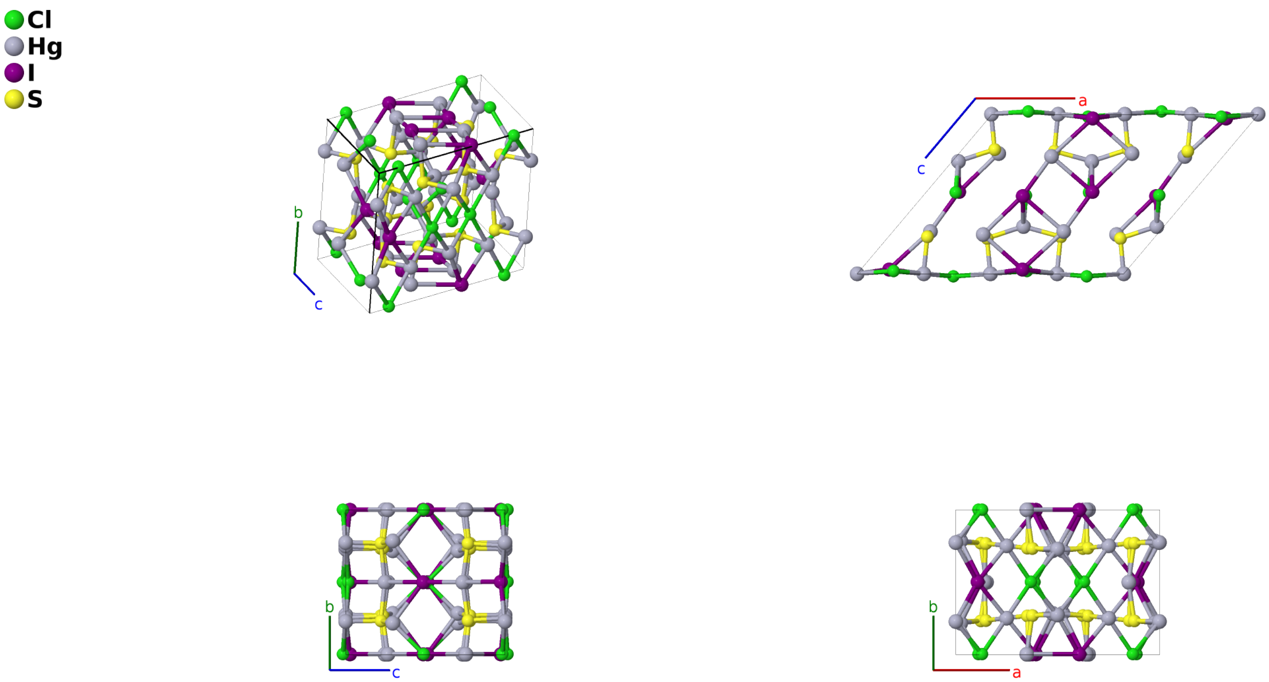
Radtkeite (Hg_3S_2ClI) Structure: AB3CD2_mC56_12_2i_eg2ij_2i_2j-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/4UG2

https://aflow.org/p/AB3CD2_mC56_12_2i_eg2ij_2i_2j-001



Prototype	$ClHg_3IS_2$
AFLOW prototype label	AB3CD2_mC56_12_2i_eg2ij_2i_2j-001
Mineral name	radtkeite
ICSD	98907
Pearson symbol	mC56
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB3CD2_mC56_12_2i_eg2ij_2i_2j-001` `--params=`$a, b/a, c/a, \beta, y_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

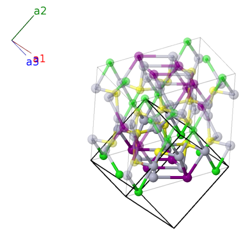
Other compounds with this structure

β-$Hg_3S_2Br_2$, $Hg_3Se_2Br_2$, $Hg_3Se_2I_2$

- We have shifted the origin by $\frac{1}{2}c\hat{z}$ from that given by (Pervukhina, 2004).

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4e)	Hg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}}$	(4e)	Hg I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$by_2\,\hat{\mathbf{y}}$	(4g)	Hg II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-by_2\,\hat{\mathbf{y}}$	(4g)	Hg II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Hg III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Hg III
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Hg IV
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Hg IV
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	I I
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	I I
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	I II
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	I II
$\mathbf{B_{17}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(8j)	Hg V
$\mathbf{B_{18}}$	=	$-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(8j)	Hg V
$\mathbf{B_{19}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(8j)	Hg V
$\mathbf{B_{20}}$	=	$(x_9 + y_9)\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(8j)	Hg V
$\mathbf{B_{21}}$	=	$(x_{10} - y_{10})\,\mathbf{a}_1 + (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S I
$\mathbf{B_{22}}$	=	$-(x_{10} + y_{10})\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S I
$\mathbf{B_{23}}$	=	$-(x_{10} - y_{10})\,\mathbf{a}_1 - (x_{10} + y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S I
$\mathbf{B_{24}}$	=	$(x_{10} + y_{10})\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S I
$\mathbf{B_{25}}$	=	$(x_{11} - y_{11})\,\mathbf{a}_1 + (x_{11} + y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II

$\mathbf{B_{26}}$	=	$-(x_{11}+y_{11})\,\mathbf{a}_1 - (x_{11}-y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II
$\mathbf{B_{27}}$	=	$-(x_{11}-y_{11})\,\mathbf{a}_1 - (x_{11}+y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II
$\mathbf{B_{28}}$	=	$(x_{11}+y_{11})\,\mathbf{a}_1 + (x_{11}-y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	S II

References

[1] N. V. Pervukhina, V. I. Vasil'ev, D. Y. Naumov, S. V. Borisov, and S. A. Magarill, *The Crystal Structure of Synthetic Radtkeite, Hg_3S_2ClI*, Can. Mineral. **42**, 87–94 (2004), doi:10.2113/gscanmin.42.1.87.