Sr_2IrO_4 Structure: AB4C2_tI56_142_a_df_d-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.

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https://aflow.org/prototype-encyclopedia/EHYC

https://aflow.org/prototype-encyclopedia/AB4C2_tI56_142_a_df_d-001

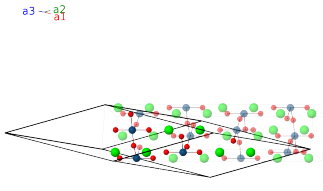
Prototype	IrO_4Sr_2
AFLOW prototype label	AB4C2_tI56_142_a_df_d-001
ICSD	78260
CCDC	1638545
Pearson symbol	tI56
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	`aflow --proto=AB4C2_tI56_142_a_df_d-001 --params=`$a, c/a, z_2, z_3, x_4$

Other compounds with this structure
Ca_2CrO_4, Ca_2MnO_4, Sr_2HfO_4, Sr_2RhO_4

- The ICSD uses Ca_2MnO_4 to represent this structure type.

Body-centered Tetragonal primitive vectors

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



Basis vectors

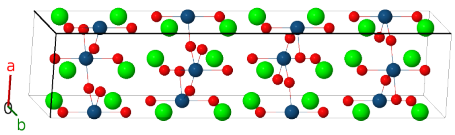
		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8a)	Ir I

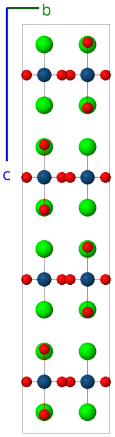
$\mathbf{B_2}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8a)	Ir I
$\mathbf{B_3}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8a)	Ir I
$\mathbf{B_4}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8a)	Ir I
$\mathbf{B_5}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_7}$	=	$-\left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_8}$	=	$-\left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_9}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_{10}}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_{11}}$	=	$\left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_{12}}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	O I
$\mathbf{B_{13}}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{14}}$	=	$z_3\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{15}}$	=	$-\left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{16}}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{17}}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{18}}$	=	$-z_3\,\mathbf{a}_1 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{19}}$	=	$\left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{20}}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16d)	Sr I
$\mathbf{B_{21}}$	=	$\left(x_4 + \frac{3}{8}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{22}}$	=	$-\left(x_4 - \frac{3}{8}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{23}}$	=	$\left(x_4 + \frac{1}{8}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{24}}$	=	$-\left(x_4 - \frac{1}{8}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{3}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{25}}$	=	$-\left(x_4 - \frac{5}{8}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{7}{8}\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{26}}$	=	$\left(x_4 + \frac{5}{8}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{7}{8}\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{27}}$	=	$-\left(x_4 - \frac{7}{8}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{5}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	O II
$\mathbf{B_{28}}$	=	$\left(x_4 + \frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{5}{8}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	O II

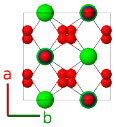
References

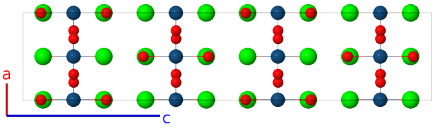
[1] M. K. Crawford, M. A. Subramanian, R. L. Harlow, J. A. Fernandez-Baca, Z. R. Wang, and D. C. Johnston, *Structural and magnetic studies of Sr_2IrO_4*, Phys. Rev. B **49**, 9198–9201 (1994), doi:10.1103/PhysRevB.87.140406.

Ir
O
Sr









Found in

[1] F. Ye, S. Chi, B. C. Chakoumakos, J. A. Fernandez-Baca, T. Qi, and G. Cao, *Magnetic and crystal structures of Sr_2IrO_4: A neutron diffraction study*, Phys. Rev. B **87**, 140406 (2013), doi:10.1103/PhysRevB.87.140406.

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