

Zr₅Ir₃ Structure:

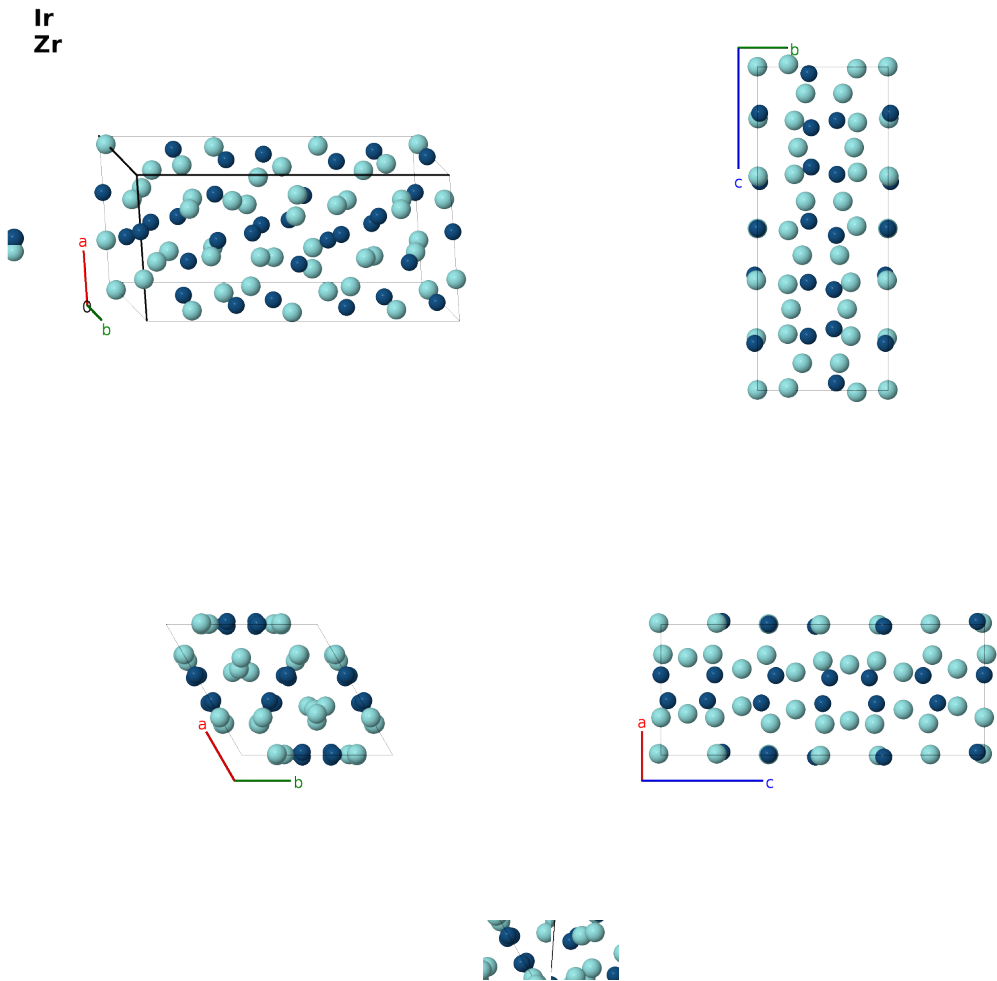
A3B5_hP48_178_ac_a2bc-001

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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.

<https://aflow.org/prototype-encyclopedia/15N7>

https://aflow.org/prototype-encyclopedia/A3B5_hP48_178_ac_a2bc-001



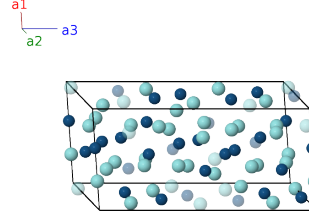
Prototype	Ir ₃ Zr ₅
AFLOW prototype label	A3B5_hP48_178_ac_a2bc-001
ICSD	104611
CCDC	1662523
Pearson symbol	hP48
Space group number	178
Space group symbol	$P6_122$

AFLOW prototype command `aflow --proto=A3B5_hP48_178_ac_a2bc-001`
 `--params=a, c/a, x1, x2, x3, x4, x5, y5, z5, x6, y6, z6`

- This structure can also be found in the enantiomorphic space group $P6_522$ #179.
- The ICSD entry sets $c = 17.701\text{\AA}$ rather than $17.01\text{\AA}$ as found in (Cenzual, 1986). We use the published value for c .

