Rb_3AsSe_{16} Structure: AB3C16_cF160_203_a_bc_eg-001

This structure originally had the label `AB3C16_cF160_203_a_bc_eg`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

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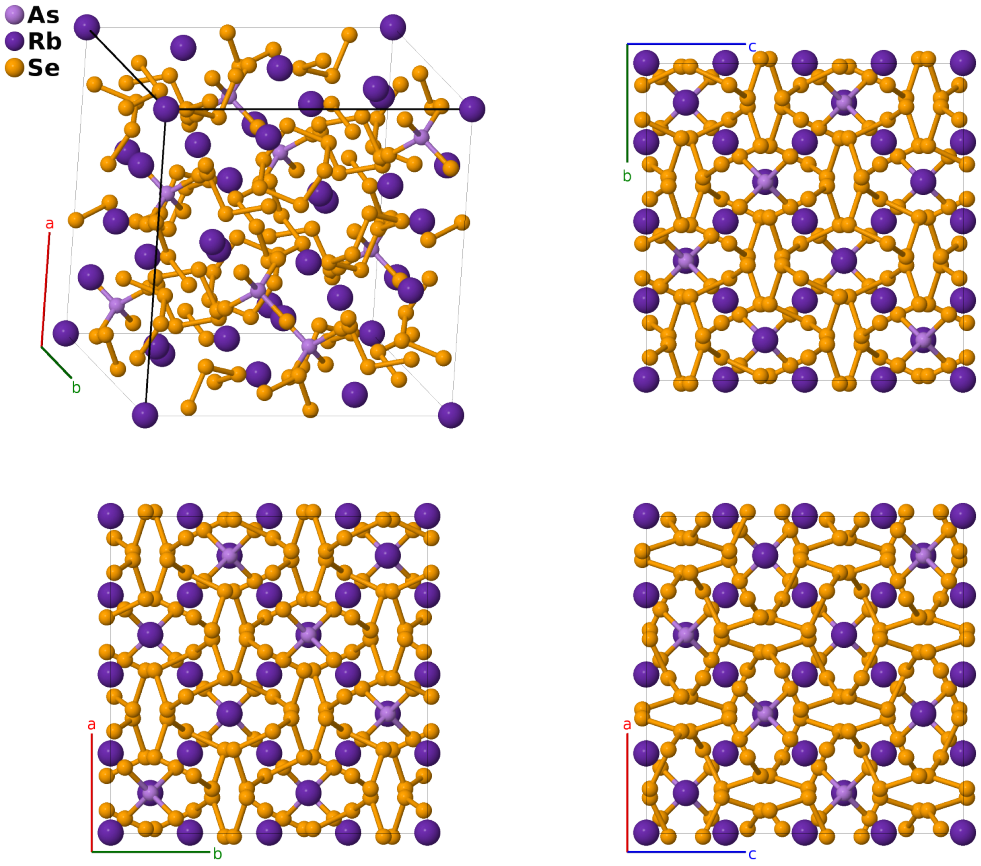
https://aflow.org/p/HAGZ

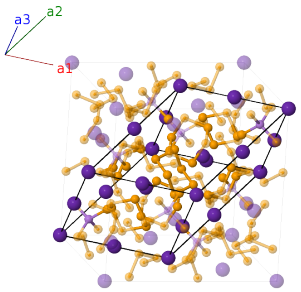
https://aflow.org/p/AB3C16_cF160_203_a_bc_eg-001



Prototype	$AsRb_3Se_{16}$
AFLOW prototype label	AB3C16_cF160_203_a_bc_eg-001
ICSD	405959
Pearson symbol	cF160
Space group number	203
Space group symbol	$Fd\bar{3}$
AFLOW prototype command	`aflow --proto=AB3C16_cF160_203_a_bc_eg-001 --params=`a, x_4, x_5, y_5, z_5

Face-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	As I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	As I
$\mathbf{B_3}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(8b)	Rb I
$\mathbf{B_4}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8b)	Rb I
$\mathbf{B_5}$	=	0	=	0	(16c)	Rb II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Rb II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Rb II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Rb II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(3x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 - \left(3x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{12}}$	=	$-\left(3x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(3x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(3x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{16}}$	=	$\left(3x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Se I
$\mathbf{B_{17}}$	=	$(-x_5 + y_5 + z_5)\,\mathbf{a}_1 + (x_5 - y_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5 - z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{18}}$	=	$(x_5 - y_5 + z_5)\,\mathbf{a}_1 + (-x_5 + y_5 + z_5)\,\mathbf{a}_2 - \left(x_5 + y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{19}}$	=	$(x_5 + y_5 - z_5)\,\mathbf{a}_1 - \left(x_5 + y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + (-x_5 + y_5 + z_5)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{20}}$	=	$-\left(x_5 + y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + (x_5 + y_5 - z_5)\,\mathbf{a}_2 + (x_5 - y_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(z_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{21}}$	=	$(x_5 + y_5 - z_5)\,\mathbf{a}_1 + (-x_5 + y_5 + z_5)\,\mathbf{a}_2 + (x_5 - y_5 + z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(96g)	Se II

