

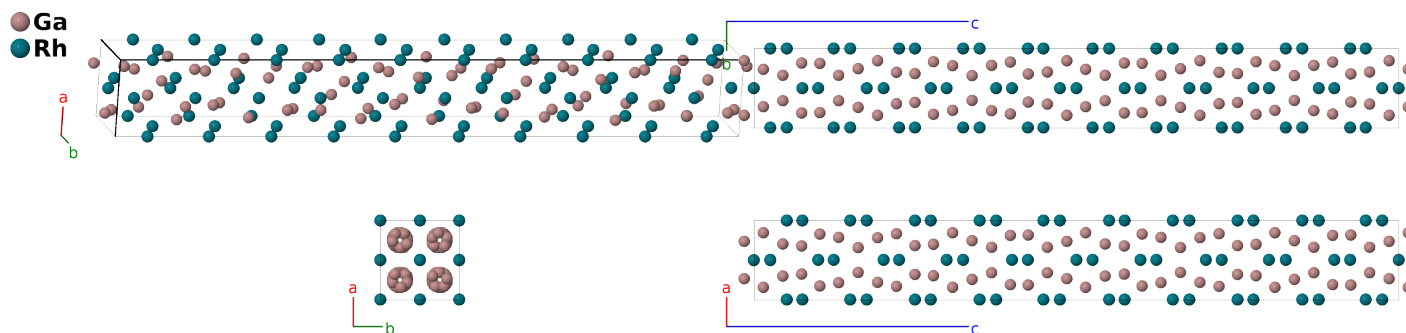
# Rh<sub>10</sub>Ga<sub>17</sub> Structure:

## A17B10\_tP108\_116\_e8j\_ad2g2h5i-001

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<https://aflow.org/p/D8JE>

[https://aflow.org/p/A17B10\\_tP108\\_116\\_e8j\\_ad2g2h5i-001](https://aflow.org/p/A17B10_tP108_116_e8j_ad2g2h5i-001)

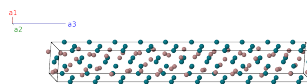


Prototype	Ga <sub>17</sub> Rh <sub>10</sub>
AFLOW prototype label	A17B10_tP108_116_e8j_ad2g2h5i-001
ICSD	103949
Pearson symbol	tP108
Space group number	116
Space group symbol	$P\bar{4}c2$
AFLOW prototype command	<pre>aflow --proto=A17B10_tP108_116_e8j_ad2g2h5i-001       --params=a, c/a, x3, z4, z5, z6, 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
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Rh I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2d)	Rh II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2d)	Rh II

$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4e)	Ga I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4e)	Ga I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4e)	Ga I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4e)	Ga I
$\mathbf{B}_9$	$= z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(4g)	Rh III
$\mathbf{B}_{10}$	$= -z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(4g)	Rh III
$\mathbf{B}_{11}$	$= (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4g)	Rh III
$\mathbf{B}_{12}$	$= -(z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4g)	Rh III
$\mathbf{B}_{13}$	$= z_5 \mathbf{a}_3$	$=$	$cz_5 \hat{\mathbf{z}}$	(4g)	Rh IV
$\mathbf{B}_{14}$	$= -z_5 \mathbf{a}_3$	$=$	$-cz_5 \hat{\mathbf{z}}$	(4g)	Rh IV
$\mathbf{B}_{15}$	$= (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4g)	Rh IV
$\mathbf{B}_{16}$	$= -(z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4g)	Rh IV
$\mathbf{B}_{17}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4h)	Rh V
$\mathbf{B}_{18}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4h)	Rh V
$\mathbf{B}_{19}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Rh V
$\mathbf{B}_{20}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Rh V
$\mathbf{B}_{21}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4h)	Rh VI
$\mathbf{B}_{22}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4h)	Rh VI
$\mathbf{B}_{23}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Rh VI
$\mathbf{B}_{24}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Rh VI
$\mathbf{B}_{25}$	$= \frac{1}{2} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4i)	Rh VII
$\mathbf{B}_{26}$	$= \frac{1}{2} \mathbf{a}_1 - z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - cz_8 \hat{\mathbf{z}}$	(4i)	Rh VII
$\mathbf{B}_{27}$	$= \frac{1}{2} \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh VII
$\mathbf{B}_{28}$	$= \frac{1}{2} \mathbf{a}_1 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh VII
$\mathbf{B}_{29}$	$= \frac{1}{2} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4i)	Rh VIII
$\mathbf{B}_{30}$	$= \frac{1}{2} \mathbf{a}_1 - z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - cz_9 \hat{\mathbf{z}}$	(4i)	Rh VIII
$\mathbf{B}_{31}$	$= \frac{1}{2} \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh VIII
$\mathbf{B}_{32}$	$= \frac{1}{2} \mathbf{a}_1 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh VIII
$\mathbf{B}_{33}$	$= \frac{1}{2} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4i)	Rh IX
$\mathbf{B}_{34}$	$= \frac{1}{2} \mathbf{a}_1 - z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - cz_{10} \hat{\mathbf{z}}$	(4i)	Rh IX
$\mathbf{B}_{35}$	$= \frac{1}{2} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh IX
$\mathbf{B}_{36}$	$= \frac{1}{2} \mathbf{a}_1 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh IX
$\mathbf{B}_{37}$	$= \frac{1}{2} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4i)	Rh X
$\mathbf{B}_{38}$	$= \frac{1}{2} \mathbf{a}_1 - z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - cz_{11} \hat{\mathbf{z}}$	(4i)	Rh X
$\mathbf{B}_{39}$	$= \frac{1}{2} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh X
$\mathbf{B}_{40}$	$= \frac{1}{2} \mathbf{a}_1 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh X
$\mathbf{B}_{41}$	$= \frac{1}{2} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(4i)	Rh XI
$\mathbf{B}_{42}$	$= \frac{1}{2} \mathbf{a}_1 - z_{12} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - cz_{12} \hat{\mathbf{z}}$	(4i)	Rh XI
$\mathbf{B}_{43}$	$= \frac{1}{2} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh XI
$\mathbf{B}_{44}$	$= \frac{1}{2} \mathbf{a}_1 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(4i)	Rh XI
$\mathbf{B}_{45}$	$= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(8j)	Ga II



$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{Ga IX}
\end{aligned}$$

## 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.