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1$	=	$\frac{1}{2}ax_1\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\hat{\mathbf{y}}$	(6a)	Ir I
$\mathbf{B}_2$	$x_1 \mathbf{a}_2 + \frac{1}{3}\mathbf{a}_3$	=	$\frac{1}{2}ax_1\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$	(6a)	Ir I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{2}{3}\mathbf{a}_3$	=	$-ax_1\hat{\mathbf{x}} + \frac{2}{3}c\hat{\mathbf{z}}$	(6a)	Ir I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(6a)	Ir I
$\mathbf{B}_5$	$-x_1 \mathbf{a}_2 + \frac{5}{6}\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\hat{\mathbf{y}} + \frac{5}{6}c\hat{\mathbf{z}}$	(6a)	Ir I
$\mathbf{B}_6$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{6}\mathbf{a}_3$	=	$ax_1\hat{\mathbf{x}} + \frac{1}{6}c\hat{\mathbf{z}}$	(6a)	Ir I
$\mathbf{B}_7$	$x_2 \mathbf{a}_1$	=	$\frac{1}{2}ax_2\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}}$	(6a)	Zr I
$\mathbf{B}_8$	$x_2 \mathbf{a}_2 + \frac{1}{3}\mathbf{a}_3$	=	$\frac{1}{2}ax_2\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$	(6a)	Zr I
$\mathbf{B}_9$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{2}{3}\mathbf{a}_3$	=	$-ax_2\hat{\mathbf{x}} + \frac{2}{3}c\hat{\mathbf{z}}$	(6a)	Zr I
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(6a)	Zr I
$\mathbf{B}_{11}$	$-x_2 \mathbf{a}_2 + \frac{5}{6}\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}} + \frac{5}{6}c\hat{\mathbf{z}}$	(6a)	Zr I
$\mathbf{B}_{12}$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{6}\mathbf{a}_3$	=	$ax_2\hat{\mathbf{x}} + \frac{1}{6}c\hat{\mathbf{z}}$	(6a)	Zr I
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6b)	Zr II
$\mathbf{B}_{14}$	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{7}{12}\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{7}{12}c\hat{\mathbf{z}}$	(6b)	Zr II
$\mathbf{B}_{15}$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{11}{12}\mathbf{a}_3$	=	$-\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{11}{12}c\hat{\mathbf{z}}$	(6b)	Zr II
$\mathbf{B}_{16}$	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6b)	Zr II
$\mathbf{B}_{17}$	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{12}\mathbf{a}_3$	=	$\frac{3}{2}ax_3\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}} + \frac{1}{12}c\hat{\mathbf{z}}$	(6b)	Zr II
$\mathbf{B}_{18}$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{5}{12}\mathbf{a}_3$	=	$\sqrt{3}ax_3\hat{\mathbf{y}} + \frac{5}{12}c\hat{\mathbf{z}}$	(6b)	Zr II
$\mathbf{B}_{19}$	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(6b)	Zr III
$\mathbf{B}_{20}$	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{7}{12}\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + \frac{7}{12}c\hat{\mathbf{z}}$	(6b)	Zr III
$\mathbf{B}_{21}$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{11}{12}\mathbf{a}_3$	=	$-\sqrt{3}ax_4\hat{\mathbf{y}} + \frac{11}{12}c\hat{\mathbf{z}}$	(6b)	Zr III
$\mathbf{B}_{22}$	$-x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(6b)	Zr III

$\mathbf{B}_{23} =$	$2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{12} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{12}c \hat{\mathbf{z}}$	(6b)	Zr III
$\mathbf{B}_{24} =$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{5}{12} \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6b)	Zr III
$\mathbf{B}_{25} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{26} =$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{27} =$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{28} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{29} =$	$y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{5}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{6}c(6z_5 + 5) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{30} =$	$(x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{6}) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{31} =$	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (z_5 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - c(z_5 - \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{32} =$	$(x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{33} =$	$-x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{34} =$	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{5}{6}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - \frac{1}{6}c(6z_5 - 5) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{35} =$	$-(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{36} =$	$x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{6}) \hat{\mathbf{z}}$	(12c)	Ir II
$\mathbf{B}_{37} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{38} =$	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{39} =$	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{40} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{41} =$	$y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{5}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{6}c(6z_6 + 5) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{42} =$	$(x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{6}) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{43} =$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (z_6 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - c(z_6 - \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{44} =$	$(x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{45} =$	$-x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - \frac{1}{3}c(3z_6 - 2) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{46} =$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{5}{6}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - \frac{1}{6}c(6z_6 - 5) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{47} =$	$-(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12c)	Zr IV
$\mathbf{B}_{48} =$	$x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{6}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{6}) \hat{\mathbf{z}}$	(12c)	Zr IV

References

- [1] K. Cenxual and E. Parthé, *Zr₅Ir₃ with a deformation superstructure of the Mn₅Si₃ structure*, Acta Crystallogr. Sect. C **42**, 1101–1105 (1986), doi:10.1107/S0108270186093253.

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