Capgaronnite [HgS·Ag(Cl,Br,I)] Structure: ABCD_oP16_18_c_c_c_c-001

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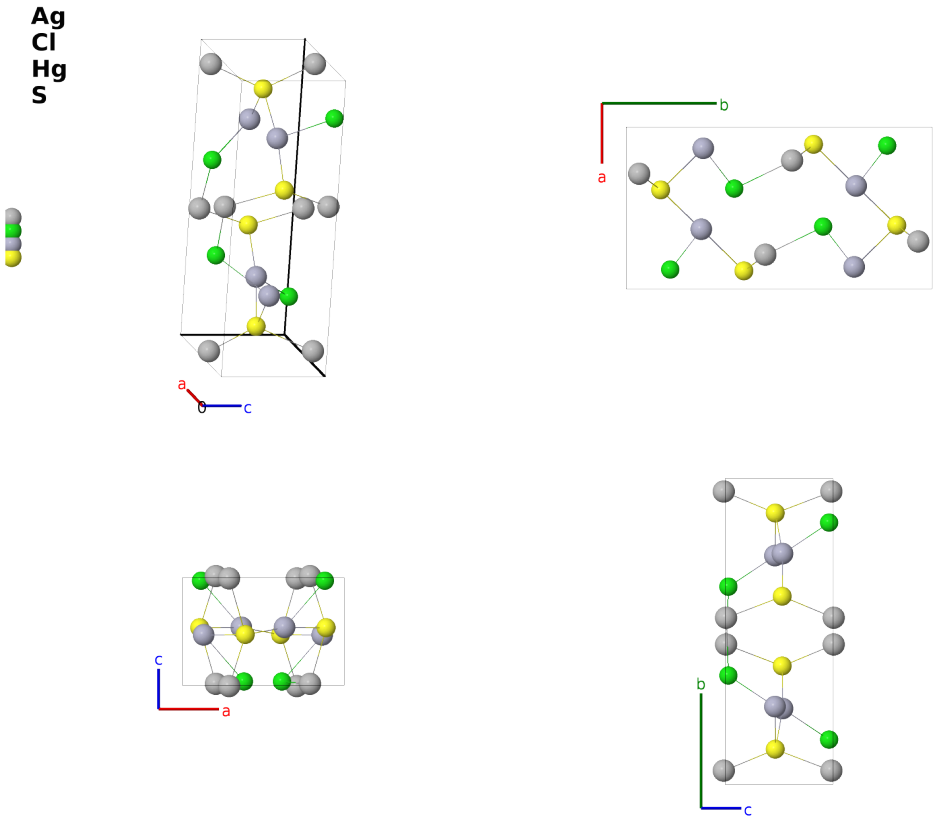
https://aflow.org/prototype-encyclopedia/HZN6

https://aflow.org/prototype-encyclopedia/ABCD_oP16_18_c_c_c_c-001

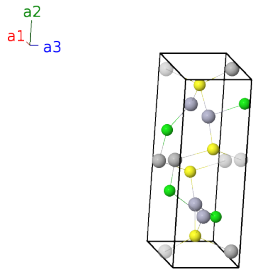


Prototype	AgClHgS
AFLOW prototype label	ABCD_oP16_18_c_c_c_c-001
Mineral name	capgaronnite
ICSD	66329
CCDC	1628410
Pearson symbol	oP16
Space group number	18
Space group symbol	$P2_12_12$
AFLOW prototype command	`aflow --proto=ABCD_oP16_18_c_c_c_c-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- The site we have labeled "Cl" is a mixture of chlorine, bromine, and iodine. We take the structural data from a sample with 82% chlorine and 18% bromine.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_3}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_7}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_8}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{11}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{12}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	Hg I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{15}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{16}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	S I

References

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