

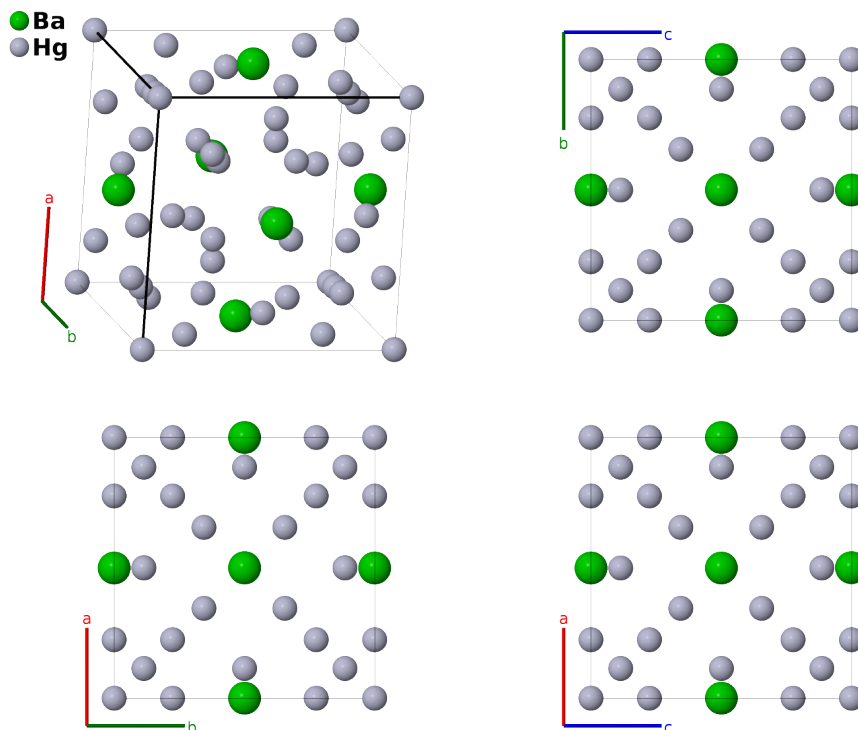
# BaHg<sub>11</sub> ( $D_{2e}$ ) Structure: AB11\_cP36\_221\_c\_agij-001

This structure originally had the label AB11\_cP36\_221\_c\_agij. Calls to that address will be redirected here.

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<https://aflow.org/p/2EDD>

[https://aflow.org/p/AB11\\_cP36\\_221\\_c\\_agij-001](https://aflow.org/p/AB11_cP36_221_c_agij-001)



Prototype	BaHg <sub>11</sub>
AFLOW prototype label	AB11_cP36_221_c_agij-001
<i>Strukturbericht</i> designation	$D_{2e}$
ICSD	58656
Pearson symbol	cP36
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB11_cP36_221_c_agij-001 --params=a, x<sub>3</sub>, y<sub>4</sub>, y<sub>5</sub></code>

## Other compounds with this structure

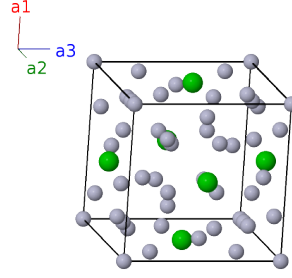
CeCd<sub>11</sub>, KHg<sub>11</sub>, LaCd<sub>11</sub>, NdCd<sub>11</sub>, PrCd<sub>11</sub>, PuCd<sub>11</sub>, RbHg<sub>11</sub>, SmCd<sub>11</sub>, SrHg<sub>11</sub>, Eu(Ag<sub>x</sub>Au<sub>11-x</sub>)

- (Pearson, 1972) state that this structure occurs in “a number of Hg and Cd phases with Group I or IIA metals or rare earths.” We lists those which we have found in the literature.

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### Simple Cubic primitive vectors

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




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1 =$	$0$	$=$	$0$	(1a)	Hg I
$\mathbf{B}_2 =$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Ba I
$\mathbf{B}_3 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Ba I
$\mathbf{B}_4 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c)	Ba I
$\mathbf{B}_5 =$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_6 =$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_7 =$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_8 =$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_9 =$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_{10} =$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_{11} =$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_{12} =$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8g)	Hg II
$\mathbf{B}_{13} =$	$y_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{14} =$	$-y_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{15} =$	$y_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{16} =$	$-y_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{17} =$	$y_4 \mathbf{a}_1 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{18} =$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{19} =$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{20} =$	$-y_4 \mathbf{a}_1 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(12i)	Hg III
$\mathbf{B}_{21} =$	$y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ay_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	(12i)	Hg III
$\mathbf{B}_{22} =$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$-ay_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	(12i)	Hg III
$\mathbf{B}_{23} =$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$ay_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	(12i)	Hg III
$\mathbf{B}_{24} =$	$-y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ay_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	(12i)	Hg III
$\mathbf{B}_{25} =$	$\frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(12j)	Hg IV
$\mathbf{B}_{26} =$	$\frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(12j)	Hg IV
$\mathbf{B}_{27} =$	$\frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(12j)	Hg IV

$$\begin{aligned}
\mathbf{B}_{28} &= \frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3 &= & \frac{1}{2} a \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{29} &= y_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_5 \mathbf{a}_3 &= & ay_5 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{30} &= y_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_5 \mathbf{a}_3 &= & ay_5 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{31} &= -y_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_5 \mathbf{a}_3 &= & -ay_5 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{32} &= -y_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_5 \mathbf{a}_3 &= & -ay_5 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{33} &= y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{34} &= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{35} &= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{Hg IV} \\
\mathbf{B}_{36} &= -y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12j) & \text{Hg IV}
\end{aligned}$$

## References

[1] G. Peyronel, *Struttura della fase BaHg<sub>11</sub>*, Gazz. Chim. Ital. **82**, 679–690 (1952).

## Found in

[1] P. Villars, *Material Phases Data System (MPDS)* (SpringerMaterials, CH-6354 Vitznau, Switzerland, 2014).

[2] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).