$\mathbf{B_{22}}$	$= -\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+ (x_5-y_5+z_5)\,\mathbf{a}_2+ (-x_5+y_5+z_5)\,\mathbf{a}_3$	$=$	$az_5\,\hat{\mathbf{x}} - a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{23}}$	$= (-x_5+y_5+z_5)\,\mathbf{a}_1+ (x_5+y_5-z_5)\,\mathbf{a}_2- \left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{24}}$	$= (x_5-y_5+z_5)\,\mathbf{a}_1- \left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+ (x_5+y_5-z_5)\,\mathbf{a}_3$	$=$	$-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{25}}$	$= (x_5-y_5+z_5)\,\mathbf{a}_1+ (x_5+y_5-z_5)\,\mathbf{a}_2+ (-x_5+y_5+z_5)\,\mathbf{a}_3$	$=$	$ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{26}}$	$= (-x_5+y_5+z_5)\,\mathbf{a}_1- \left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+ (x_5-y_5+z_5)\,\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{27}}$	$= -\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+ (-x_5+y_5+z_5)\,\mathbf{a}_2+ (x_5+y_5-z_5)\,\mathbf{a}_3$	$=$	$ay_5\,\hat{\mathbf{x}} - a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{28}}$	$= (x_5+y_5-z_5)\,\mathbf{a}_1+ (x_5-y_5+z_5)\,\mathbf{a}_2- \left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{29}}$	$= (x_5-y_5-z_5)\,\mathbf{a}_1- (x_5-y_5+z_5)\,\mathbf{a}_2- (x_5+y_5-z_5)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{30}}$	$= -(x_5-y_5+z_5)\,\mathbf{a}_1+ (x_5-y_5-z_5)\,\mathbf{a}_2+ \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{31}}$	$= -(x_5+y_5-z_5)\,\mathbf{a}_1+ \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2+ (x_5-y_5-z_5)\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{32}}$	$= \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1- (x_5+y_5-z_5)\,\mathbf{a}_2- (x_5-y_5+z_5)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{33}}$	$= -(x_5+y_5-z_5)\,\mathbf{a}_1+ (x_5-y_5-z_5)\,\mathbf{a}_2- (x_5-y_5+z_5)\,\mathbf{a}_3$	$=$	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{34}}$	$= \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1- (x_5-y_5+z_5)\,\mathbf{a}_2+ (x_5-y_5-z_5)\,\mathbf{a}_3$	$=$	$-az_5\,\hat{\mathbf{x}} + a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{35}}$	$= (x_5-y_5-z_5)\,\mathbf{a}_1- (x_5+y_5-z_5)\,\mathbf{a}_2+ \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{36}}$	$= -(x_5-y_5+z_5)\,\mathbf{a}_1+ \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2- (x_5+y_5-z_5)\,\mathbf{a}_3$	$=$	$a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{37}}$	$= -(x_5-y_5+z_5)\,\mathbf{a}_1- (x_5+y_5-z_5)\,\mathbf{a}_2+ (x_5-y_5-z_5)\,\mathbf{a}_3$	$=$	$-ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{38}}$	$= (x_5-y_5-z_5)\,\mathbf{a}_1+ \left(x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2- (x_5-y_5+z_5)\,\mathbf{a}_3$	$=$	$a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II

$\mathbf{B_{39}}$	$=$	$\left(x_5 + y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 - y_5 - z_5\right)\,\mathbf{a}_2 - \left(x_5 + y_5 - z_5\right)\,\mathbf{a}_3$	$=$	$-ay_5\,\hat{\mathbf{x}} + a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Se II
$\mathbf{B_{40}}$	$=$	$-\left(x_5 + y_5 - z_5\right)\,\mathbf{a}_1 - \left(x_5 - y_5 + z_5\right)\,\mathbf{a}_2 + \left(x_5 + y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$a\left(y_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96g)	Se II

References

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.