

P₄Se₃ Structure:

A4B3_oP112_62_8c4d_4c4d-001

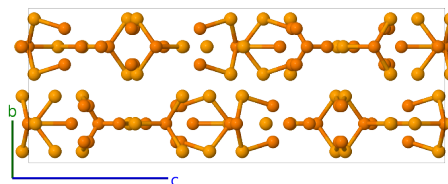
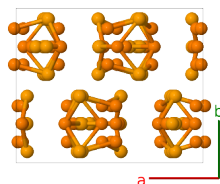
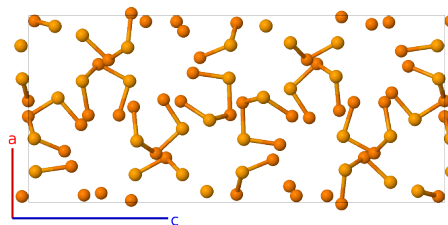
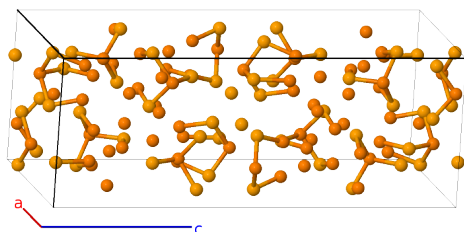
This structure originally had the label **A4B3_oP112.62.8c4d_4c4d**. Calls to that address will be redirected here.

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

https://aflow.org/p/A4B3_oP112_62_8c4d_4c4d-001

● P
● Se

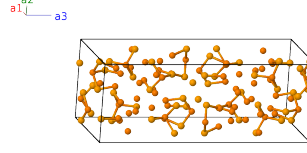


Prototype	P ₄ Se ₃
AFLOW prototype label	A4B3_oP112_62_8c4d_4c4d-001
ICSD	26483
Pearson symbol	oP112
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<pre>aflow --proto=A4B3_oP112_62_8c4d_4c4d-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, z6, x7, z7,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

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	P I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	P I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	P II
\mathbf{B}_6	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	P II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	P III
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P III
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	P III
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	P IV
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P IV
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	P IV
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	P V
\mathbf{B}_{18}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P V
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	P V
\mathbf{B}_{20}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P V
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	P VI
\mathbf{B}_{22}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P VI
\mathbf{B}_{23}	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	P VI

$$\begin{aligned}
\mathbf{B}_{86} &= \begin{pmatrix} (x_{17} + \frac{1}{2}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 - \\ (z_{17} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se V} \\
\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) & \text{Se V} \\
\mathbf{B}_{88} &= - (x_{17} - \frac{1}{2}) \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 + \\ & \quad (z_{17} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & \quad c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se V} \\
\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) & \text{Se VI} \\
\mathbf{B}_{90} &= - (x_{18} - \frac{1}{2}) \mathbf{a}_1 - y_{18} \mathbf{a}_2 + \\ & \quad (z_{18} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{18} - \frac{1}{2}) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VI} \\
\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) & \text{Se VI} \\
\mathbf{B}_{92} &= (x_{18} + \frac{1}{2}) \mathbf{a}_1 - (y_{18} - \frac{1}{2}) \mathbf{a}_2 - \\ & \quad (z_{18} - \frac{1}{2}) \mathbf{a}_3 = a(x_{18} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{18} - \frac{1}{2}) \hat{\mathbf{y}} - \\ & \quad c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VI} \\
\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) & \text{Se VI} \\
\mathbf{B}_{94} &= (x_{18} + \frac{1}{2}) \mathbf{a}_1 + y_{18} \mathbf{a}_2 - \\ & \quad (z_{18} - \frac{1}{2}) \mathbf{a}_3 = a(x_{18} + \frac{1}{2}) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VI} \\
\mathbf{B}_{95} &= 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) & \text{Se VI} \\
\mathbf{B}_{96} &= - (x_{18} - \frac{1}{2}) \mathbf{a}_1 + (y_{18} + \frac{1}{2}) \mathbf{a}_2 + \\ & \quad (z_{18} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{18} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{18} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & \quad c(z_{18} + \frac{1}{2}) \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} &= - (x_{19} - \frac{1}{2}) \mathbf{a}_1 - y_{19} \mathbf{a}_2 + \\ & \quad (z_{19} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{19} - \frac{1}{2}) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{99} &= -x_{19} \mathbf{a}_1 + (y_{19} + \frac{1}{2}) \mathbf{a}_2 - z_{19} \mathbf{a}_3 = -ax_{19} \hat{\mathbf{x}} + b(y_{19} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{100} &= (x_{19} + \frac{1}{2}) \mathbf{a}_1 - (y_{19} - \frac{1}{2}) \mathbf{a}_2 - \\ & \quad (z_{19} - \frac{1}{2}) \mathbf{a}_3 = a(x_{19} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{19} - \frac{1}{2}) \hat{\mathbf{y}} - \\ & \quad c(z_{19} - \frac{1}{2}) \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} &= (x_{19} + \frac{1}{2}) \mathbf{a}_1 + y_{19} \mathbf{a}_2 - \\ & \quad (z_{19} - \frac{1}{2}) \mathbf{a}_3 = a(x_{19} + \frac{1}{2}) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - c(z_{19} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{103} &= x_{19} \mathbf{a}_1 - (y_{19} - \frac{1}{2}) \mathbf{a}_2 + z_{19} \mathbf{a}_3 = ax_{19} \hat{\mathbf{x}} - b(y_{19} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8d) & \text{Se VII} \\
\mathbf{B}_{104} &= - (x_{19} - \frac{1}{2}) \mathbf{a}_1 + (y_{19} + \frac{1}{2}) \mathbf{a}_2 + \\ & \quad (z_{19} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{19} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{19} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & \quad c(z_{19} + \frac{1}{2}) \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} &= - (x_{20} - \frac{1}{2}) \mathbf{a}_1 - y_{20} \mathbf{a}_2 + \\ & \quad (z_{20} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{20} - \frac{1}{2}) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c(z_{20} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{107} &= -x_{20} \mathbf{a}_1 + (y_{20} + \frac{1}{2}) \mathbf{a}_2 - z_{20} \mathbf{a}_3 = -ax_{20} \hat{\mathbf{x}} + b(y_{20} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{108} &= (x_{20} + \frac{1}{2}) \mathbf{a}_1 - (y_{20} - \frac{1}{2}) \mathbf{a}_2 - \\ & \quad (z_{20} - \frac{1}{2}) \mathbf{a}_3 = a(x_{20} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{20} - \frac{1}{2}) \hat{\mathbf{y}} - \\ & \quad c(z_{20} - \frac{1}{2}) \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} &= (x_{20} + \frac{1}{2}) \mathbf{a}_1 + y_{20} \mathbf{a}_2 - \\ & \quad (z_{20} - \frac{1}{2}) \mathbf{a}_3 = a(x_{20} + \frac{1}{2}) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - c(z_{20} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{111} &= x_{20} \mathbf{a}_1 - (y_{20} - \frac{1}{2}) \mathbf{a}_2 + z_{20} \mathbf{a}_3 = ax_{20} \hat{\mathbf{x}} - b(y_{20} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8d) & \text{Se VIII} \\
\mathbf{B}_{112} &= - (x_{20} - \frac{1}{2}) \mathbf{a}_1 + (y_{20} + \frac{1}{2}) \mathbf{a}_2 + \\ & \quad (z_{20} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{20} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{20} + \frac{1}{2}) \hat{\mathbf{y}} + \\ & \quad c(z_{20} + \frac{1}{2}) \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.