

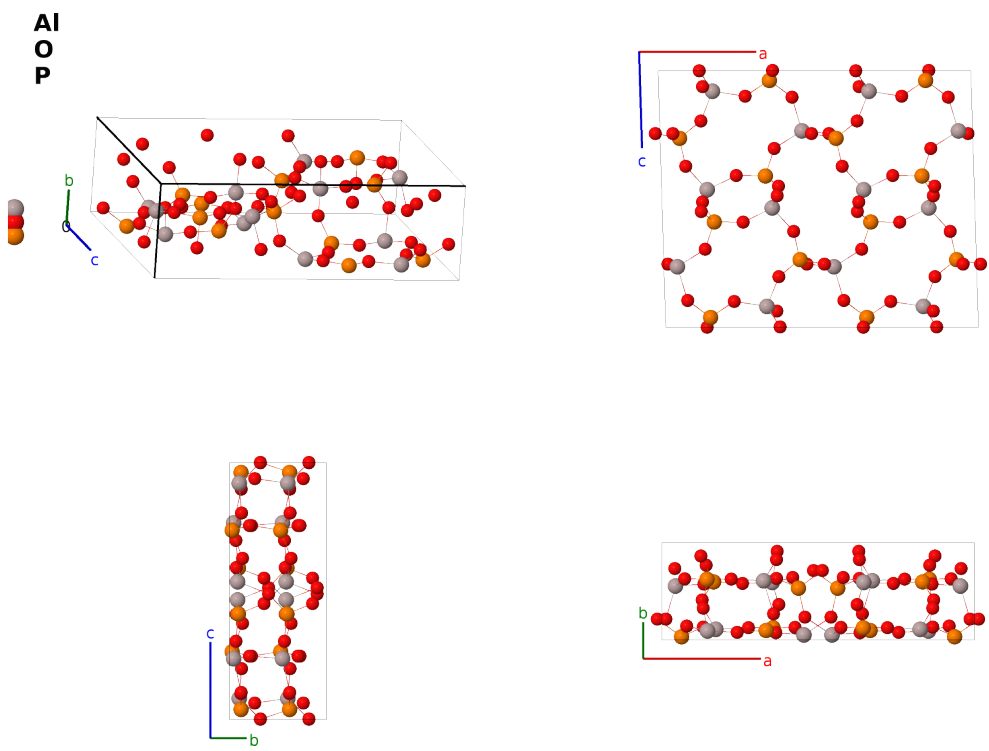
Monoclinic AlPO_4 -53(C) Structure: AB4C_mC72_5_3c_12c_3c-001

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- 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/AQSC>

https://aflow.org/prototype-encyclopedia/AB4C_mC72_5_3c_12c_3c-001

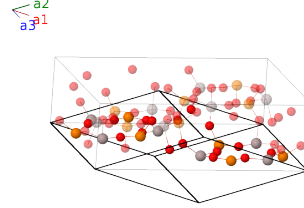


Prototype	AlO_4P
AFLOW prototype label	AB4C_mC72_5_3c_12c_3c-001
ICSD	91681
CCDC	1651206
Pearson symbol	mC72
Space group number	5
Space group symbol	$C2$
AFLOW prototype command	<pre>aflow --proto=AB4C_mC72_5_3c_12c_3c-001 --params=a,b/a,c/a,β,$x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3,x_4,y_4,z_4,x_5,y_5,z_5,x_6,y_6,z_6,x_7,y_7,z_7,x_8,y_8,z_8,x_9,y_9,z_9,x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},z_{15},x_{16},y_{16},z_{16},x_{17},y_{17},z_{17},x_{18},y_{18},z_{18}$</pre>

- (Kirchner, 2000) found the aluminum phosphates zeolite $\text{AlPO}_4\text{-53}$ in three states:
 - As-synthesized $\text{AlPO}_4\text{-53(A)}$ $[24(\text{AlPO}_4) \cdot 8.5\text{CH}_3\text{NH}_2 \cdot 14\text{H}_2\text{O}]$ includes methyl and ammonium ions as well as water.
 - Orthorhombic $\text{AlPO}_4\text{-53(B)}$ is calcined (heated below the melting temperature) to remove those ions and molecules, leaving the framework structure.
 - Monoclinic $\text{AlPO}_4\text{-53(C)}$ (this structure) is produced by heating $\text{AlPO}_4\text{-53(B)}$ above 700°C .

