

Zr₂₁Re₂₅ Structure:

A25B21_hR92_167_b2e3f_e3f-001

This structure previously used the label(s) **A25B21_hR92_167_b2e3f_e3f**. Calls to these addresses will be redirected here.

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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/1BVC>

https://aflow.org/prototype-encyclopedia/A25B21_hR92_167_b2e3f_e3f-001

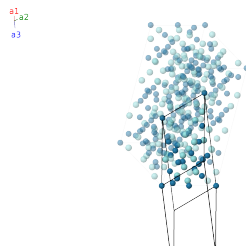
Prototype	Re ₂₅ Zr ₂₁
AFLOW prototype label	A25B21_hR92_167_b2e3f_e3f-001
ICSD	105909
CCDC	1663776
Pearson symbol	hR92
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	<pre>aflow --proto=A25B21_hR92_167_b2e3f_e3f-001 --params=a,c/a,x₂,x₃,x₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀</pre>

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

$\mathbf{B}_{35} =$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{36} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 - 3) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{37} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 - 3) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{38} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 - 3) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{39} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{40} =$	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{41} =$	$-y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{42} =$	$(z_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (x_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{43} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{44} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 + (y_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}}$	(12f)	Re V
$\mathbf{B}_{45} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{46} =$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{47} =$	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{48} =$	$-(z_7 - \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 - 3) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{49} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} - \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 - 3) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{50} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 - (y_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} - \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 - 3) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{51} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{52} =$	$-z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{53} =$	$-y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{54} =$	$(z_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}}$	(12f)	Re VI
$\mathbf{B}_{55} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$ </				

$$\begin{aligned}
\mathbf{B}_{81} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{82} &= z_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + y_{10} \mathbf{a}_3 = -\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}} & (12f) & \text{Zr IV} \\
\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}} - \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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{84} &= -\left(z_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_3 = \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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{85} &= -\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 = -\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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{86} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_3 = -\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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{87} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -\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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{88} &= -z_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - y_{10} \mathbf{a}_3 = \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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{89} &= -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}} + \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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{90} &= \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_3 = -\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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{91} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 = \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}} & (12f) & \text{Zr IV} \\
\mathbf{B}_{92} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_3 = \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}} & (12f) & \text{Zr IV}
\end{aligned}$$

References

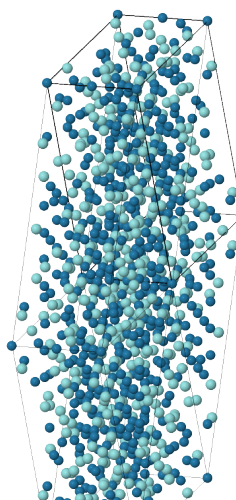
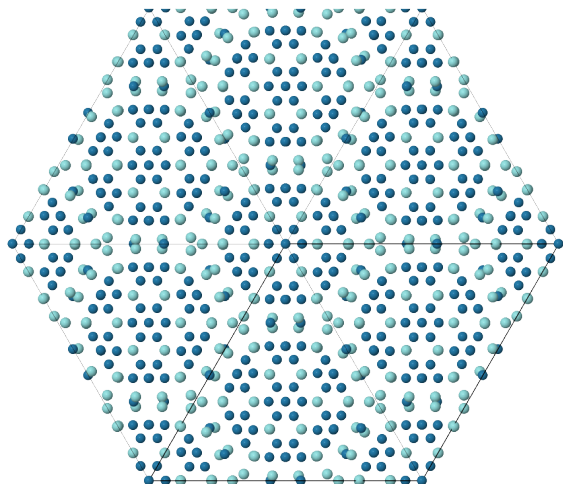
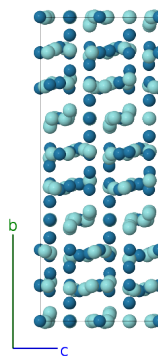
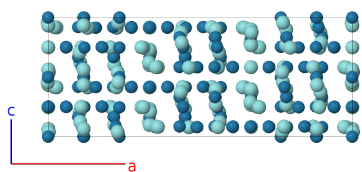
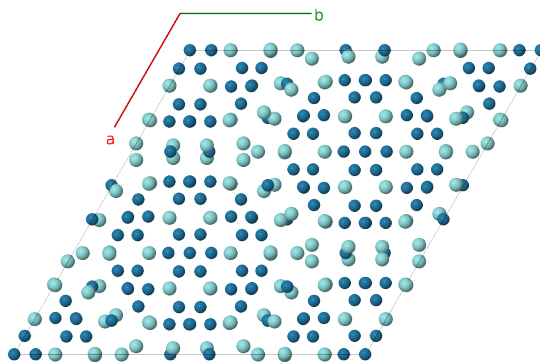
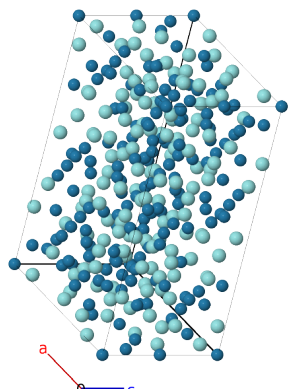
- [1] K. Cenxual, E. Parthé, and R. M. Waterstrat, *Zr₂₁Re₂₅, a new rhombohedral structure type containing 12Å-thick infinite MgZn₂(Laves)-type columns*, Acta Crystallogr. Sect. C **42**, 261–266 (1986), doi:10.1107/S0108270186096555.

Found in

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

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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.