HgCl$_2$ ($C25$) Structure: A2B_oP12_62_2c_c-002
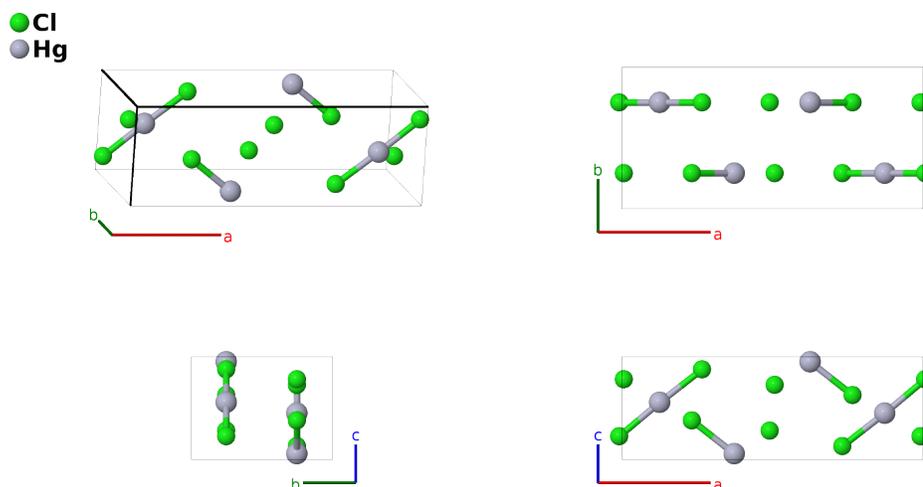
This structure originally had the label `A2B_oP12_62_2c_c.HgCl2`. Calls to that address will be redirected here.

https://aflow.org/p/DNGY

https://aflow.org/p/A2B_oP12_62_2c_c-002

Prototype	Cl$_2$Hg
AFLOW prototype label	A2B_oP12_62_2c_c-002
***Strukturbericht* designation**	$C25$
ICSD	26722
Pearson symbol	oP12
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	aflow --proto=A2B_oP12_62_2c_c-002 --params=$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3$

Other compounds with this structure

FeO$_2$ (goethite)

- (Hermann, 1937) gave HgCl$_2$ the *Strukturbericht* designation $C25$. Later that year (Gottfried, 1937) gave the same compound the designation $C28$. We will use $C25$, although some other references, *e.g.* (Parthé, 1993) use the $C28$ designation.

- PbCl$_2$ ($C23$), HgCl$_2$ ($C25$), SrH$_2$ ($C29$), Co$_2$Si ($C37$), and SrBr$_2$ ($C53$) all share the same AFLOW label, A2B_oP12_62_2c_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
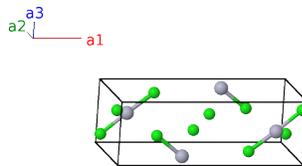
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} + z_1\mathbf{a_3}$	$=$	$ax_1\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_2}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_3}$	$=$	$-x_1\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} - z_1\mathbf{a_3}$	$=$	$-ax_1\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_1\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_4}$	$=$	$\left(x_1 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_5}$	$=$	$x_2\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} + z_2\mathbf{a_3}$	$=$	$ax_2\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B_6}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B_7}$	$=$	$-x_2\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} - z_2\mathbf{a_3}$	$=$	$-ax_2\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Cl II
$\mathbf{B_9}$	$=$	$x_3\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} + z_3\mathbf{a_3}$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{11}}$	$=$	$-x_3\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} - z_3\mathbf{a_3}$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Hg I

References

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