Calomel (Hg_2Cl_2, $D3_1$) Structure: AB_tI8_139_e_e-001

This structure originally had the label `AB_tI8_139_e_e`. Calls to that address will be redirected here.

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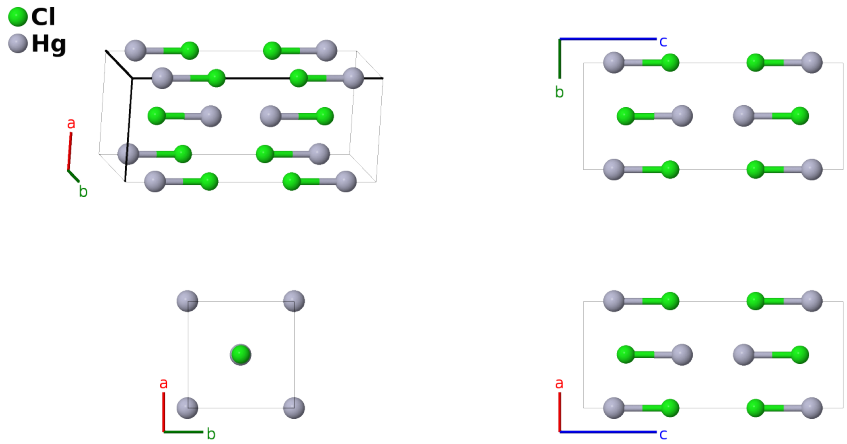
https://aflow.org/p/T1KN

https://aflow.org/p/AB_tI8_139_e_e-001



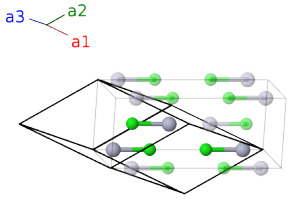
Prototype	ClHg
AFLOW prototype label	AB_tI8_139_e_e-001
***Strukturbericht* designation**	$D3_1$
Mineral name	calomel
ICSD	65441
Pearson symbol	tI8
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB_tI8_139_e_e-001 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure

Hg_2I_2

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Hg I
$\mathbf{B_4}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Hg I

References

[1] N. J. Calos, C. H. L. Kennard, and R. L. Davis, *The structure of calomel, Hg_2Cl_2, derived from neutron powder data*, Z. Krystallogr. **187**, 305–307 (1989), doi:10.1524/zkri.1989.187.14.305.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).