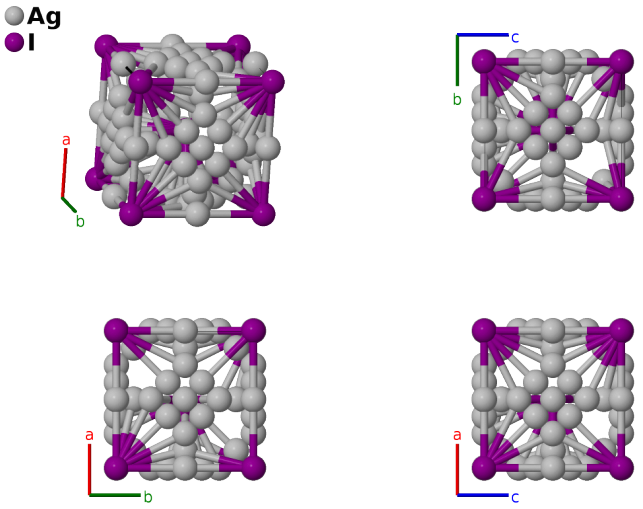
α-AgI ($B23$) Structure: A21B_cI44_229_bdh_a-001

This structure originally had the label `A21B_cI44_229_bdh_a`. Calls to that address will be redirected here.

Cite this page as: 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/p/QV5K

https://aflow.org/p/A21B_cI44_229_bdh_a-001



Prototype	AgI
AFLOW prototype label	A21B_cI44_229_bdh_a-001
***Strukturbericht* designation**	$B23$
ICSD	33262
Pearson symbol	cI44
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A21B_cI44_229_bdh_a-001 --params=`a, y_4

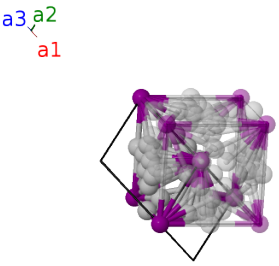
Other compounds with this structure
Ag_2S, Ag_2Se

- Under ambient conditions, silver iodide exists as a mixture of β-AgI, which has the wurtzite ($B4$) structure, and γ-AgI, which has the zincblende ($B3$) structure (Hull, 2004). Above 420K AgI transforms to this superionic α phase. The iodine atom sits at the (2a) site of the bcc lattice of space group $Im\bar{3}m$ #229, while the silver atom is randomly distributed on one of the (6b), (12d), and (24h) Wyckoff sites in each unit cell. On average, then, each of the 21 Ag sites listed below is occupied only 4.762% of the time in any given primitive cell. This easy transport between sites drives the superionic behavior of α-AgI. Ag_2S and Ag_2Se have higher concentrations of silver on each site.

- There is no ICSD entry for (Strock, 1934), so we use that from (Rahlfs, 1936). The two are identical except for the lattice constant (a = 5.034Å for Strock, 4.88Å for Rahlfs.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	I I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6b)	Ag I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(6b)	Ag I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{z}}$	(6b)	Ag I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Ag II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12d)	Ag II
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(12d)	Ag II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Ag II
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Ag II
$\mathbf{B_{10}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Ag II
$\mathbf{B_{11}}$	=	$2y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{12}}$	=	$y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{13}}$	=	$-y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{14}}$	=	$-2y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{15}}$	=	$y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{16}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{17}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{18}}$	=	$-y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Ag III
$\mathbf{B_{19}}$	=	$y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + 2y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(24h)	Ag III
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(24h)	Ag III
$\mathbf{B_{21}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(24h)	Ag III
$\mathbf{B_{22}}$	=	$-y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - 2y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(24h)	Ag III

References

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