

P₄Se₃ Structure:

A4B3_oP112_62_8c4d_4c4d-001

This structure previously used the label(s) **A4B3_oP112_62_8c4d_4c4d**. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/DMDS>

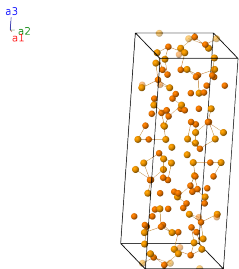
https://aflow.org/prototype-encyclopedia/A4B3_oP112_62_8c4d_4c4d-001

Prototype	P ₄ Se ₃
AFLOW prototype label	A4B3_oP112_62_8c4d_4c4d-001
ICSD	26483
CCDC	1258713
Pearson symbol	oP112
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<pre>aflow --proto=A4B3_oP112_62_8c4d_4c4d-001 --params=a,b/a,c/a,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀, z₁₀,x₁₁,z₁₁,x₁₂,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</pre>

- (Keulen, 1959) give this structure in the *Pmnb* setting of space group #62. We used FINDSYM to translate this into the standard *Pnma* setting.
- The original version of this structure (Hicks, 1999) had errors in the positions of several atoms. These have now been corrected.

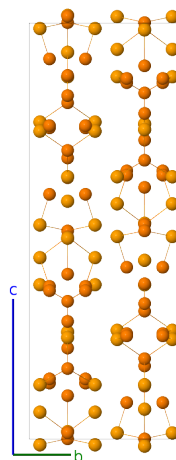
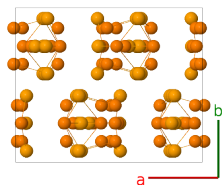
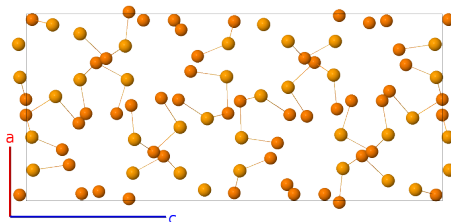
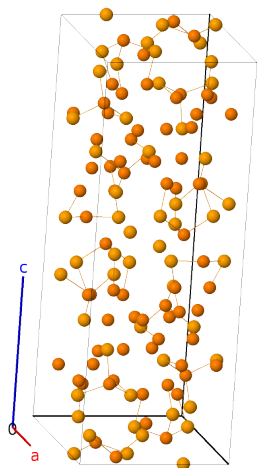
Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

P
Se



$\mathbf{B}_{34} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{35} =$	$-x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{36} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{37} =$	$x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{38} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{40} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{42} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{43} =$	$-x_{11} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{44} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{45} =$	$x_{12} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(4c)	Se IV
$\mathbf{B}_{46} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se IV
$\mathbf{B}_{47} =$	$-x_{12} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(4c)	Se IV
$\mathbf{B}_{48} =$	$(x_{12} + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se IV
$\mathbf{B}_{49} =$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{50} =$	$-(x_{13} - \frac{1}{2}) \mathbf{a}_1 - y_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{51} =$	$-x_{13} \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} + b(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{52} =$	$(x_{13} + \frac{1}{2}) \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{13} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{53} =$	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{54} =$	$(x_{13} + \frac{1}{2}) \mathbf{a}_1 + y_{13} \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{13} + \frac{1}{2}) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{55} =$	$x_{13} \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} - b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{56} =$	$-(x_{13} - \frac{1}{2}) \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P IX
$\mathbf{B}_{57} =$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$	(8d)	P X
$\mathbf{B}_{58} =$	$-(x_{14} - \frac{1}{2}) \mathbf{a}_1 - y_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{14} - \frac{1}{2}) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P X
$\mathbf{B}_{59} =$	$-x_{14} \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-ax_{14} \hat{\mathbf{x}} + b(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}}$	(8d)	P X
$\mathbf{B}_{60} =$	$(x_{14} + \frac{1}{2}) \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{14} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P X
$\mathbf{B}_{61} =$	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}}$	(8d)	P X
$\mathbf{B}_{62} =$	$(x_{14} + \frac{1}{2}) \mathbf{a}_1 + y_{14} \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_{14} + \frac{1}{2}) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	P X
$\mathbf{B}_{63} =$	$x_{14} \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$ax_{14} \hat{\mathbf{x}} - b(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$	(8d)	P X

