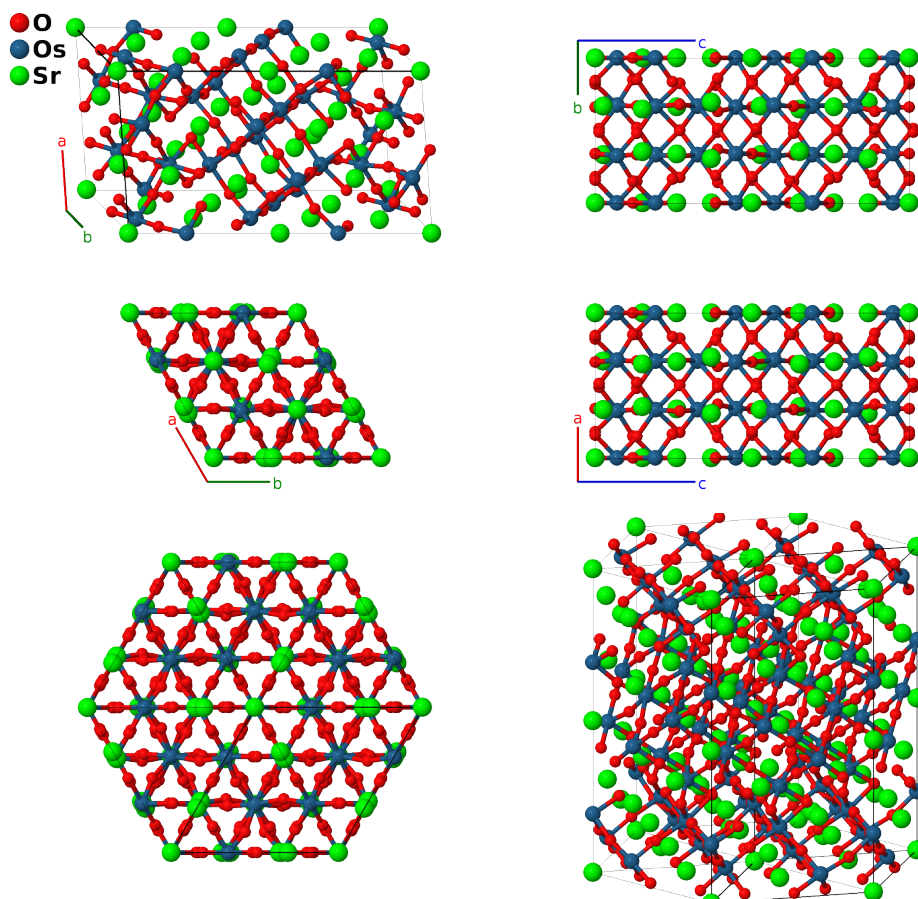


Sr₈Os_{6.3}O₂₄ Structure: A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001

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<https://afLOW.org/p/AL94>

https://afLOW.org/p/A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001



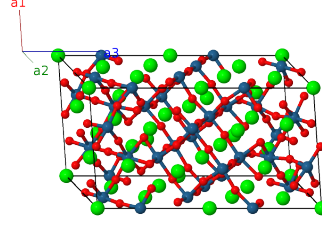
Prototype	O ₂₄ Os _{6.3} Sr ₈
AFLOW prototype label	A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001
ICSD	112868
Pearson symbol	hP118
Space group number	185
Space group symbol	<i>P6₃cm</i>
AFLOW prototype command	afLOW --proto=A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001 --params=a, c/a, z ₁ , z ₂ , z ₃ , z ₄ , z ₅ , x ₆ , z ₆ , x ₇ , z ₇ , x ₈ , z ₈ , x ₉ , z ₉ , x ₁₀ , z ₁₀ , x ₁₁ , z ₁₁ , x ₁₂ , z ₁₂ , x ₁₃ , z ₁₃ , x 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

- The first osmium (4b) site (Os-II) has an occupancy of 93.1%, while the next (4b) site (Os-III) has 27.9% occupancy.

