γ-$SrIrO_3$ Double Perovskite Structure: AB3C_tP10_123_g_abi_cd-001

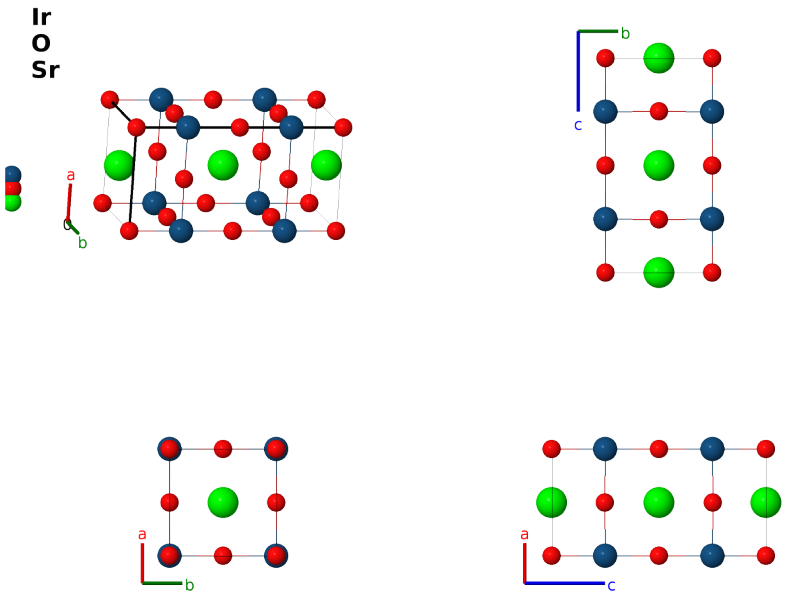
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/2HYS

https://aflow.org/prototype-encyclopedia/AB3C_tP10_123_g_abi_cd-001



Prototype	$IrSrO_3$
AFLOW prototype label	AB3C_tP10_123_g_abi_cd-001
Pearson symbol	tP10
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB3C_tP10_123_g_abi_cd-001 --params=`$a, c/a, z_5, z_6$

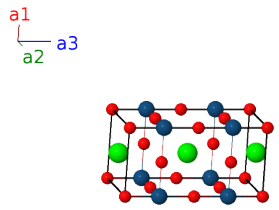
- The structural transitions in $SrIrO_3$ are less certain than for other perovskites.
  - The ground state is usually believed to be monoclinic with space group $C2/c$ #15, however
  - (Schmalle, 1990) found a somewhat disordered room temperature cubic phase.
  - (Longo, 1971) found that to the right 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 (this structure), 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.
- (Wang, 2024) found the current structure to be metastable under ambient conditions and made their structureal measurements at room temperature.
- When c = 2 a and $z_4 = z_5 = 1/4$ this becomes the cubic perovskite ($E2_1$) structure.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	O II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	Sr I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Sr II
$\mathbf{B_5}$	=	$z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(2g)	Ir I
$\mathbf{B_6}$	=	$-z_5\,\mathbf{a}_3$	=	$-cz_5\,\hat{\mathbf{z}}$	(2g)	Ir I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(4i)	O III

References

[1] H. Wang, A. de la Torre, J. T. Race, Q. Wang, J. P. C. Ruff, P. M. Woodward, K. W. Plumb, D. Walker, and W. Xie, *Pseudosymmetry in Tetragonal Perovskite $SrIrO_3$ Synthesized under High Pressure*, ACS App. Electron. Mater. **6**, 6820–6825 (2024), doi:10.1021/acsaelm.4c01214.

[2] H. Schmalle, C. Gurtner, H. R. Oswald, and A. Reller, *The crystal structure of $SrIrO_3$*, Z. Krystallogr. **191**, 239–247 (1990), doi:10.1524/zkri.1990.191.14.239.

[3] J. M. Longo, J. A. Kafalas, and R. Arnott, *Structure and properties of the high and low pressure forms of $SrIrO_3$*, J. Solid State Chem. **3**, 174–179 (1971), doi:10.1016/0022-4596(71)90022-3.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).