

Sr₈Os_{6.3}O₂₄ Structure:

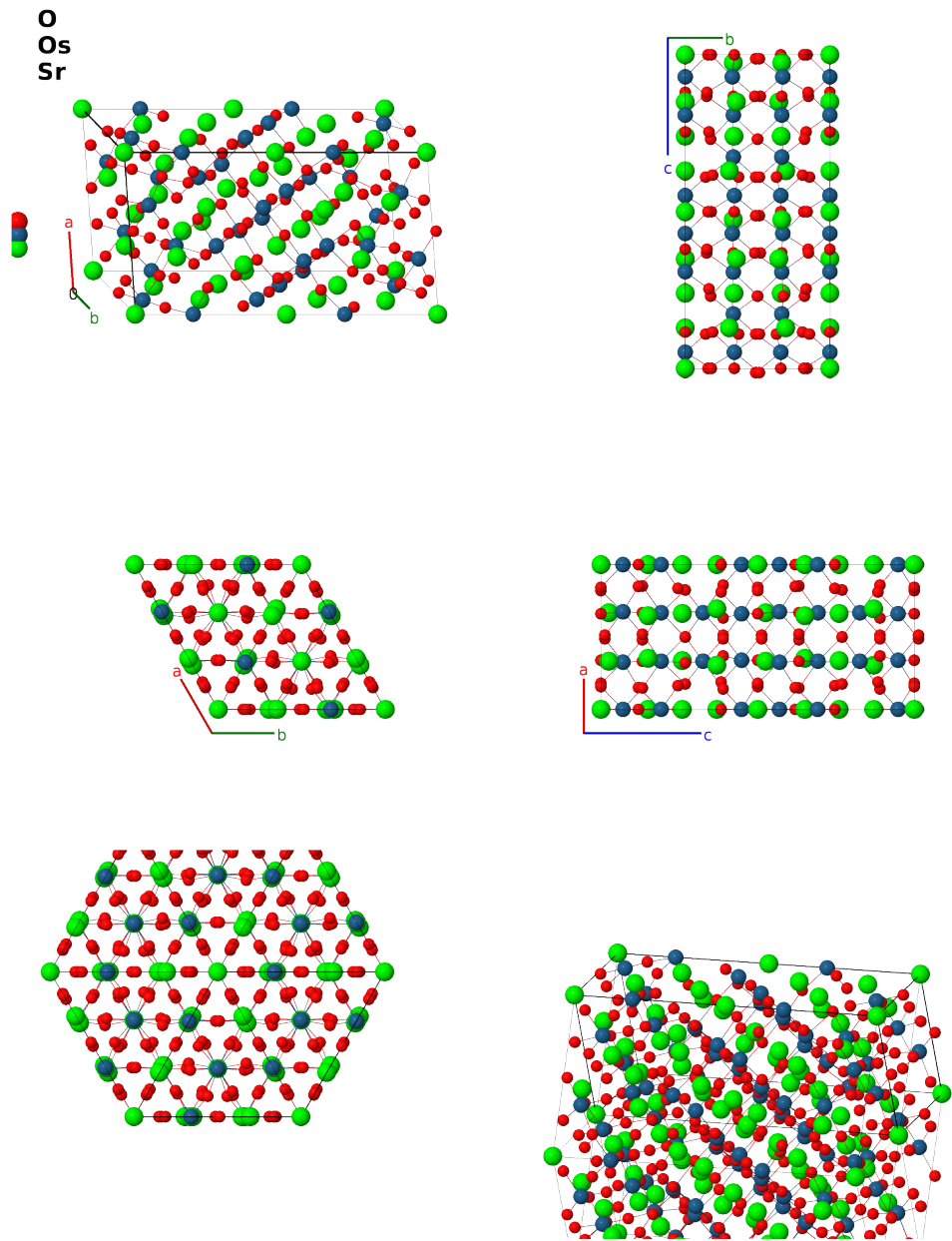
A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001

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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/AL94>

https://aflow.org/prototype-encyclopedia/A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001



Prototype

O₂₄Os_{6.3}Sr₈

AFLOW prototype label

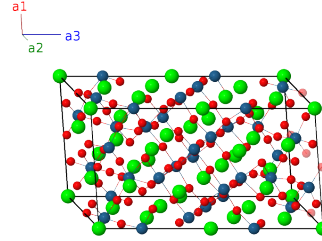
A36B11C12_hP118_185_4c4d_a2b2c_ab3c-001

ICSD	112868
CCDC	2059167
Pearson symbol	hP118
Space group number	185
Space group symbol	$P6_3cm$
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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Os I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Os I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	Sr I
$\mathbf{B}_4$	$= \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Sr I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Os II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Os II
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Os II
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Os II
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4b)	Os III
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Os III
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Os III
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4b)	Os III
$\mathbf{B}_{13}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4b)	Sr II
$\mathbf{B}_{14}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Sr II
$\mathbf{B}_{15}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Sr II
$\mathbf{B}_{16}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4b)	Sr II