- Space group $P6_3cm$ does not specify the origin of the z axis, we follow (Thakur, 2021) and set $z_2 = 0$ for the Sr-I atom.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	Os I
\mathbf{B}_2	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Os I
\mathbf{B}_3	$z_2 \mathbf{a}_3$	=	$cz_2 \hat{\mathbf{z}}$	(2a)	Sr I
\mathbf{B}_4	$(z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Sr I
\mathbf{B}_5	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	Os II
\mathbf{B}_6	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Os II
\mathbf{B}_7	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Os II
\mathbf{B}_8	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	Os II
\mathbf{B}_9	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	Os III
\mathbf{B}_{10}	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Os III
\mathbf{B}_{11}	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Os III
\mathbf{B}_{12}	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	Os III
\mathbf{B}_{13}	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4b)	Sr II
\mathbf{B}_{14}	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Sr II
\mathbf{B}_{15}	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Sr II
\mathbf{B}_{16}	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4b)	Sr II
\mathbf{B}_{17}	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	=	$\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{18}	$x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{19}	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{20}	$-x_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{21}	$-x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{22}	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{23}	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_3$	=	$\frac{1}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{24}	$x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$\frac{1}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{25}	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} + cz_7 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{26}	$-x_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{27}	$-x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{28}	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{29}	$x_8 \mathbf{a}_1 + z_8 \mathbf{a}_3$	=	$\frac{1}{2}ax_8 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{30}	$x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$\frac{1}{2}ax_8 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6c)	O III

$$\begin{aligned}
\mathbf{B}_{99} &= y_{17} \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{17} + 2y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{100} &= (x_{17} - y_{17}) \mathbf{a}_1 + x_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{101} &= -y_{17} \mathbf{a}_1 - x_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{102} &= -(x_{17} - y_{17}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{17} + 2y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{103} &= x_{17} \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{104} &= y_{17} \mathbf{a}_1 + x_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = \frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{105} &= (x_{17} - y_{17}) \mathbf{a}_1 - y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = \frac{1}{2}a(x_{17} - 2y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{106} &= -x_{17} \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 = -\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (12d) & \text{O VII} \\
\mathbf{B}_{107} &= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = \frac{1}{2}a(x_{18} + y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{18} - y_{18}) \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{108} &= -y_{18} \mathbf{a}_1 + (x_{18} - y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = \frac{1}{2}a(x_{18} - 2y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{109} &= -(x_{18} - y_{18}) \mathbf{a}_1 - x_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = -\frac{1}{2}a(2x_{18} - y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{110} &= -x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_{18} + y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{18} - y_{18}) \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{111} &= y_{18} \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{18} + 2y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{112} &= (x_{18} - y_{18}) \mathbf{a}_1 + x_{18} \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{18} - y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{113} &= -y_{18} \mathbf{a}_1 - x_{18} \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_{18} + y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{18} - y_{18}) \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{114} &= -(x_{18} - y_{18}) \mathbf{a}_1 + y_{18} \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{18} + 2y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{115} &= x_{18} \mathbf{a}_1 + (x_{18} - y_{18}) \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(2x_{18} - y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{116} &= y_{18} \mathbf{a}_1 + x_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = \frac{1}{2}a(x_{18} + y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{18} - y_{18}) \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{117} &= (x_{18} - y_{18}) \mathbf{a}_1 - y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = \frac{1}{2}a(x_{18} - 2y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (12d) & \text{O VIII} \\
\mathbf{B}_{118} &= -x_{18} \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = -\frac{1}{2}a(2x_{18} - y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (12d) & \text{O VIII}
\end{aligned}$$

References

- [1] G. S. Thakur, T. Doert, S. Mohitkar, W. Schnelle, C. Felser, and M. Jansen, *Crystal Growth of a New 8H Perovskite Sr₈O_{s6.3}O₂₄ Exhibiting High T_c Ferromagnetism*, Cryst. Growth Des. **21**, 2459–2464 (2021), doi:10.1021/acs.cgd.1c00057.