

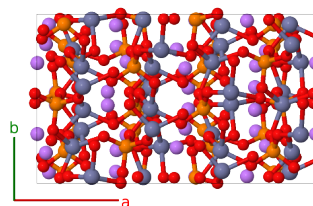
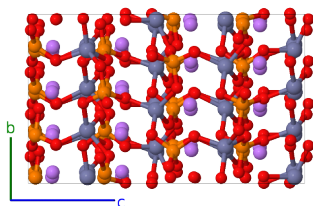
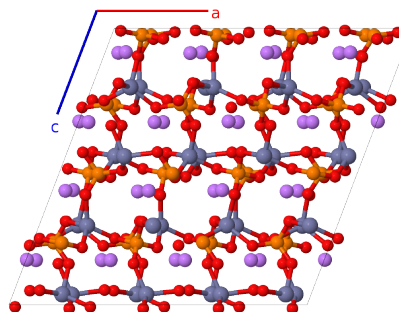
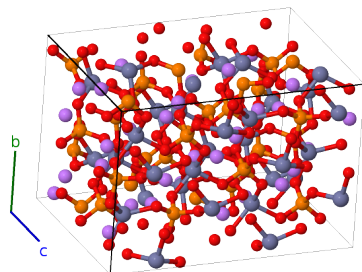
α -LiZnPO₄ Structure: AB4CD_mC224_9_8a_32a_8a_8a-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/L704>

https://aflow.org/p/AB4CD_mC224_9_8a_32a_8a_8a-001

● Li
● O
● P
● Zn



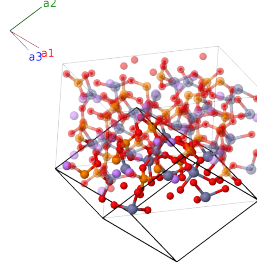
Prototype	LiO ₄ PZn
AFLOW prototype label	AB4CD_mC224_9_8a_32a_8a_8a-001
ICSD	65764
Pearson symbol	mC224
Space group number	9
Space group symbol	<i>Cc</i>
AFLOW prototype command	<pre>aflow --proto=AB4CD_mC224_9_8a_32a_8a_8a-001 --params=a,b/a,c/a,beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16,x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22,z22,x23,y23,z23,x24,y24,z24,x25,y25,z25,x26,y26,z26,x27,y27,z27,x28,y28,z28,x29,y29,z29,x30,y30,z30,x31,y31,z31,x32,y32,z32,x33,y33,z33,x34,y34,z34,x35,y35,z35,x36,y36,z36,x37,y37,z37,x38,y38,z38,x39,y39,z39,x40,y40,z40,x41,y41,z41,x42,y42,z42,x43,y43,z43,x44,y44,z44,x45,y45,z45,x46,y46,z46,x47,y47,z47,x48,y48,z48,x49,y49,z49,x50,y50,z50,x51,y51,z51,x52,y52,z52,x53,y53,z53,x54,y54,z54,x55,y55,z55,x56,y56,z56</pre>

• LiZnPO₄ has been observed in a variety of structures. We list those which have know crystal structures:

- α -LiZnPO₄ (this structure)
- δ_1 -LiZnPO₄, and
- rhombohedral LiZnPO₄.

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	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4a)	Li I
\mathbf{B}_2	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li I
\mathbf{B}_3	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4a)	Li II
\mathbf{B}_4	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li II
\mathbf{B}_5	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4a)	Li III
\mathbf{B}_6	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li III
\mathbf{B}_7	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4a)	Li IV
\mathbf{B}_8	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li IV
\mathbf{B}_9	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4a)	Li V
\mathbf{B}_{10}	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li V
\mathbf{B}_{11}	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4a)	Li VI
\mathbf{B}_{12}	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li VI
\mathbf{B}_{13}	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4a)	Li VII
\mathbf{B}_{14}	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Li VII
\mathbf{B}_{15}	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4a)	Li VIII

