Dyscrasite ($Ag_{3.15}Sb_{0.85}$) Structure: A3B_oP4_25_abc_d-001

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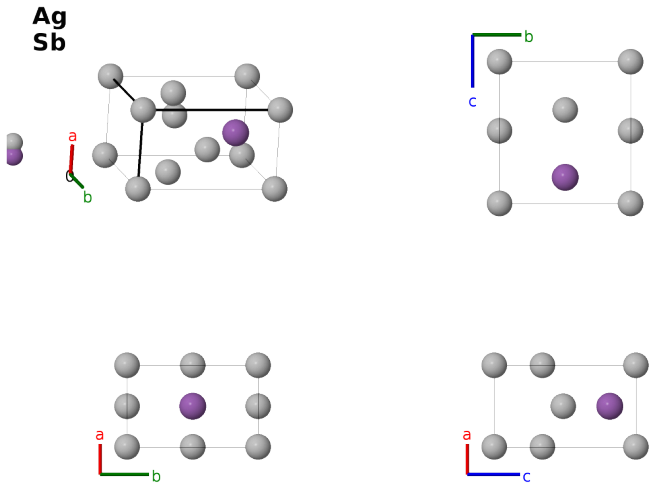
https://aflow.org/prototype-encyclopedia/KFCF

https://aflow.org/prototype-encyclopedia/A3B_oP4_25_abc_d-001

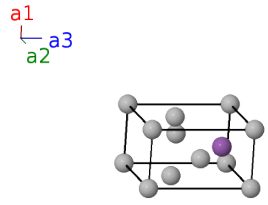


Prototype	Ag_3Sb
AFLOW prototype label	A3B_oP4_25_abc_d-001
Mineral name	dyscrasite
ICSD	64698
CCDC	1626881
Pearson symbol	oP4
Space group number	25
Space group symbol	$Pmm2$
AFLOW prototype command	`aflow --proto=A3B_oP4_25_abc_d-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, z_4$

- We have reordered the Wyckoff positions of this structure to match the AFLOW standard. What (Scott, 1976) designated as the Sb (1a) site is now (1d). That site is actually 85% antimony and 15% silver.
- Space group $Pmm2$ #25 allows an arbitary choice of the origin of the z-axis. We set $z_1 = 0$ for the (1a) site.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Ag I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(1b)	Ag II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(1c)	Ag III
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(1d)	Sb I

References

[1] J. D. Scott, *Refinement of the crystal structure of dyscrasite, and its implications for the structure of allargentum*, Can. Mineral. **14**, 139–142 (1976).

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

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