$\mathbf{B}_{64} =$	$-(x_{14} - \frac{1}{2}) \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{14} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} +$	$(8d)$	P X
	$(z_{14} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{65} =$	$x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$ax_{15} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}}$	$(8d)$	P XI
$\mathbf{B}_{66} =$	$-(x_{15} - \frac{1}{2}) \mathbf{a}_1 - y_{15} \mathbf{a}_2 +$	$=$	$-a(x_{15} - \frac{1}{2}) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	P XI
	$(z_{15} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{67} =$	$-x_{15} \mathbf{a}_1 + (y_{15} + \frac{1}{2}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-ax_{15} \hat{\mathbf{x}} + b(y_{15} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}}$	$(8d)$	P XI
$\mathbf{B}_{68} =$	$(x_{15} + \frac{1}{2}) \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{15} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} -$	$(8d)$	P XI
	$(z_{15} - \frac{1}{2}) \mathbf{a}_3$		$c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{69} =$	$-x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}}$	$(8d)$	P XI
$\mathbf{B}_{70} =$	$(x_{15} + \frac{1}{2}) \mathbf{a}_1 + y_{15} \mathbf{a}_2 -$	$=$	$a(x_{15} + \frac{1}{2}) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	P XI
	$(z_{15} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{71} =$	$x_{15} \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$ax_{15} \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}}$	$(8d)$	P XI
$\mathbf{B}_{72} =$	$-(x_{15} - \frac{1}{2}) \mathbf{a}_1 + (y_{15} + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{15} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{15} + \frac{1}{2}) \hat{\mathbf{y}} +$	$(8d)$	P XI
	$(z_{15} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{73} =$	$x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$ax_{16} \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$	$(8d)$	P XII
$\mathbf{B}_{74} =$	$-(x_{16} - \frac{1}{2}) \mathbf{a}_1 - y_{16} \mathbf{a}_2 +$	$=$	$-a(x_{16} - \frac{1}{2}) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	P XII
	$(z_{16} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{75} =$	$-x_{16} \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-ax_{16} \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}}$	$(8d)$	P XII
$\mathbf{B}_{76} =$	$(x_{16} + \frac{1}{2}) \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{16} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} -$	$(8d)$	P XII
	$(z_{16} - \frac{1}{2}) \mathbf{a}_3$		$c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{77} =$	$-x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-ax_{16} \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}}$	$(8d)$	P XII
$\mathbf{B}_{78} =$	$(x_{16} + \frac{1}{2}) \mathbf{a}_1 + y_{16} \mathbf{a}_2 -$	$=$	$a(x_{16} + \frac{1}{2}) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	P XII
	$(z_{16} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{79} =$	$x_{16} \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$ax_{16} \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$	$(8d)$	P XII
$\mathbf{B}_{80} =$	$-(x_{16} - \frac{1}{2}) \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{16} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} +$	$(8d)$	P XII
	$(z_{16} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{81} =$	$x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$ax_{17} \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	$(8d)$	Se V
$\mathbf{B}_{82} =$	$-(x_{17} - \frac{1}{2}) \mathbf{a}_1 - y_{17} \mathbf{a}_2 +$	$=$	$-a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	Se V
	$(z_{17} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{83} =$	$-x_{17} \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-ax_{17} \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}}$	$(8d)$	Se V
$\mathbf{B}_{84} =$	$(x_{17} + \frac{1}{2}) \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} -$	$(8d)$	Se V
	$(z_{17} - \frac{1}{2}) \mathbf{a}_3$		$c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{85} =$	$-x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-ax_{17} \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}}$	$(8d)$	Se V
$\mathbf{B}_{86} =$	$(x_{17} + \frac{1}{2}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 -$	$=$	$a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	Se V
	$(z_{17} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{87} =$	$x_{17} \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$ax_{17} \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	$(8d)$	Se V
$\mathbf{B}_{88} =$	$-(x_{17} - \frac{1}{2}) \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} +$	$(8d)$	Se V
	$(z_{17} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{89} =$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$ax_{18} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	$(8d)$	Se VI
$\mathbf{B}_{90} =$	$-(x_{18} - \frac{1}{2}) \mathbf{a}_1 - y_{18} \mathbf{a}_2 +$	$=$	$-a(x_{18} - \frac{1}{2}) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}}$	$(8d)$	Se VI
	$(z_{18} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{91} =$	$-x_{18} \mathbf{a}_1 + (y_{18} + \frac{1}{2}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} + b(y_{18} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}}$	$(8d)$	Se VI
$\mathbf{B}_{92} =$	$(x_{18} + \frac{1}{2}) \mathbf{a}_1 - (y_{18} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{18} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{18} - \frac{1}{2}) \hat{\mathbf{y}} -$	$(8d)$	Se VI
	$(z_{18} - \frac{1}{2}) \mathbf{a}_3$		$c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{93} =$	$-x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}}$	$(8d)$	Se VI

