Monoclinic (I) $Ba_3CoIr_2O_9$ Structure: A3BC2D9_mC60_15_ef_a_f_e4f-001

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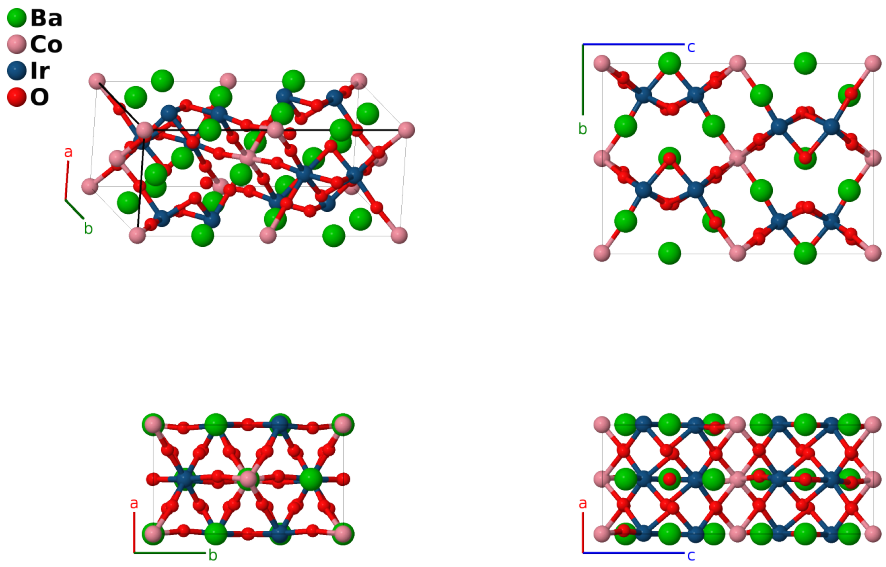
https://aflow.org/p/G3XE

https://aflow.org/p/A3BC2D9_mC60_15_ef_a_f_e4f-001



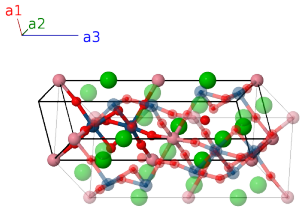
Prototype	$Ba_3CoIr_2O_9$
AFLOW prototype label	A3BC2D9_mC60_15_ef_a_f_e4f-001
ICSD	35995
Pearson symbol	mC60
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A3BC2D9_mC60_15_ef_a_f_e4f-001 --params=`$a, b/a, c/a, \beta, y_2, y_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- $Ba_3CoIr_2O_9$ has been observed in three phases (Garg, 2020):
  - Above 107K it is in the hexagonal $Ba_3CoIr_2O_9$ structure, an ordered quaternary form of the hexagonal $BaTiO_3$ structure.
  - Below 107K it transforms into this monoclinic (I) $Ba_3CoIr_2O_9$ structure.
  - "On further reduction of temperature," apparently at some point above 60K, the primitive cell doubles and the monoclinic (II) $Ba_3CoIr_2O_9$ structure appears. The monoclinic (I) and monoclinic (II) structures coexist down to absolute zero.

- Data for this structure was taken at 60K.

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	(4a)	Co I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Co I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ba II
$\mathbf{B_8}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ba II
$\mathbf{B_9}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ba II
$\mathbf{B_{10}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ba II
$\mathbf{B_{11}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ir I
$\mathbf{B_{12}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ir I
$\mathbf{B_{13}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ir I
$\mathbf{B_{14}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Ir I
$\mathbf{B_{15}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{16}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{17}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{18}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{19}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III

$\mathbf{B_{20}}$	=	$-(x_7+y_7)\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_7+c\left(z_7-\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{21}}$	=	$-(x_7-y_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-(ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{22}}$	=	$(x_7+y_7)\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_7+c\left(z_7+\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{23}}$	=	$(x_8-y_8)\,\mathbf{a}_1+(x_8+y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{24}}$	=	$-(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_8+c\left(z_8-\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{25}}$	=	$-(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{26}}$	=	$(x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_8+c\left(z_8+\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{27}}$	=	$(x_9-y_9)\,\mathbf{a}_1+(x_9+y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{28}}$	=	$-(x_9+y_9)\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_9+c\left(z_9-\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{29}}$	=	$-(x_9-y_9)\,\mathbf{a}_1-(x_9+y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$-(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{30}}$	=	$(x_9+y_9)\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_9+c\left(z_9+\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V

References

[1] C. Garg, D. Roy, M. Lonsky, P. Manuel, A. Cervellino, J. Müller, M. Kabir, and S. Nair, *Evolution of the structural, magnetic and electronic properties of the triple perovskite* $Ba_3CoIr_2O_9$, Phys. Rev. B **103**, 014437 (2021), doi:10.1103/PhysRevB.103.014437.