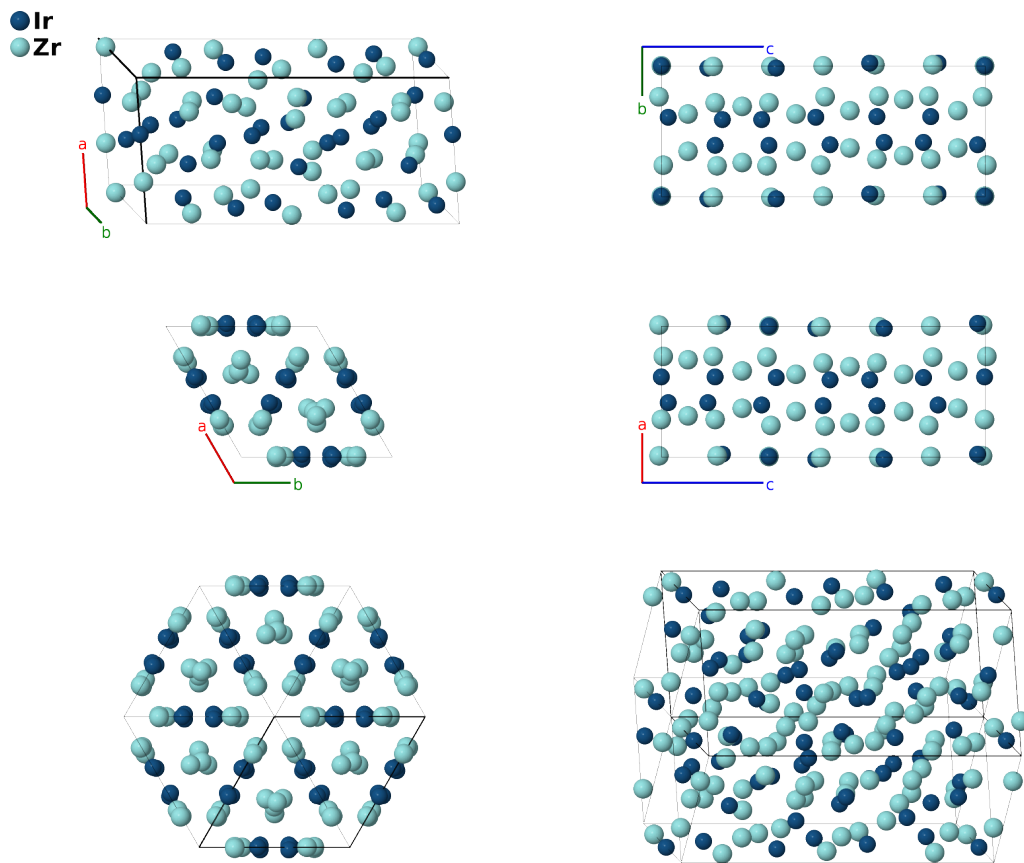


# Zr<sub>5</sub>Ir<sub>3</sub> Structure: A3B5\_hP48\_178\_ac\_a2bc-001

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<https://afLOW.org/p/15N7>

[https://afLOW.org/p/A3B5\\_hP48\\_178\\_ac\\_a2bc-001](https://afLOW.org/p/A3B5_hP48_178_ac_a2bc-001)



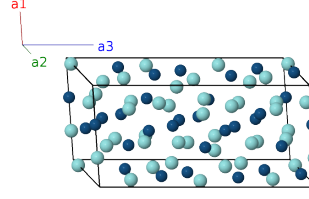
Prototype	Ir <sub>3</sub> Zr <sub>5</sub>
AFLOW prototype label	A3B5_hP48_178_ac_a2bc-001
ICSD	104611
Pearson symbol	hP48
Space group number	178
Space group symbol	<i>P</i> 6 <sub>1</sub> 22
AFLOW prototype command	<code>afLOW --proto=A3B5_hP48_178_ac_a2bc-001 --params=a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></code>

- This structure can also be found in the enantiomorphic space group *P*6<sub>5</sub>22 #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

$$\begin{aligned}
\mathbf{B}_{29} &= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{5}{6}\right) \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) & \text{Ir II} \\
\mathbf{B}_{30} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{6}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{6}\right) \hat{\mathbf{z}} & (12c) & \text{Ir II} \\
\mathbf{B}_{31} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{3}\right) \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\left(z_5 - \frac{1}{3}\right) \hat{\mathbf{z}} & (12c) & \text{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) & \text{Ir II} \\
\mathbf{B}_{33} &= -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - \left(z_5 - \frac{2}{3}\right) \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) & \text{Ir II} \\
\mathbf{B}_{34} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{5}{6}\right) \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) & \text{Ir II} \\
\mathbf{B}_{35} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (12c) & \text{Ir II} \\
\mathbf{B}_{36} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - \left(z_5 - \frac{1}{6}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{6}\right) \hat{\mathbf{z}} & (12c) & \text{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) & \text{Zr IV} \\
\mathbf{B}_{38} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(z_6 + \frac{1}{3}\right) \mathbf{a}_3 = \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{3}\right) \hat{\mathbf{z}} & (12c) & \text{Zr IV} \\
\mathbf{B}_{39} &= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(z_6 + \frac{2}{3}\right) \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) & \text{Zr IV} \\
\mathbf{B}_{40} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \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\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (12c) & \text{Zr IV} \\
\mathbf{B}_{41} &= y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \left(z_6 + \frac{5}{6}\right) \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) & \text{Zr IV} \\
\mathbf{B}_{42} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{6}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{6}\right) \hat{\mathbf{z}} & (12c) & \text{Zr IV} \\
\mathbf{B}_{43} &= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{3}\right) \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\left(z_6 - \frac{1}{3}\right) \hat{\mathbf{z}} & (12c) & \text{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) & \text{Zr IV} \\
\mathbf{B}_{45} &= -x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - \left(z_6 - \frac{2}{3}\right) \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) & \text{Zr IV} \\
\mathbf{B}_{46} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - \left(z_6 - \frac{5}{6}\right) \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) & \text{Zr IV} \\
\mathbf{B}_{47} &= -(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (12c) & \text{Zr IV} \\
\mathbf{B}_{48} &= x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - \left(z_6 - \frac{1}{6}\right) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{6}\right) \hat{\mathbf{z}} & (12c) & \text{Zr IV}
\end{aligned}$$

## References

- [1] K. Cenzual and E. Parthé, *Zr<sub>5</sub>Ir<sub>3</sub> with a deformation superstructure of the Mn<sub>5</sub>Si<sub>3</sub> structure*, Acta Crystallogr. Sect. C **42**, 1101–1105 (1986), doi:10.1107/S0108270186093253.