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_2$	$-(x_1 + y_1) \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_3$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B}_4$	$-(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B}_5$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Al III
$\mathbf{B}_6$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4c)	Al III
$\mathbf{B}_7$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_8$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_9$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{10}$	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{11}$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{12}$	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{13}$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{14}$	$-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4c)	O IV

$\mathbf{B}_{15}$	$=$	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 +$ $z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{16}$	$=$	$-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 -$ $z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{17}$	$=$	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 +$ $z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{18}$	$=$	$-(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 -$ $z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4c)	O VI
$\mathbf{B}_{19}$	$=$	$(x_{10} - y_{10}) \mathbf{a}_1 +$ $(x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{20}$	$=$	$-(x_{10} + y_{10}) \mathbf{a}_1 -$ $(x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} -$ $cz_{10} \sin \beta \hat{\mathbf{z}}$	(4c)	O VII
$\mathbf{B}_{21}$	$=$	$(x_{11} - y_{11}) \mathbf{a}_1 +$ $(x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	O VIII
$\mathbf{B}_{22}$	$=$	$-(x_{11} + y_{11}) \mathbf{a}_1 -$ $(x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} -$ $cz_{11} \sin \beta \hat{\mathbf{z}}$	(4c)	O VIII
$\mathbf{B}_{23}$	$=$	$(x_{12} - y_{12}) \mathbf{a}_1 +$ $(x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	O IX
$\mathbf{B}_{24}$	$=$	$-(x_{12} + y_{12}) \mathbf{a}_1 -$ $(x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(4c)	O IX
$\mathbf{B}_{25}$	$=$	$(x_{13} - y_{13}) \mathbf{a}_1 +$ $(x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	O X
$\mathbf{B}_{26}$	$=$	$-(x_{13} + y_{13}) \mathbf{a}_1 -$ $(x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(4c)	O X
$\mathbf{B}_{27}$	$=$	$(x_{14} - y_{14}) \mathbf{a}_1 +$ $(x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(4c)	O XI
$\mathbf{B}_{28}$	$=$	$-(x_{14} + y_{14}) \mathbf{a}_1 -$ $(x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} -$ $cz_{14} \sin \beta \hat{\mathbf{z}}$	(4c)	O XI
$\mathbf{B}_{29}$	$=$	$(x_{15} - y_{15}) \mathbf{a}_1 +$ $(x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(4c)	O XII
$\mathbf{B}_{30}$	$=$	$-(x_{15} + y_{15}) \mathbf{a}_1 -$ $(x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} -$ $cz_{15} \sin \beta \hat{\mathbf{z}}$	(4c)	O XII
$\mathbf{B}_{31}$	$=$	$(x_{16} - y_{16}) \mathbf{a}_1 +$ $(x_{16} + y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_{32}$	$=$	$-(x_{16} + y_{16}) \mathbf{a}_1 -$ $(x_{16} - y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} -$ $cz_{16} \sin \beta \hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B}_{33}$	$=$	$(x_{17} - y_{17}) \mathbf{a}_1 +$ $(x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(4c)	P II
$\mathbf{B}_{34}$	$=$	$-(x_{17} + y_{17}) \mathbf{a}_1 -$ $(x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} -$ $cz_{17} \sin \beta \hat{\mathbf{z}}$	(4c)	P II
$\mathbf{B}_{35}$	$=$	$(x_{18} - y_{18}) \mathbf{a}_1 +$ $(x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(4c)	P III
$\mathbf{B}_{36}$	$=$	$-(x_{18} + y_{18}) \mathbf{a}_1 -$ $(x_{18} - y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} -$ $cz_{18} \sin \beta \hat{\mathbf{z}}$	(4c)	P III

References

- [1] R. M. Kirchner, R. W. Grosse-Kunstleve, J. J. Pluth, S. T. Wilson, R. W. Broach, and J. V. Smith, *The structures of as-synthesized $\text{AlPO}_4\text{-53(A)}$, calcined dehydrated $\text{AlPO}_4\text{-53(B)}$, and $\text{AlPO}_4\text{-53(C)}$, a new phase determined by the FOCUS*

method, Micro. Meso. Mater. **39**, 319–332 (2000), doi:10.1016/S1387-1811(00)00205-5.

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