$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(1a)	Al VI
$\mathbf{B}_7$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(1a)	Al VII
$\mathbf{B}_8$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(1a)	Al VIII
$\mathbf{B}_9$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(1a)	Al IX
$\mathbf{B}_{10}$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(1a)	Al X

$\mathbf{B}_{59}$	$=$	$x_{59} \mathbf{a}_1 + y_{59} \mathbf{a}_2 + z_{59} \mathbf{a}_3$	$=$	$(ax_{59} + by_{59} \cos \gamma + c_x z_{59}) \hat{\mathbf{x}} + (by_{59} \sin \gamma + c_y z_{59}) \hat{\mathbf{y}} + c_z z_{59} \hat{\mathbf{z}}$	(1a)	O XIX
$\mathbf{B}_{60}$	$=$	$x_{60} \mathbf{a}_1 + y_{60} \mathbf{a}_2 + z_{60} \mathbf{a}_3$	$=$	$(ax_{60} + by_{60} \cos \gamma + c_x z_{60}) \hat{\mathbf{x}} + (by_{60} \sin \gamma + c_y z_{60}) \hat{\mathbf{y}} + c_z z_{60} \hat{\mathbf{z}}$	(1a)	O XX
$\mathbf{B}_{61}$	$=$	$x_{61} \mathbf{a}_1 + y_{61} \mathbf{a}_2 + z_{61} \mathbf{a}_3$	$=$	$(ax_{61} + by_{61} \cos \gamma + c_x z_{61}) \hat{\mathbf{x}} + (by_{61} \sin \gamma + c_y z_{61}) \hat{\mathbf{y}} + c_z z_{61} \hat{\mathbf{z}}$	(1a)	O XXI
$\mathbf{B}_{62}$	$=$	$x_{62} \mathbf{a}_1 + y_{62} \mathbf{a}_2 + z_{62} \mathbf{a}_3$	$=$	$(ax_{62} + by_{62} \cos \gamma + c_x z_{62}) \hat{\mathbf{x}} + (by_{62} \sin \gamma + c_y z_{62}) \hat{\mathbf{y}} + c_z z_{62} \hat{\mathbf{z}}$	(1a)	O XXII
$\mathbf{B}_{63}$	$=$	$x_{63} \mathbf{a}_1 + y_{63} \mathbf{a}_2 + z_{63} \mathbf{a}_3$	$=$	$(ax_{63} + by_{63} \cos \gamma + c_x z_{63}) \hat{\mathbf{x}} + (by_{63} \sin \gamma + c_y z_{63}) \hat{\mathbf{y}} + c_z z_{63} \hat{\mathbf{z}}$	(1a)	O XXIII
$\mathbf{B}_{64}$	$=$	$x_{64} \mathbf{a}_1 + y_{64} \mathbf{a}_2 + z_{64} \mathbf{a}_3$	$=$	$(ax_{64} + by_{64} \cos \gamma + c_x z_{64}) \hat{\mathbf{x}} + (by_{64} \sin \gamma + c_y z_{64}) \hat{\mathbf{y}} + c_z z_{64} \hat{\mathbf{z}}$	(1a)	O XXIV
$\mathbf{B}_{65}$	$=$	$x_{65} \mathbf{a}_1 + y_{65} \mathbf{a}_2 + z_{65} \mathbf{a}_3$	$=$	$(ax_{65} + by_{65} \cos \gamma + c_x z_{65}) \hat{\mathbf{x}} + (by_{65} \sin \gamma + c_y z_{65}) \hat{\mathbf{y}} + c_z z_{65} \hat{\mathbf{z}}$	(1a)	O XXV
$\mathbf{B}_{66}$	$=$	$x_{66} \mathbf{a}_1 + y_{66} \mathbf{a}_2 + z_{66} \mathbf{a}_3$	$=$	$(ax_{66} + by_{66} \cos \gamma + c_x z_{66}) \hat{\mathbf{x}} + (by_{66} \sin \gamma + c_y z_{66}) \hat{\mathbf{y}} + c_z z_{66} \hat{\mathbf{z}}$	(1a)	O XXVI
$\mathbf{B}_{67}$	$=$	$x_{67} \mathbf{a}_1 + y_{67} \mathbf{a}_2 + z_{67} \mathbf{a}_3$	$=$	$(ax_{67} + by_{67} \cos \gamma + c_x z_{67}) \hat{\mathbf{x}} + (by_{67} \sin \gamma + c_y z_{67}) \hat{\mathbf{y}} + c_z z_{67} \hat{\mathbf{z}}$	(1a)	O XXVII