$\mathbf{B}_{90} =$	$-(x_{16} - y_{16}) \mathbf{a}_1 + y_{16} \mathbf{a}_2 +$	$=$	$\frac{1}{2}a(-x_{16} + 2y_{16}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{16} \hat{\mathbf{y}} +$	$(12d)$	O VI
	$(z_{16} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{91} =$	$x_{16} \mathbf{a}_1 + (x_{16} - y_{16}) \mathbf{a}_2 +$	$=$	$\frac{1}{2}a(2x_{16} - y_{16}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{16} \hat{\mathbf{y}} +$	$(12d)$	O VI
	$(z_{16} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{92} =$	$y_{16} \mathbf{a}_1 + x_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{16} + y_{16}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{16} - y_{16}) \hat{\mathbf{y}} +$	$(12d)$	O VI
			$cz_{16} \hat{\mathbf{z}}$		
$\mathbf{B}_{93} =$	$(x_{16} - y_{16}) \mathbf{a}_1 - y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{16} - 2y_{16}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$	$(12d)$	O VI
$\mathbf{B}_{94} =$	$-x_{16} \mathbf{a}_1 - (x_{16} - y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{16} - y_{16}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$	$(12d)$	O VI
$\mathbf{B}_{95} =$	$x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} +$	$(12d)$	O VII
			$cz_{17} \hat{\mathbf{z}}$		
$\mathbf{B}_{96} =$	$-y_{17} \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{17} - 2y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	$(12d)$	O VII
$\mathbf{B}_{97} =$	$-(x_{17} - y_{17}) \mathbf{a}_1 - x_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	$(12d)$	O VII
$\mathbf{B}_{98} =$	$-x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} +$	$(12d)$	O VII
			$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{99} =$	$y_{17} \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 +$	$=$	$\frac{1}{2}a(-x_{17} + 2y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} +$	$(12d)$	O VII
	$(z_{17} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{100} =$	$(x_{17} - y_{17}) \mathbf{a}_1 + x_{17} \mathbf{a}_2 +$	$=$	$\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} +$	$(12d)$	O VII
	$(z_{17} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{101} =$	$-y_{17} \mathbf{a}_1 - x_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} +$	$(12d)$	O VII
			$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{102} =$	$-(x_{17} - y_{17}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 +$	$=$	$\frac{1}{2}a(-x_{17} + 2y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} +$	$(12d)$	O VII
	$(z_{17} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{103} =$	$x_{17} \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 +$	$=$	$\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} +$	$(12d)$	O VII
	$(z_{17} + \frac{1}{2}) \mathbf{a}_3$		$c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$		
$\mathbf{B}_{104} =$	$y_{17} \mathbf{a}_1 + x_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{17} + y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{17} - y_{17}) \hat{\mathbf{y}} +$	$(12d)$	O VII
			$cz_{17} \hat{\mathbf{z}}$		
$\mathbf{B}_{105} =$	$(x_{17} - y_{17}) \mathbf{a}_1 - y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{17} - 2y_{17}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	$(12d)$	O VII
$\mathbf{B}_{106} =$	$-x_{17} \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{17} - y_{17}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	$(12d)$	O VII
$\mathbf{B}_{107} =$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{18} + y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{18} - y_{18}) \hat{\mathbf{y}} +$	$(12d)$	O VIII
			$cz_{18} \hat{\mathbf{z}}$		
$\mathbf{B}_{108} =$	$-y_{18} \mathbf{a}_1 + (x_{18} - y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{18} - 2y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	$(12d)$	O VIII
$\mathbf{B}_{109} =$	$-(x_{18} - y_{18}) \mathbf{a}_1 - x_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{18} - y_{18}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{18}$		

$$\mathbf{B}_{118} = -x_{18} \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 = -\frac{1}{2}a (2x_{18} - y_{18}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} \quad (12d) \quad \text{O VIII}$$

References

- [1] G. S. Thakur, T. Doert, S. Mohitkar, W. Schnelle, C. Felser, and M. Jansen, *Crystal Growth of a New 8H Perovskite $\text{Sr}_8\text{Os}_{6.3}\text{O}_{24}$ Exhibiting High T_c Ferromagnetism*, Cryst. Growth Des. **21**, 2459–2464 (2021), doi:10.1021/acs.cgd.1c00057.

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