$Ag_{13}OsO_6$ Structure: A13B6C_cF160_226_bi_f_a-001

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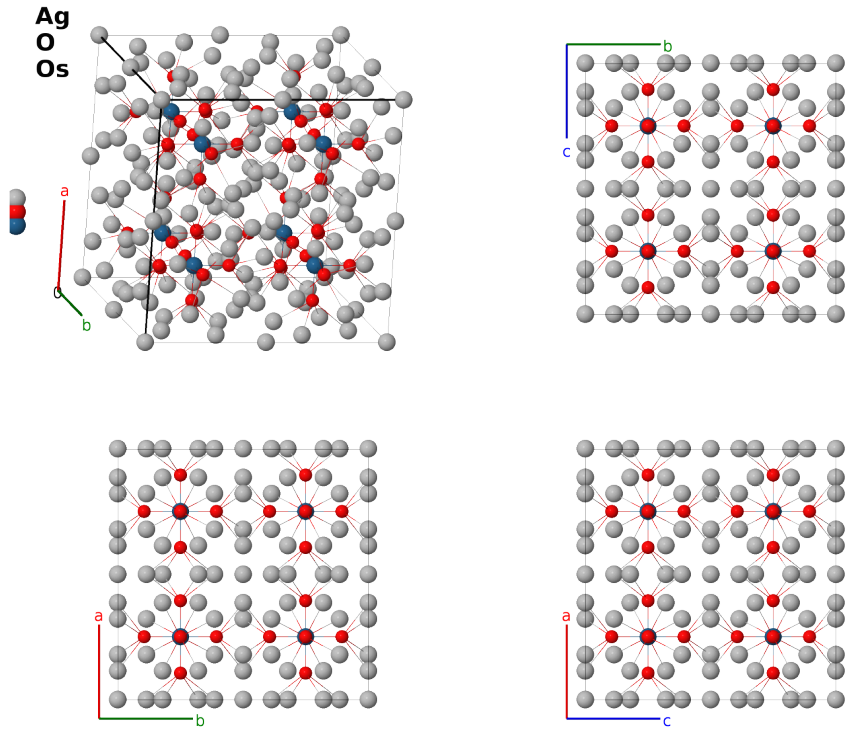
https://aflow.org/prototype-encyclopedia/1RP0

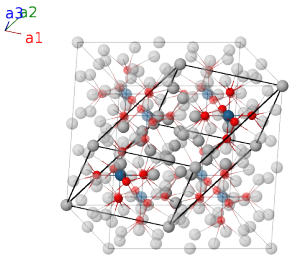
https://aflow.org/prototype-encyclopedia/A13B6C_cF160_226_bi_f_a-001



Prototype	$Ag_{13}O_6Os$
AFLOW prototype label	A13B6C_cF160_226_bi_f_a-001
ICSD	413193
CCDC	1663064
Pearson symbol	cF160
Space group number	226
Space group symbol	$Fm\bar{3}c$
AFLOW prototype command	`aflow --proto=A13B6C_cF160_226_bi_f_a-001 --params=`a, x_3, y_4, z_4

Face-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8a)	Os I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8a)	Os I
$\mathbf{B_3}$	=	0	=	0	(8b)	Ag I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(8b)	Ag I
$\mathbf{B_5}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_8}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{11}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{14}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{16}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(48f)	O I
$\mathbf{B_{17}}$	=	$(y_4 + z_4)\,\mathbf{a}_1 - (y_4 - z_4)\,\mathbf{a}_2 + (y_4 - z_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{18}}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 - (y_4 + z_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{19}}$	=	$(y_4 - z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{20}}$	=	$-(y_4 + z_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{21}}$	=	$(y_4 - z_4)\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(96i)	Ag II

$\mathbf{B_{22}}$	$=$	$-\left(y_4+z_4\right)\,\mathbf{a}_1-\left(y_4-z_4\right)\,\mathbf{a}_2+\left(y_4+z_4\right)\,\mathbf{a}_3$	$=$	$az_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{23}}$	$=$	$\left(y_4+z_4\right)\,\mathbf{a}_1+\left(y_4-z_4\right)\,\mathbf{a}_2-\left(y_4+z_4\right)\,\mathbf{a}_3$	$=$	$-az_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{24}}$	$=$	$-\left(y_4-z_4\right)\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2+\left(y_4-z_4\right)\,\mathbf{a}_3$	$=$	$-az_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{25}}$	$=$	$-\left(y_4-z_4\right)\,\mathbf{a}_1+\left(y_4-z_4\right)\,\mathbf{a}_2+\left(y_4+z_4\right)\,\mathbf{a}_3$	$=$	$ay_4\,\hat{\mathbf{x}}+az_4\,\hat{\mathbf{y}}$	(96i)	Ag II
$\mathbf{B_{26}}$	$=$	$\left(y_4+z_4\right)\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2-\left(y_4-z_4\right)\,\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{x}}+az_4\,\hat{\mathbf{y}}$	(96i)	Ag II
$\mathbf{B_{27}}$	$=$	$-\left(y_4+z_4\right)\,\mathbf{a}_1+\left(y_4+z_4\right)\,\mathbf{a}_2+\left(y_4-z_4\right)\,\mathbf{a}_3$	$=$	$ay_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}$	(96i)	Ag II
$\mathbf{B_{28}}$	$=$	$\left(y_4-z_4\right)\,\mathbf{a}_1-\left(y_4-z_4\right)\,\mathbf{a}_2-\left(y_4+z_4\right)\,\mathbf{a}_3$	$=$	$-ay_4\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}$	(96i)	Ag II
$\mathbf{B_{29}}$	$=$	$-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-a\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{30}}$	$=$	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-a\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{31}}$	$=$	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{32}}$	$=$	$\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{33}}$	$=$	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{34}}$	$=$	$\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{35}}$	$=$	$-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}-a\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{36}}$	$=$	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}-a\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{37}}$	$=$	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{38}}$	$=$	$-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(96i)	Ag II
$\mathbf{B_{39}}$	$=$	$\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4+z_4-\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(96i)	Ag II

$\mathbf{B_{40}}$	$= \left(-y_4 + z_4 + \frac{1}{2}\right)\mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\mathbf{a}_2 - \left(y_4 + z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$= -a\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(96i)	Ag II

References

[1] S. Ahlert, W. Klein, O. Jepsen, O. Gunnarsson, O. K. Andersen, and M. Jansen, *$Ag_{13}OsO_6$: A Silver Oxide with Interconnected Icosahedral $Ag_{13}4^+$ Clusters and Dispersed $[OsO_6]^{4-}$ Octahedra*, Angew. Chem. Int. Ed. **42**, 4322–4325 (2003), doi:10.1002/anie.200351740.

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