β-$BaIrO_3$ Perovskite Structure: ABC3_mC50_12_a2i_c2i_be2i2j-001

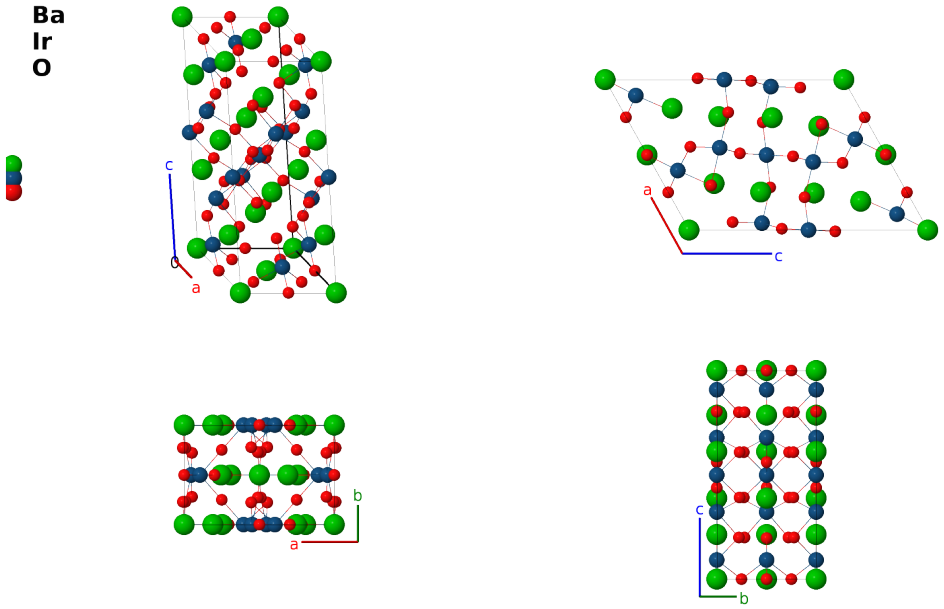
Cite this page as:

- 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/4SZ0

https://aflow.org/prototype-encyclopedia/ABC3_mC50_12_a2i_c2i_be2i2j-001



Prototype	$BaIrO_3$
AFLOW prototype label	ABC3_mC50_12_a2i_c2i_be2i2j-001
ICSD	173849
CCDC	1688750
Pearson symbol	mC50
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=ABC3_mC50_12_a2i_c2i_be2i2j-001 --params=`$a, b/a, c/a, \beta, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

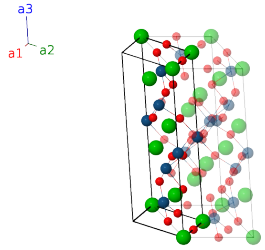
- $BaIrO_3$ is a distorted perovskite which has a number of phase transitions with increasing pressure (Cheng, 2009; Cheng, 2013).
- (Cheng, 2009) label the structures by the approximate stacking of the BaO_3 layers.

– 0-3 GPa: the ground state α-$BaIrO_3$ "9R" structure, in space group $C2/m$ #12.
– 3-5 GPa: β-$BaIrO_3$ "5H" structure, also in space group $C2/m$ #12. (this structure)
– 5-18 GPa: γ-$BaIrO_3$, which has the $SrIrO_3$ "6H" structure.
– 18-?? GPa: δ-$BaIrO_3$ is in the tetragonal γ-$SrZrO_3$ structure.
– Presumably at some point above 25 GPa the compound transforms into the cubic perovskite ($E2_1$) "3C" structure.

- AFLOW moved the origin from the Ir I site to the Ba I site, a shift of $1/2(\mathbf{a_1}+\mathbf{a_2}+\mathbf{a_3})$.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	Ir I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4e)	O II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}}$	(4e)	O II
$\mathbf{B_6}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ba II
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ba II
$\mathbf{B_8}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ba III
$\mathbf{B_9}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ba III
$\mathbf{B_{10}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ir II
$\mathbf{B_{11}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ir II
$\mathbf{B_{12}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ir III
$\mathbf{B_{13}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ir III
$\mathbf{B_{14}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{15}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{16}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{17}}$	=	$-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{18}}$	=	$(x_{11} - y_{11})\,\mathbf{a}_1 + (x_{11} + y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B_{19}}$	=	$-(x_{11} + y_{11})\,\mathbf{a}_1 - (x_{11} - y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B_{20}}$	=	$-(x_{11} - y_{11})\,\mathbf{a}_1 - (x_{11} + y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O V

$\mathbf{B_{21}}$	$=$	$(x_{11}+y_{11})\,\mathbf{a}_1+$ $(x_{11}-y_{11})\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3$	$=$	$(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O V
$\mathbf{B_{22}}$	$=$	$(x_{12}-y_{12})\,\mathbf{a}_1+$ $(x_{12}+y_{12})\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	$=$	$(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O VI
$\mathbf{B_{23}}$	$=$	$-(x_{12}+y_{12})\,\mathbf{a}_1-$ $(x_{12}-y_{12})\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	$=$	$-(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}-$ $cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O VI
$\mathbf{B_{24}}$	$=$	$-(x_{12}-y_{12})\,\mathbf{a}_1-$ $(x_{12}+y_{12})\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	$=$	$-(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}-$ $cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O VI
$\mathbf{B_{25}}$	$=$	$(x_{12}+y_{12})\,\mathbf{a}_1+$ $(x_{12}-y_{12})\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	$=$	$(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O VI

References

[1] J.-G. Cheng, J. A. Alonso, E. Suard, J.-S. Zhou, and J. B. Goodenough, *A New Perovskite Polytype in the High-Pressure Sequence of $BaIrO_3$*, J. Am. Chem. Soc. **131**, 7461–7469 (2009), doi:10.1021/ja901829e.

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).