$$\begin{aligned}
\mathbf{B}_{94} &= \begin{pmatrix} x_{18} + \frac{1}{2} \\ z_{18} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{18} \mathbf{a}_2 - \begin{pmatrix} z_{18} - \frac{1}{2} \\ z_{18} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_{18} + \frac{1}{2} \right) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - c \left(z_{18} - \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VI} \\
\mathbf{B}_{95} &= x_{18} \mathbf{a}_1 - \left(y_{18} - \frac{1}{2} \right) \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= ax_{18} \hat{\mathbf{x}} - b \left(y_{18} - \frac{1}{2} \right) \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (8d) & \text{Se VI} \\
\mathbf{B}_{96} &= - \left(x_{18} - \frac{1}{2} \right) \mathbf{a}_1 + \left(y_{18} + \frac{1}{2} \right) \mathbf{a}_2 + \begin{pmatrix} z_{18} + \frac{1}{2} \\ z_{18} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_{18} - \frac{1}{2} \right) \hat{\mathbf{x}} + b \left(y_{18} + \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_{18} + \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VI} \\
\mathbf{B}_{97} &= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= ax_{19} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{98} &= - \left(x_{19} - \frac{1}{2} \right) \mathbf{a}_1 - y_{19} \mathbf{a}_2 + \begin{pmatrix} z_{19} - \frac{1}{2} \\ z_{19} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_{19} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{99} &= -x_{19} \mathbf{a}_1 + \left(y_{19} + \frac{1}{2} \right) \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= -ax_{19} \hat{\mathbf{x}} + b \left(y_{19} + \frac{1}{2} \right) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{100} &= \left(x_{19} + \frac{1}{2} \right) \mathbf{a}_1 - \left(y_{19} - \frac{1}{2} \right) \mathbf{a}_2 - \begin{pmatrix} z_{19} - \frac{1}{2} \\ z_{19} - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_{19} + \frac{1}{2} \right) \hat{\mathbf{x}} - b \left(y_{19} - \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{101} &= -x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= -ax_{19} \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{102} &= \begin{pmatrix} x_{19} + \frac{1}{2} \\ z_{19} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{19} \mathbf{a}_2 - \begin{pmatrix} z_{19} - \frac{1}{2} \\ z_{19} - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_{19} + \frac{1}{2} \right) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{103} &= x_{19} \mathbf{a}_1 - \left(y_{19} - \frac{1}{2} \right) \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= ax_{19} \hat{\mathbf{x}} - b \left(y_{19} - \frac{1}{2} \right) \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{104} &= - \left(x_{19} - \frac{1}{2} \right) \mathbf{a}_1 + \left(y_{19} + \frac{1}{2} \right) \mathbf{a}_2 + \begin{pmatrix} z_{19} + \frac{1}{2} \\ z_{19} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_{19} - \frac{1}{2} \right) \hat{\mathbf{x}} + b \left(y_{19} + \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{105} &= x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= ax_{20} \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{106} &= - \left(x_{20} - \frac{1}{2} \right) \mathbf{a}_1 - y_{20} \mathbf{a}_2 + \begin{pmatrix} z_{20} + \frac{1}{2} \\ z_{20} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_{20} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{107} &= -x_{20} \mathbf{a}_1 + \left(y_{20} + \frac{1}{2} \right) \mathbf{a}_2 - z_{20} \mathbf{a}_3 &= -ax_{20} \hat{\mathbf{x}} + b \left(y_{20} + \frac{1}{2} \right) \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{108} &= \begin{pmatrix} x_{20} + \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \left(y_{20} - \frac{1}{2} \right) \mathbf{a}_2 - \begin{pmatrix} z_{20} - \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_{20} + \frac{1}{2} \right) \hat{\mathbf{x}} - b \left(y_{20} - \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_{20} - \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{109} &= -x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3 &= -ax_{20} \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{110} &= \begin{pmatrix} x_{20} + \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{20} \mathbf{a}_2 - \begin{pmatrix} z_{20} - \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_{20} + \frac{1}{2} \right) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - c \left(z_{20} - \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{111} &= x_{20} \mathbf{a}_1 - \left(y_{20} - \frac{1}{2} \right) \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= ax_{20} \hat{\mathbf{x}} - b \left(y_{20} - \frac{1}{2} \right) \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{112} &= - \left(x_{20} - \frac{1}{2} \right) \mathbf{a}_1 + \left(y_{20} + \frac{1}{2} \right) \mathbf{a}_2 + \begin{pmatrix} z_{20} + \frac{1}{2} \\ z_{20} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_{20} - \frac{1}{2} \right) \hat{\mathbf{x}} + b \left(y_{20} + \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2} \right) \hat{\mathbf{z}} & (8d) & \text{Se VIII}
\end{aligned}$$

References

- [1] E. Keulen and A. Vos, *The Crystal Structure of P_4Se_3* , Acta Cryst. **12**, 323–329 (1959), doi:10.1107/S0365110X59000950.
- [2] 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.

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