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

This structure previously used the label(s) `AB_tI8_139_e_e`. Calls to these addresses will be redirected here.

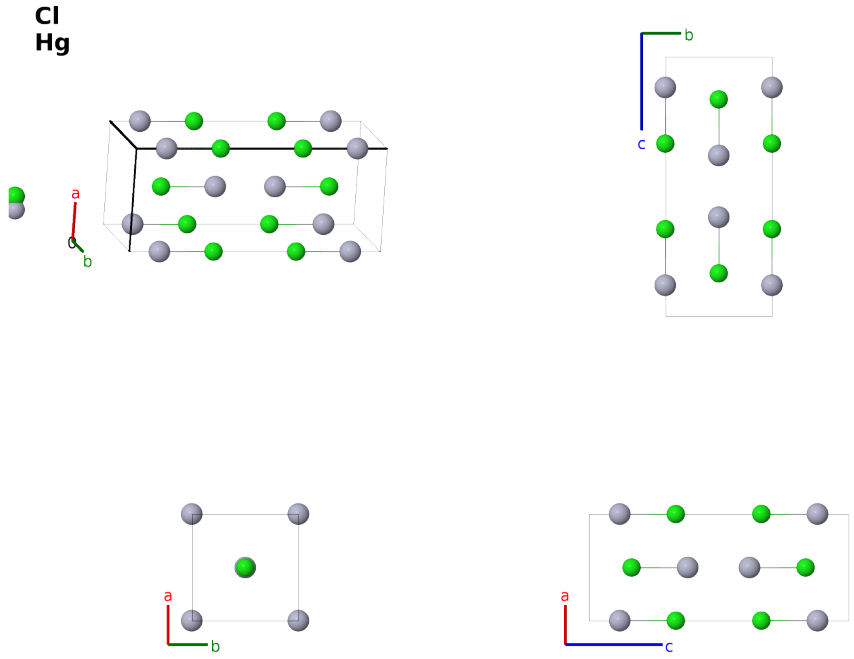
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/T1KN

https://aflow.org/prototype-encyclopedia/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
CCDC	1627563
Pearson symbol	tI8
Space group number	139
Space group symbol	$I4/mmm$

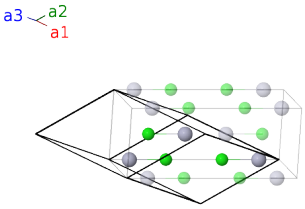
AFLOW prototype command `aflow --proto=AB_tI8_139_e_e-001 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure

Hg_2I_2

Body-centered Tetragonal primitive vectors

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



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).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043