$\mathbf{B}_{68}$	$=$	$x_{68} \mathbf{a}_1 + y_{68} \mathbf{a}_2 + z_{68} \mathbf{a}_3$	$=$	$(ax_{68} + by_{68} \cos \gamma + c_x z_{68}) \hat{\mathbf{x}} + (by_{68} \sin \gamma + c_y z_{68}) \hat{\mathbf{y}} + c_z z_{68} \hat{\mathbf{z}}$	(1a)	O XXVIII
$\mathbf{B}_{69}$	$=$	$x_{69} \mathbf{a}_1 + y_{69} \mathbf{a}_2 + z_{69} \mathbf{a}_3$	$=$	$(ax_{69} + by_{69} \cos \gamma + c_x z_{69}) \hat{\mathbf{x}} + (by_{69} \sin \gamma + c_y z_{69}) \hat{\mathbf{y}} + c_z z_{69} \hat{\mathbf{z}}$	(1a)	O XXIX
$\mathbf{B}_{70}$	$=$	$x_{70} \mathbf{a}_1 + y_{70} \mathbf{a}_2 + z_{70} \mathbf{a}_3$	$=$	$(ax_{70} + by_{70} \cos \gamma + c_x z_{70}) \hat{\mathbf{x}} + (by_{70} \sin \gamma + c_y z_{70}) \hat{\mathbf{y}} + c_z z_{70} \hat{\mathbf{z}}$	(1a)	O XXX
$\mathbf{B}_{71}$	$=$	$x_{71} \mathbf{a}_1 + y_{71} \mathbf{a}_2 + z_{71} \mathbf{a}_3$	$=$	$(ax_{71} + by_{71} \cos \gamma + c_x z_{71}) \hat{\mathbf{x}} + (by_{71} \sin \gamma + c_y z_{71}) \hat{\mathbf{y}} + c_z z_{71} \hat{\mathbf{z}}$	(1a)	O XXXI
$\mathbf{B}_{72}$	$=$	$x_{72} \mathbf{a}_1 + y_{72} \mathbf{a}_2 + z_{72} \mathbf{a}_3$	$=$	$(ax_{72} + by_{72} \cos \gamma + c_x z_{72}) \hat{\mathbf{x}} + (by_{72} \sin \gamma + c_y z_{72}) \hat{\mathbf{y}} + c_z z_{72} \hat{\mathbf{z}}$	(1a)	O XXXII
$\mathbf{B}_{73}$	$=$	$x_{73} \mathbf{a}_1 + y_{73} \mathbf{a}_2 + z_{73} \mathbf{a}_3$	$=$	$(ax_{73} + by_{73} \cos \gamma + c_x z_{73}) \hat{\mathbf{x}} + (by_{73} \sin \gamma + c_y z_{73}) \hat{\mathbf{y}} + c_z z_{73} \hat{\mathbf{z}}$	(1a)	O XXXIII
$\mathbf{B}_{74}$	$=$	$x_{74} \mathbf{a}_1 + y_{74} \mathbf{a}_2 + z_{74} \mathbf{a}_3$	$=$	$(ax_{74} + by_{74} \cos \gamma + c_x z_{74}) \hat{\mathbf{x}} + (by_{74} \sin \gamma + c_y z_{74}) \hat{\mathbf{y}} + c_z z_{74} \hat{\mathbf{z}}$	(1a)	O XXXIV
$\mathbf{B}_{75}$	$=$	$x_{75} \mathbf{a}_1 + y_{75} \mathbf{a}_2 + z_{75} \mathbf{a}_3$	$=$	$(ax_{75} + by_{75} \cos \gamma + c_x z_{75}) \hat{\mathbf{x}} + (by_{75} \sin \gamma + c_y z_{75}) \hat{\mathbf{y}} + c_z z_{75} \hat{\mathbf{z}}$	(1a)	O XXXV
$\mathbf{B}_{76}$	$=$	$x_{76} \mathbf{a}_1 + y_{76} \mathbf{a}_2 + z_{76} \mathbf{a}_3$	$=$	$(ax_{76} + by_{76} \cos \gamma + c_x z_{76}) \hat{\mathbf{x}} + (by_{76} \sin \gamma + c_y z_{76}) \hat{\mathbf{y}} + c_z z_{76} \hat{\mathbf{z}}$	(1a)	O XXXVI
$\mathbf{B}_{77}$	$=$	$x_{77} \mathbf{a}_1 + y_{77} \mathbf{a}_2 + z_{77} \mathbf{a}_3$	$=$	$(ax_{77} + by_{77} \cos \gamma + c_x z_{77}) \hat{\mathbf{x}} + (by_{77} \sin \gamma + c_y z_{77}) \hat{\mathbf{y}} + c_z z_{77} \hat{\mathbf{z}}$	(1a)	O XXXVII