$$\begin{aligned}
\mathbf{B}_{16} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 &= (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{Li VIII} \\
\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}} &(4a) &\text{O I} \\
\mathbf{B}_{18} &= (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O I} \\
\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}} &(4a) &\text{O II} \\
\mathbf{B}_{20} &= (x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O II} \\
\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}} &(4a) &\text{O III} \\
\mathbf{B}_{22} &= (x_{11} + y_{11}) \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O III} \\
\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}} &(4a) &\text{O IV} \\
\mathbf{B}_{24} &= (x_{12} + y_{12}) \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{12} + c(z_{12} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O IV} \\
\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}} &(4a) &\text{O V} \\
\mathbf{B}_{26} &= (x_{13} + y_{13}) \mathbf{a}_1 + (x_{13} - y_{13}) \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{13} + c(z_{13} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O V} \\
\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}} &(4a) &\text{O VI} \\
\mathbf{B}_{28} &= (x_{14} + y_{14}) \mathbf{a}_1 + (x_{14} - y_{14}) \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{14} + c(z_{14} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O VI} \\
\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}} &(4a) &\text{O VII} \\
\mathbf{B}_{30} &= (x_{15} + y_{15}) \mathbf{a}_1 + (x_{15} - y_{15}) \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{15} + c(z_{15} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O VII} \\
\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}} &(4a) &\text{O VIII} \\
\mathbf{B}_{32} &= (x_{16} + y_{16}) \mathbf{a}_1 + (x_{16} - y_{16}) \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{16} + c(z_{16} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O VIII} \\
\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}} &(4a) &\text{O IX} \\
\mathbf{B}_{34} &= (x_{17} + y_{17}) \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{17} + c(z_{17} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O IX} \\
\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}} &(4a) &\text{O X} \\
\mathbf{B}_{36} &= (x_{18} + y_{18}) \mathbf{a}_1 + (x_{18} - y_{18}) \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{18} + c(z_{18} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O X} \\
\mathbf{B}_{37} &= (x_{19} - y_{19}) \mathbf{a}_1 + (x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= (ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}} &(4a) &\text{O XI} \\
\mathbf{B}_{38} &= (x_{19} + y_{19}) \mathbf{a}_1 + (x_{19} - y_{19}) \mathbf{a}_2 + (z_{19} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{19} + c(z_{19} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{O XI}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{108} &= \begin{pmatrix} (x_{54} + y_{54}) \mathbf{a}_1 + \\ (x_{54} - y_{54}) \mathbf{a}_2 + (z_{54} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{54} + c(z_{54} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{54} \hat{\mathbf{y}} + \\ c(z_{54} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{Zn VI} \\
\mathbf{B}_{109} &= \begin{pmatrix} (x_{55} - y_{55}) \mathbf{a}_1 + \\ (x_{55} + y_{55}) \mathbf{a}_2 + z_{55} \mathbf{a}_3 \end{pmatrix} = (ax_{55} + cz_{55} \cos \beta) \hat{\mathbf{x}} + by_{55} \hat{\mathbf{y}} + cz_{55} \sin \beta \hat{\mathbf{z}} & (4a) & \text{Zn VII} \\
\mathbf{B}_{110} &= \begin{pmatrix} (x_{55} + y_{55}) \mathbf{a}_1 + \\ (x_{55} - y_{55}) \mathbf{a}_2 + (z_{55} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{55} + c(z_{55} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{55} \hat{\mathbf{y}} + \\ c(z_{55} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{Zn VII} \\
\mathbf{B}_{111} &= \begin{pmatrix} (x_{56} - y_{56}) \mathbf{a}_1 + \\ (x_{56} + y_{56}) \mathbf{a}_2 + z_{56} \mathbf{a}_3 \end{pmatrix} = (ax_{56} + cz_{56} \cos \beta) \hat{\mathbf{x}} + by_{56} \hat{\mathbf{y}} + cz_{56} \sin \beta \hat{\mathbf{z}} & (4a) & \text{Zn VIII} \\
\mathbf{B}_{112} &= \begin{pmatrix} (x_{56} + y_{56}) \mathbf{a}_1 + \\ (x_{56} - y_{56}) \mathbf{a}_2 + (z_{56} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} (ax_{56} + c(z_{56} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{56} \hat{\mathbf{y}} + \\ c(z_{56} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4a) & \text{Zn VIII}
\end{aligned}$$

References

- [1] L. Elammari and B. Elouadi, *Structure of α -LiZnPO₄*, Acta Crystallogr. Sect. C **45**, 1864–1867 (1989), doi:10.1107/S0108270189003094.