

Rh₁₀Ga₁₇ Structure:

A17B10_tP108_116_e8j_ad2g2h5i-001

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<https://aflow.org/prototype-encyclopedia/D8JE>

https://aflow.org/prototype-encyclopedia/A17B10_tP108_116_e8j_ad2g2h5i-001

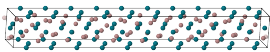
Prototype	Ga ₁₇ Rh ₁₀
AFLOW prototype label	A17B10_tP108_116_e8j_ad2g2h5i-001
ICSD	103949
CCDC	1661877
Pearson symbol	tP108
Space group number	116
Space group symbol	$P\bar{4}c2$
AFLOW prototype command	<pre>aflow --proto=A17B10_tP108_116_e8j_ad2g2h5i-001 --params=a, c/a, x₃, z₄, z₅, z₆, z₇, z₈, z₉, z₁₀, z₁₁, z₁₂, x₁₃, y₁₃, z₁₃, x₁₄, y₁₄, z₁₄, x₁₅, y₁₅, z₁₅, x₁₆, y₁₆, z₁₆, x₁₇, y₁₇, z₁₇, x₁₈, y₁₈, z₁₈, x₁₉, y₁₉, z₁₉, x₂₀, y₂₀, z₂₀</pre>

- We have shifted the origin used by (Vollenkle, 1967) to place the Rh I atom on the (2a) site rather than the (2b) site.

Simple Tetragonal primitive vectors



$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$\frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2a) Rh I

$\mathbf{B}_{84} =$	$-y_{17} \mathbf{a}_1 - x_{17} \mathbf{a}_2 - \left(z_{17} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} - c \left(z_{17} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VI
$\mathbf{B}_{85} =$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$ax_{18} \hat{\mathbf{x}} + ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{86} =$	$-x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} - ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{87} =$	$y_{18} \mathbf{a}_1 - x_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$ay_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{88} =$	$-y_{18} \mathbf{a}_1 + x_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-ay_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{89} =$	$x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_{18} \hat{\mathbf{x}} - ay_{18} \hat{\mathbf{y}} + c \left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{90} =$	$-x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} + ay_{18} \hat{\mathbf{y}} + c \left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{91} =$	$y_{18} \mathbf{a}_1 + x_{18} \mathbf{a}_2 - \left(z_{18} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_{18} \hat{\mathbf{x}} + ax_{18} \hat{\mathbf{y}} - c \left(z_{18} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{92} =$	$-y_{18} \mathbf{a}_1 - x_{18} \mathbf{a}_2 - \left(z_{18} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} - c \left(z_{18} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VII
$\mathbf{B}_{93} =$	$x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} + ay_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{94} =$	$-x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{95} =$	$y_{19} \mathbf{a}_1 - x_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$ay_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{96} =$	$-y_{19} \mathbf{a}_1 + x_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-ay_{19} \hat{\mathbf{x}} + ax_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{97} =$	$x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{98} =$	$-x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} + ay_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{99} =$	$y_{19} \mathbf{a}_1 + x_{19} \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_{19} \hat{\mathbf{x}} + ax_{19} \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{100} =$	$-y_{19} \mathbf{a}_1 - x_{19} \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga VIII
$\mathbf{B}_{101} =$	$x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{102} =$	$-x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{103} =$	$y_{20} \mathbf{a}_1 - x_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3$	$=$	$ay_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{104} =$	$-y_{20} \mathbf{a}_1 + x_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3$	$=$	$-ay_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{105} =$	$x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{106} =$	$-x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{107} =$	$y_{20} \mathbf{a}_1 + x_{20} \mathbf{a}_2 - \left(z_{20} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} - c \left(z_{20} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga IX
$\mathbf{B}_{108} =$	$-y_{20} \mathbf{a}_1 - x_{20} \mathbf{a}_2 - \left(z_{20} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} - c \left(z_{20} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8j)	Ga IX

References

- [1] H. Völlenkle, A. Wittmann, and H. Nowotny, *Die Kristallstrukturen von $Rh_{10}Ga_{17}$ und Ir_3Ga_5* , Monatsh. Chem **98**, 176–183 (1967), doi:10.1007/BF00901115.

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Ga
Rh