$\mathbf{B}_{78}$	$=$	$x_{78} \mathbf{a}_1 + y_{78} \mathbf{a}_2 + z_{78} \mathbf{a}_3$	$=$	$(ax_{78} + by_{78} \cos \gamma + c_x z_{78}) \hat{\mathbf{x}} + (by_{78} \sin \gamma + c_y z_{78}) \hat{\mathbf{y}} + c_z z_{78} \hat{\mathbf{z}}$	(1a)	O XXXVIII
$\mathbf{B}_{79}$	$=$	$x_{79} \mathbf{a}_1 + y_{79} \mathbf{a}_2 + z_{79} \mathbf{a}_3$	$=$	$(ax_{79} + by_{79} \cos \gamma + c_x z_{79}) \hat{\mathbf{x}} + (by_{79} \sin \gamma + c_y z_{79}) \hat{\mathbf{y}} + c_z z_{79} \hat{\mathbf{z}}$	(1a)	O XXXIX
$\mathbf{B}_{80}$	$=$	$x_{80} \mathbf{a}_1 + y_{80} \mathbf{a}_2 + z_{80} \mathbf{a}_3$	$=$	$(ax_{80} + by_{80} \cos \gamma + c_x z_{80}) \hat{\mathbf{x}} + (by_{80} \sin \gamma + c_y z_{80}) \hat{\mathbf{y}} + c_z z_{80} \hat{\mathbf{z}}$	(1a)	O XL
$\mathbf{B}_{81}$	$=$	$x_{81} \mathbf{a}_1 + y_{81} \mathbf{a}_2 + z_{81} \mathbf{a}_3$	$=$	$(ax_{81} + by_{81} \cos \gamma + c_x z_{81}) \hat{\mathbf{x}} + (by_{81} \sin \gamma + c_y z_{81}) \hat{\mathbf{y}} + c_z z_{81} \hat{\mathbf{z}}$	(1a)	O XLI
$\mathbf{B}_{82}$	$=$	$x_{82} \mathbf{a}_1 + y_{82} \mathbf{a}_2 + z_{82} \mathbf{a}_3$	$=$	$(ax_{82} + by_{82} \cos \gamma + c_x z_{82}) \hat{\mathbf{x}} + (by_{82} \sin \gamma + c_y z_{82}) \hat{\mathbf{y}} + c_z z_{82} \hat{\mathbf{z}}$	(1a)	O XLII

$\mathbf{B}_{227} =$	$x_{227} \mathbf{a}_1 + y_{227} \mathbf{a}_2 + z_{227} \mathbf{a}_3$	$=$	$(ax_{227} + by_{227} \cos \gamma + c_x z_{227}) \hat{\mathbf{x}} + (by_{227} \sin \gamma + c_y z_{227}) \hat{\mathbf{y}} + c_z z_{227} \hat{\mathbf{z}}$	(1a)	P XXVII
$\mathbf{B}_{228} =$	$x_{228} \mathbf{a}_1 + y_{228} \mathbf{a}_2 + z_{228} \mathbf{a}_3$	$=$	$(ax_{228} + by_{228} \cos \gamma + c_x z_{228}) \hat{\mathbf{x}} + (by_{228} \sin \gamma + c_y z_{228}) \hat{\mathbf{y}} + c_z z_{228} \hat{\mathbf{z}}$	(1a)	P XXVIII
$\mathbf{B}_{229} =$	$x_{229} \mathbf{a}_1 + y_{229} \mathbf{a}_2 + z_{229} \mathbf{a}_3$	$=$	$(ax_{229} + by_{229} \cos \gamma + c_x z_{229}) \hat{\mathbf{x}} + (by_{229} \sin \gamma + c_y z_{229}) \hat{\mathbf{y}} + c_z z_{229} \hat{\mathbf{z}}$	(1a)	P XXIX
$\mathbf{B}_{230} =$	$x_{230} \mathbf{a}_1 + y_{230} \mathbf{a}_2 + z_{230} \mathbf{a}_3$	$=$	$(ax_{230} + by_{230} \cos \gamma + c_x z_{230}) \hat{\mathbf{x}} + (by_{230} \sin \gamma + c_y z_{230}) \hat{\mathbf{y}} + c_z z_{230} \hat{\mathbf{z}}$	(1a)	P XXX
$\mathbf{B}_{231} =$	$x_{231} \mathbf{a}_1 + y_{231} \mathbf{a}_2 + z_{231} \mathbf{a}_3$	$=$	$(ax_{231} + by_{231} \cos \gamma + c_x z_{231}) \hat{\mathbf{x}} + (by_{231} \sin \gamma + c_y z_{231}) \hat{\mathbf{y}} + c_z z_{231} \hat{\mathbf{z}}$	(1a)	P XXXI
