

Zr₂₁Re₂₅ Structure:

A25B21_hR92_167_b2e3f_e3f-001

This structure originally had the label `A25B21_hR92_167_b2e3f_e3f`. Calls to that address will be redirected here.

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<https://afLOW.org/p/1BVC>

https://afLOW.org/p/A25B21_hR92_167_b2e3f_e3f-001

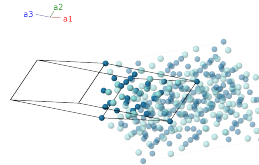
Prototype	Re ₂₅ Zr ₂₁
AFLOW prototype label	A25B21_hR92_167_b2e3f_e3f-001
ICSD	105909
Pearson symbol	hR92
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	<code>afLOW --proto=A25B21_hR92_167_b2e3f_e3f-001</code> <code>--params=a, c/a, x₂, x₃, x₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀</code>

Other compounds with this structure

Hf₂₁Re₂₅, Mg₂₁Zn₂₅, Ti₂₁Mn₂₅, Ti₂₁Re₂₅

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(2b)	Re I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Re I
\mathbf{B}_3	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_2 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a (4x_2 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Re II
\mathbf{B}_4	$= \frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_2 - 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a (4x_2 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Re II
\mathbf{B}_5	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Re II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_2 + 3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a (12x_2 + 1) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	Re II
\mathbf{B}_7	$= \frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_2 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a (12x_2 + 5) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	Re II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	Re II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	Re III

$$\begin{aligned}
\mathbf{B}_{83} &= y_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3 = -\frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} - & (12f) & \text{Zr IV} \\
& & & \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} + \\
& & & \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} \\
\mathbf{B}_{84} &= -\left(z_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - & (12f) & \text{Zr IV} \\
& & & \frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} + \\
& & & \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} - \\
& & & \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} - 3) \hat{\mathbf{z}} \\
\mathbf{B}_{85} &= -\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 - & (12f) & \text{Zr IV} \\
& & & -\frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} - \\
& & & \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} - \\
& & & \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} - 3) \hat{\mathbf{z}} \\
\mathbf{B}_{86} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_2 - & (12f) & \text{Zr IV} \\
& & & -\frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} + \\
& & & \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} - \\
& & & \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} - 3) \hat{\mathbf{z}} \\
\mathbf{B}_{87} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = & (12f) & \text{Zr IV} \\
& & & -\frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} + \\
& & & \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} - \\
& & & \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} \\
\mathbf{B}_{88} &= -z_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - y_{10} \mathbf{a}_3 = & (12f) & \text{Zr IV} \\
& & & \frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} - \\
& & & \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} - \\
& & & \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} \\
\mathbf{B}_{89} &= -y_{10} \mathbf{a}_1 - z_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3 = & (12f) & \text{Zr IV} \\
& & & \frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} + \\
& & & \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} - \\
& & & \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} \\
\mathbf{B}_{90} &= \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + & (12f) & \text{Zr IV} \\
& & & -\frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} - \\
& & & \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} + \\
& & & \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} + 3) \hat{\mathbf{z}} \\
\mathbf{B}_{91} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 + & (12f) & \text{Zr IV} \\
& & & \frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} + \\
& & & \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} + \\
& & & \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} + 3) \hat{\mathbf{z}} \\
\mathbf{B}_{92} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_2 + & (12f) & \text{Zr IV} \\
& & & \frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} - \\
& & & \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} + \\
& & & \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} + 3) \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] K. Cenzual, E. Parthé, and R. M. Waterstrat, *Zr₂₁Re₂₅, a new rhombohedral structure type containing 12Å-thick infinite MgZn₂(Laves)-type columns*, Acta Crystallogr. Sect. C **42**, 261–266 (1986), doi:10.1107/S0108270186096555.

Found in

- [1] R. Cerný and G. Renaudin, *The intermetallic compound Mg₂₁Zn₂₅*, Acta Crystallogr. Sect. C **58**, i154–i155 (2002), doi:10.1107/S0108270102018103.

● Re
● Zr

