$BaHg_{11}$ ($D2_e$) Structure: AB11_cP36_221_c_agij-001

This structure previously used the label(s) `AB11_cP36_221_c_agij`. Calls to these addresses will be redirected here.

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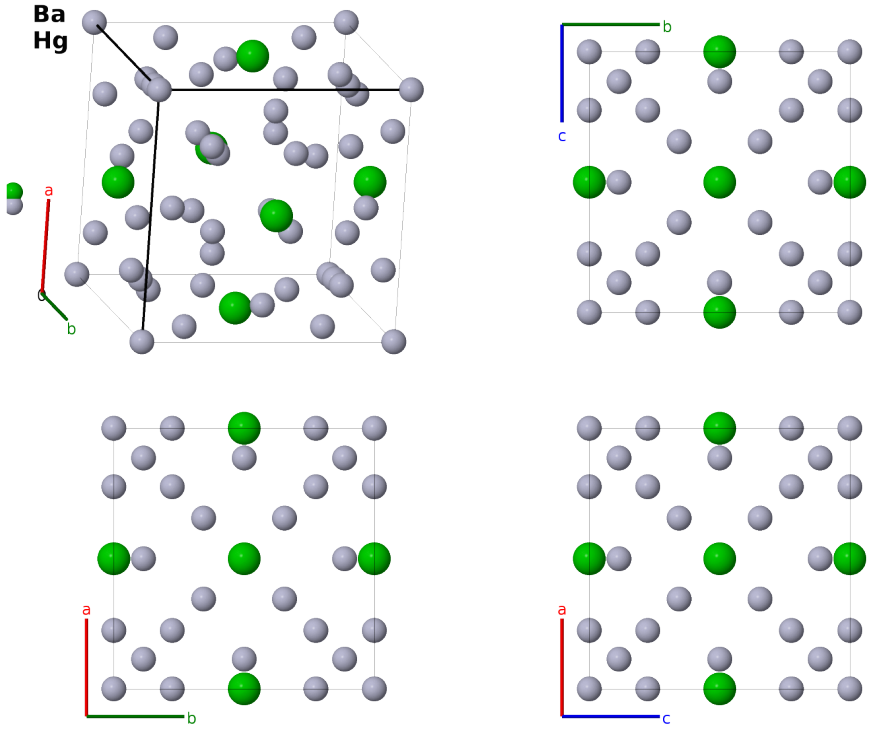
https://aflow.org/prototype-encyclopedia/2EDD

https://aflow.org/prototype-encyclopedia/AB11_cP36_221_c_agij-001



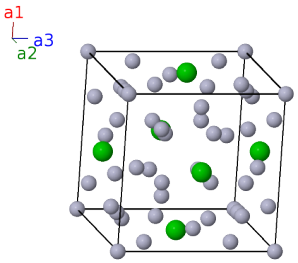
Prototype	$BaHg_{11}$
AFLOW prototype label	AB11_cP36_221_c_agij-001
***Strukturbericht* designation**	$D2_e$
ICSD	58656
CCDC	1622661
Pearson symbol	cP36
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB11_cP36_221_c_agij-001 --params=`a, x_3, y_4, y_5

Other compounds with this structure
$CeCd_{11}$, KHg_{11}, $LaCd_{11}$, $NdCd_{11}$, $PrCd_{11}$, $PuCd_{11}$, $RbHg_{11}$, $SmCd_{11}$, $SrHg_{11}$, $Eu(Ag_xAu_{11-x})$

- (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.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



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
$\mathbf{B_{28}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(12j)	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)	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)	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)	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)	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)	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)	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)	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)	Hg IV

References

[1] G. Peyronel, *Struttura della fase $BaHg_{11}$*, 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, Tornoto, 1972).

First cited in

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