Kenhsuite (γ-$Hg_3S_2Cl_2$) Structure: AB2C_oP16_51_2e_bfi_j-001

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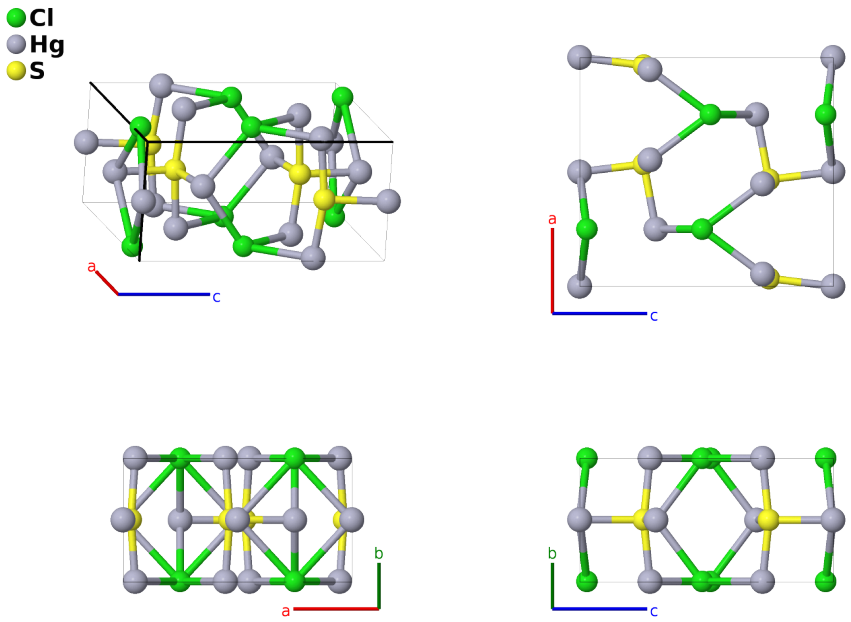
https://aflow.org/p/LQ5X

https://aflow.org/p/AB2C_oP16_51_2e_bfi_j-001



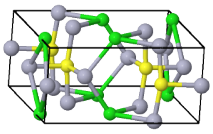
Prototype	$Cl_2Hg_3S_2$
AFLOW prototype label	AB2C_oP16_51_2e_bfi_j-001
Mineral name	kenhsuite
ICSD	29252
Pearson symbol	oP16
Space group number	51
Space group symbol	*Pmma*
AFLOW prototype command	`aflow --proto=AB2C_oP16_51_2e_bfi_j-001 --params=`$a, b/a, c/a, z_2, z_3, z_4, x_5, z_5, x_6, z_6$

- $Hg_3Cl_2S_2$ is found in three forms (Carlson, 1967):
  - Corderoite (α-$Hg_3Cl_2S_2$), the cubic ground state.
  - β-$Hg_3Cl_2S_2$, which appears above 340°C, another cubic phase with a much larger unit cell.
  - Kenhsuite (γ-$Hg_3Cl_2S_2$), which on average has an orthorhombic lattice. This state is apparently metastable. (this structure)

- (Ďurovič, 1961) found that Kenhsuite was composed of blocks of periodic structure in space group $C2/m$ #12, with lattice constants $(a', b', c') = (2a, 2b, c)$, where (a, b, c) are the lattice constants given here. This page shows what Ďurovič refers to as the "composite structure," essentially averaging all of the periodic structures. The data for this structure was originally given in the *Pbmm* setting of space group #51. We used FINDSYM to transform it to the standard *Pmma* setting, which involved a rotation and a translation.
- The Hg-III (4i) site is only half occupied, giving the observed stoichiometry.

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
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Hg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Hg I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(2e)	Cl I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(2e)	Cl I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(2e)	Cl II
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(2e)	Cl II
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2f)	Hg II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2f)	Hg II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4i)	Hg III
$\mathbf{B_{10}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4i)	Hg III
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(4i)	Hg III
$\mathbf{B_{12}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(4i)	Hg III
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4j)	S I
$\mathbf{B_{14}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4j)	S I
$\mathbf{B_{15}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4j)	S I
$\mathbf{B_{16}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4j)	S I

References

[1] S. Ďurovič, *The Crystal Structure of γ-$Hg_3S_2Cl_2$*, Acta Crystallogr. Sect. B **24**, 1661–1670 (1961), doi:10.1107/S0567740868004814.

[2] E. H. Carlson, *The growth of HgS and $Hg_3S_2Cl_2$ single crystals by a vapor phase method* **1**, 271–277 (1967), doi:10.1016/0022-0248(67)90033-4.

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