Monoclinic (II) $Ba_3CoIr_2O_9$ Structure: A3BC2D9_mP60_13_ef2g_ab_2g_ef8g-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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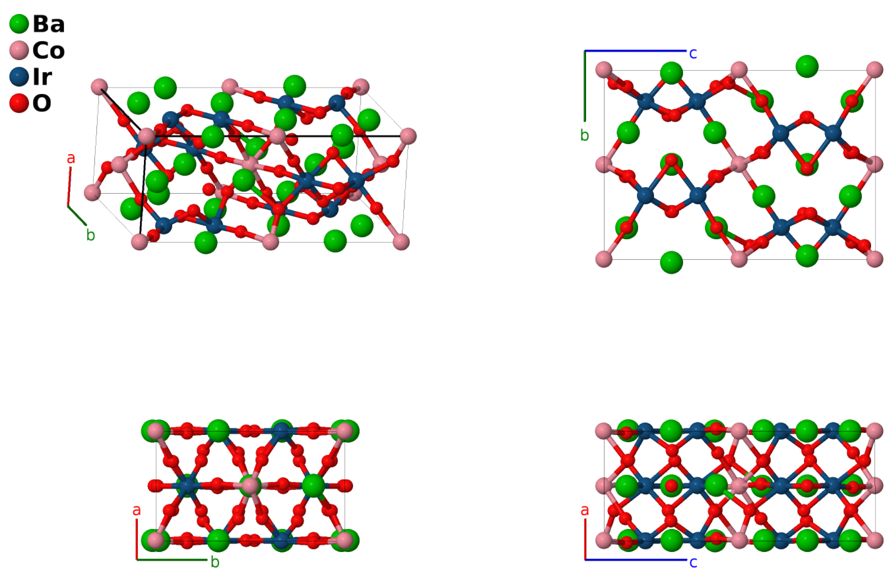
https://aflow.org/p/2BLQ

https://aflow.org/p/A3BC2D9_mP60_13_ef2g_ab_2g_ef8g-001



Prototype	$Ba_3CoIr_2O_9$
AFLOW prototype label	A3BC2D9_mP60_13_ef2g_ab_2g_ef8g-001
ICSD	35996
Pearson symbol	mP60
Space group number	13
Space group symbol	$P2/c$
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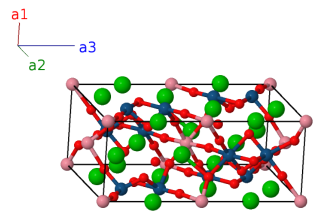
- $Ba_3CoIr_2O_9$ has been observed in three phases (Garg, 2020):
  - Above 107K it is in the hexagonal $Ba_3CoIr_2O_9$ structure, an ordered quaternary form of the hexagonal $BaTiO_3$ structure.
  - Below 107K it transforms into the monoclinic (I) $Ba_3CoIr_2O_9$ structure.
  - "On further reduction of temperature," apparently at some point above 60K, the primitive cell doubles and this 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.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Co I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Co II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}\left(a + c\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2b)	Co II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	Ba I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	Ba I
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{c\cos\beta}{4}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	Ba II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{3c\cos\beta}{4}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	Ba II
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{c\cos\beta}{4}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	O II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\left(\frac{a}{2} + \frac{3c\cos\beta}{4}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(2f)	O II
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba III
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba III
$\mathbf{B_{15}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba III
$\mathbf{B_{16}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba III
$\mathbf{B_{17}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba IV
$\mathbf{B_{18}}$	=	$-x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba IV
$\mathbf{B_{19}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba IV
$\mathbf{B_{20}}$	=	$x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ba IV
$\mathbf{B_{21}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir I
$\mathbf{B_{22}}$	=	$-x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_9 + c\left(z_9 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir I
$\mathbf{B_{23}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir I
$\mathbf{B_{24}}$	=	$x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_9 + c\left(z_9 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir I

$\mathbf{B_{25}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir II
$\mathbf{B_{26}}$	=	$-x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{10} + c\left(z_{10} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir II
$\mathbf{B_{27}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir II
$\mathbf{B_{28}}$	=	$x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{10} + c\left(z_{10} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	Ir II
$\mathbf{B_{29}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{30}}$	=	$-x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{11} + c\left(z_{11} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{31}}$	=	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{32}}$	=	$x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{11} + c\left(z_{11} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O III
$\mathbf{B_{33}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{34}}$	=	$-x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{12} + c\left(z_{12} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{35}}$	=	$-x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{36}}$	=	$x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{12} + c\left(z_{12} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IV
$\mathbf{B_{37}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{38}}$	=	$-x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{13} + c\left(z_{13} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{39}}$	=	$-x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{40}}$	=	$x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{13} + c\left(z_{13} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O V
$\mathbf{B_{41}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{42}}$	=	$-x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{14} + c\left(z_{14} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{43}}$	=	$-x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	=	$-(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{44}}$	=	$x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{14} + c\left(z_{14} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VI
$\mathbf{B_{45}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VII
$\mathbf{B_{46}}$	=	$-x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 - \left(z_{15} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{15} + c\left(z_{15} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - c\left(z_{15} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VII
$\mathbf{B_{47}}$	=	$-x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$-(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VII
$\mathbf{B_{48}}$	=	$x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{15} + c\left(z_{15} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + c\left(z_{15} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VII
$\mathbf{B_{49}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VIII
$\mathbf{B_{50}}$	=	$-x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 - \left(z_{16} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{16} + c\left(z_{16} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - c\left(z_{16} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VIII

$\mathbf{B_{51}}$	=	$-x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$-\left(ax_{16} + cz_{16}\cos\beta\right)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VIII
$\mathbf{B_{52}}$	=	$x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + \left(z_{16} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{16} + c\left(z_{16} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + c\left(z_{16} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O VIII
$\mathbf{B_{53}}$	=	$x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$\left(ax_{17} + cz_{17}\cos\beta\right)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} + cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IX
$\mathbf{B_{54}}$	=	$-x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 - \left(z_{17} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{17} + c\left(z_{17} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} - c\left(z_{17} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IX
$\mathbf{B_{55}}$	=	$-x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3$	=	$-\left(ax_{17} + cz_{17}\cos\beta\right)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IX
$\mathbf{B_{56}}$	=	$x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + \left(z_{17} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{17} + c\left(z_{17} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} + c\left(z_{17} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O IX
$\mathbf{B_{57}}$	=	$x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$\left(ax_{18} + cz_{18}\cos\beta\right)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} + cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O X
$\mathbf{B_{58}}$	=	$-x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 - \left(z_{18} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{18} + c\left(z_{18} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} - c\left(z_{18} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O X
$\mathbf{B_{59}}$	=	$-x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3$	=	$-\left(ax_{18} + cz_{18}\cos\beta\right)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(4g)	O X
$\mathbf{B_{60}}$	=	$x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{18} + c\left(z_{18} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} + c\left(z_{18} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4g)	O X

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.