$\mathbf{B}_{232} =$	$x_{232} \mathbf{a}_1 + y_{232} \mathbf{a}_2 + z_{232} \mathbf{a}_3$	$=$	$(ax_{232} + by_{232} \cos \gamma + c_x z_{232}) \hat{\mathbf{x}} + (by_{232} \sin \gamma + c_y z_{232}) \hat{\mathbf{y}} + c_z z_{232} \hat{\mathbf{z}}$	(1a)	P XXXII
$\mathbf{B}_{233} =$	$x_{233} \mathbf{a}_1 + y_{233} \mathbf{a}_2 + z_{233} \mathbf{a}_3$	$=$	$(ax_{233} + by_{233} \cos \gamma + c_x z_{233}) \hat{\mathbf{x}} + (by_{233} \sin \gamma + c_y z_{233}) \hat{\mathbf{y}} + c_z z_{233} \hat{\mathbf{z}}$	(1a)	P XXXIII
$\mathbf{B}_{234} =$	$x_{234} \mathbf{a}_1 + y_{234} \mathbf{a}_2 + z_{234} \mathbf{a}_3$	$=$	$(ax_{234} + by_{234} \cos \gamma + c_x z_{234}) \hat{\mathbf{x}} + (by_{234} \sin \gamma + c_y z_{234}) \hat{\mathbf{y}} + c_z z_{234} \hat{\mathbf{z}}$	(1a)	P XXXIV
$\mathbf{B}_{235} =$	$x_{235} \mathbf{a}_1 + y_{235} \mathbf{a}_2 + z_{235} \mathbf{a}_3$	$=$	$(ax_{235} + by_{235} \cos \gamma + c_x z_{235}) \hat{\mathbf{x}} + (by_{235} \sin \gamma + c_y z_{235}) \hat{\mathbf{y}} + c_z z_{235} \hat{\mathbf{z}}$	(1a)	P XXXV
$\mathbf{B}_{236} =$	$x_{236} \mathbf{a}_1 + y_{236} \mathbf{a}_2 + z_{236} \mathbf{a}_3$	$=$	$(ax_{236} + by_{236} \cos \gamma + c_x z_{236}) \hat{\mathbf{x}} + (by_{236} \sin \gamma + c_y z_{236}) \hat{\mathbf{y}} + c_z z_{236} \hat{\mathbf{z}}$	(1a)	P XXXVI
$\mathbf{B}_{237} =$	$x_{237} \mathbf{a}_1 + y_{237} \mathbf{a}_2 + z_{237} \mathbf{a}_3$	$=$	$(ax_{237} + by_{237} \cos \gamma + c_x z_{237}) \hat{\mathbf{x}} + (by_{237} \sin \gamma + c_y z_{237}) \hat{\mathbf{y}} + c_z z_{237} \hat{\mathbf{z}}$	(1a)	P XXXVII
$\mathbf{B}_{238} =$	$x_{238} \mathbf{a}_1 + y_{238} \mathbf{a}_2 + z_{238} \mathbf{a}_3$	$=$	$(ax_{238} + by_{238} \cos \gamma + c_x z_{238}) \hat{\mathbf{x}} + (by_{238} \sin \gamma + c_y z_{238}) \hat{\mathbf{y}} + c_z z_{238} \hat{\mathbf{z}}$	(1a)	P XXXVIII
$\mathbf{B}_{239} =$	$x_{239} \mathbf{a}_1 + y_{239} \mathbf{a}_2 + z_{239} \mathbf{a}_3$	$=$	$(ax_{239} + by_{239} \cos \gamma + c_x z_{239}) \hat{\mathbf{x}} + (by_{239} \sin \gamma + c_y z_{239}) \hat{\mathbf{y}} + c_z z_{239} \hat{\mathbf{z}}$	(1a)	P XXXIX
$\mathbf{B}_{240} =$	$x_{240} \mathbf{a}_1 + y_{240} \mathbf{a}_2 + z_{240} \mathbf{a}_3$	$=$	$(ax_{240} + by_{240} \cos \gamma + c_x z_{240}) \hat{\mathbf{x}} + (by_{240} \sin \gamma + c_y z_{240}) \hat{\mathbf{y}} + c_z z_{240} \hat{\mathbf{z}}$	(1a)	P XL

References

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First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).