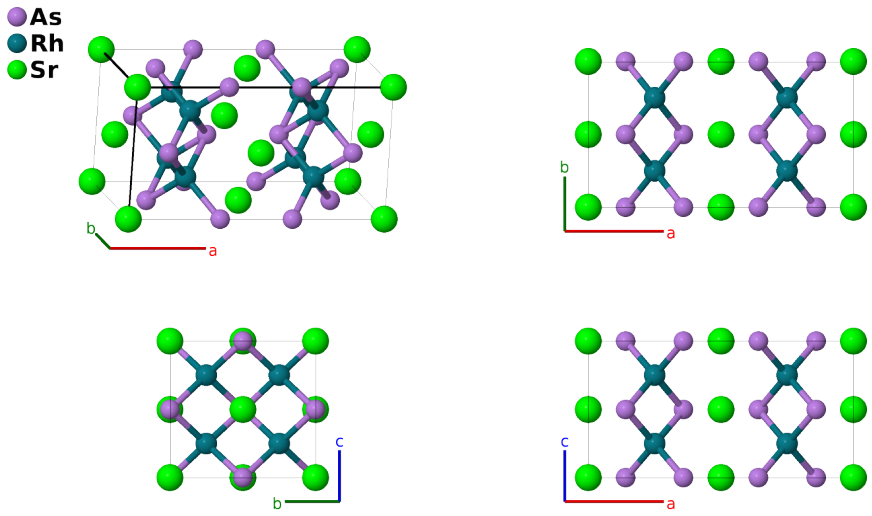
β-$SrRh_2As_2$ Structure: A2B2C_oF20_69_g_f_a-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/DY16

https://aflow.org/p/A2B2C_oF20_69_g_f_a-001



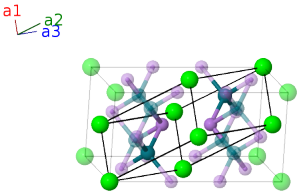
Prototype	As_2Rh_2Sr
AFLOW prototype label	A2B2C_oF20_69_g_f_a-001
ICSD	417001
Pearson symbol	oF20
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=A2B2C_oF20_69_g_f_a-001 --params=`$a, b/a, c/a, x_3$

Other compounds with this structure
$EuRh_2As_2$

- $SrRh_2As_2$ is known to have two temperature-driven structural phase transitions (Zinth, 2012):
  - Below 463K it is in the monoclinic α-$SrRh_2As_2$ structure.
  - In the range 463-555K it is in this orthorhombic β-$SrRh_2As_2$ structure.
  - Above 555K γ-$SrRh_2As_2$ is in the tetragonal $ThCr_2Si_2$ structure.
- (Zinth, 2012) have incorrect Wyckoff symbols for the structure of β-$SrRh_2As_2$ in Table IV. We assume the actual positions are correct, and shift the position of the strontium atom to the origin.
- The ICSD entry is from the earlier work of (Hellman, 2007).

Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Sr I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Rh I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	Rh I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8g)	As I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8g)	As I

References

[1] V. Zinth, V. Petricek, M. Dusek, and D. Johrendt, *Structural phase transitions in $SrRh_2As_2$*, Phys. Rev. B **85**, 014109 (2012), doi:10.1103/PhysRevB.85.014109.

[2] A. Hellmann, A. Löhken, A. Wurth, and A. Mewis, *New Arsenides with $ThCr_2Si_2$-type or Related Structures: The Compounds ARh_2As_2 (A: Eu, Sr, Ba) and $BaZn_2As_2$*, Z. Naturforsch. B **62**, 155–161 (2007), doi:10.1515/znb-2007-0203.