β-$SrIrO_3$ Perovskite Structure: A2B6C7_cI90_204_e_dg_ac2f-001

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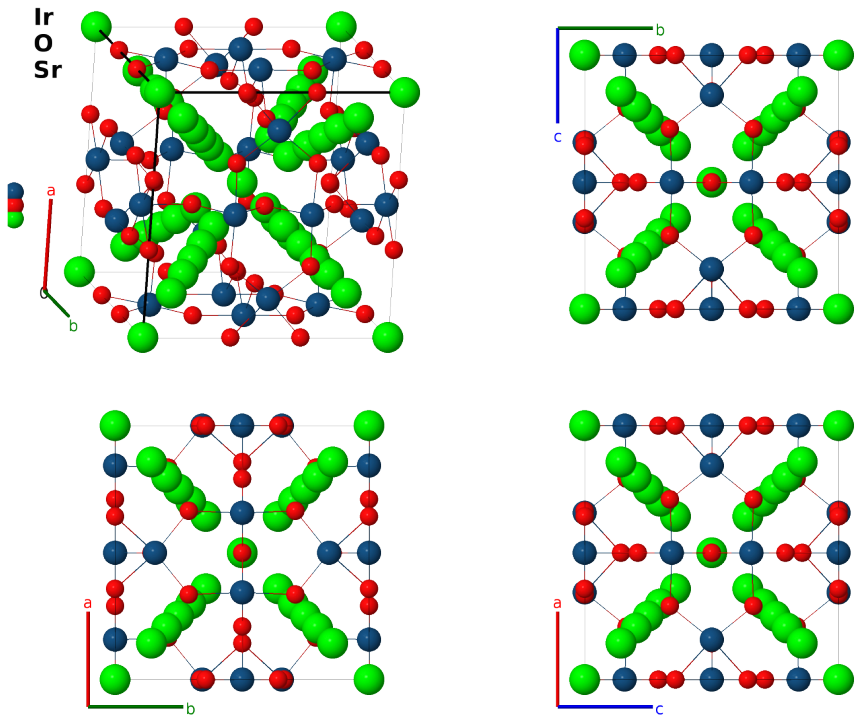
https://aflow.org/prototype-encyclopedia/1EJ0

https://aflow.org/prototype-encyclopedia/A2B6C7_cI90_204_e_dg_ac2f-001



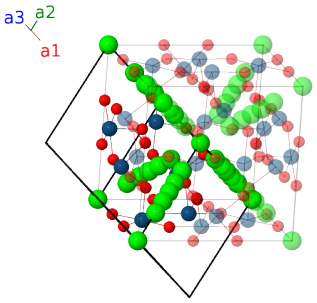
Prototype	$IrSrO_3$
AFLOW prototype label	A2B6C7_cI90_204_e_dg_ac2f-001
ICSD	33738
CCDC	1606480
Pearson symbol	cI90
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	`aflow --proto=A2B6C7_cI90_204_e_dg_ac2f-001 --params=`$a, x_3, x_4, x_5, x_6, y_7, z_7$

- The structural transitions in $SrIrO_3$ are less certain than for other perovskites.

  - The ground state is usually believed to be monoclinic with space group $C2/c$ #15, however
  - (Schmalle, 1990) found a somewhat disordered room temperature cubic phase (this structure).
  - (Longo, 1971) found that to the right of a line from (700°C, 5GPa) to (1650°, 2GPa) there is a transformation to the orthorhombic $CaTiO_3$ structure, but
  - (Wang, 2024) found a tetragonal double perovskite structure formed at 1400°C and 6GPa, well into the range where (Longo, 1971) found the orthorhombic structure. This structure is very close to cubic perovskite ($E2_1$), which may well be the structure found at higher pressures and temperatures.
- The Greek letters used to designate the phase are arbitrarily assigned in the order of the first publication describing the phases.
- All of the strontium sites in this structure are sparsely populated. The occupation numbers from (Schmalle, 1990) do not give the correct stoichiometry, so we use the values from the ICSD entry. The occupations are:
  - Sr I 33.6%
  - Sr II 12.0%
  - Sr III 23.4%
  - Sr IV 30.0%
- These values give a stoichiometry of $Sr_{0.848}IrO_3$.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Sr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(12d)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(12d)	O I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(12d)	O I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(12d)	O I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12e)	Ir I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12e)	Ir I

$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}$	(12e)	Ir I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}$	(12e)	Ir I
$\mathbf{B_{16}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(12e)	Ir I
$\mathbf{B_{17}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(12e)	Ir I
$\mathbf{B_{18}}$	=	$2x_5\,\mathbf{a}_1+2x_5\,\mathbf{a}_2+2x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{19}}$	=	$-2x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{20}}$	=	$-2x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{21}}$	=	$-2x_5\,\mathbf{a}_1$	=	$ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{22}}$	=	$-2x_5\,\mathbf{a}_1-2x_5\,\mathbf{a}_2-2x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{23}}$	=	$2x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{24}}$	=	$2x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{25}}$	=	$2x_5\,\mathbf{a}_1$	=	$-ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(16f)	Sr III
$\mathbf{B_{26}}$	=	$2x_6\,\mathbf{a}_1+2x_6\,\mathbf{a}_2+2x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{27}}$	=	$-2x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{28}}$	=	$-2x_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{29}}$	=	$-2x_6\,\mathbf{a}_1$	=	$ax_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{30}}$	=	$-2x_6\,\mathbf{a}_1-2x_6\,\mathbf{a}_2-2x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{31}}$	=	$2x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{32}}$	=	$2x_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{33}}$	=	$2x_6\,\mathbf{a}_1$	=	$-ax_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+ax_6\,\hat{\mathbf{z}}$	(16f)	Sr IV
$\mathbf{B_{34}}$	=	$(y_7+z_7)\,\mathbf{a}_1+z_7\,\mathbf{a}_2+y_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{y}}+az_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{35}}$	=	$-(y_7-z_7)\,\mathbf{a}_1+z_7\,\mathbf{a}_2-y_7\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{y}}+az_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{36}}$	=	$(y_7-z_7)\,\mathbf{a}_1-z_7\,\mathbf{a}_2+y_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{y}}-az_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{37}}$	=	$-(y_7+z_7)\,\mathbf{a}_1-z_7\,\mathbf{a}_2-y_7\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{y}}-az_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{38}}$	=	$y_7\,\mathbf{a}_1+(y_7+z_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$az_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{39}}$	=	$-y_7\,\mathbf{a}_1-(y_7-z_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$az_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{40}}$	=	$y_7\,\mathbf{a}_1+(y_7-z_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-az_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{41}}$	=	$-y_7\,\mathbf{a}_1-(y_7+z_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-az_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{z}}$	(24g)	O II
$\mathbf{B_{42}}$	=	$z_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+(y_7+z_7)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}}+az_7\,\hat{\mathbf{y}}$	(24g)	O II
$\mathbf{B_{43}}$	=	$z_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2-(y_7-z_7)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+az_7\,\hat{\mathbf{y}}$	(24g)	O II
$\mathbf{B_{44}}$	=	$-z_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+(y_7-z_7)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}}-az_7\,\hat{\mathbf{y}}$	(24g)	O II
$\mathbf{B_{45}}$	=	$-z_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2-(y_7+z_7)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}-az_7\,\hat{\mathbf{y}}$	(24g)	O II

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