

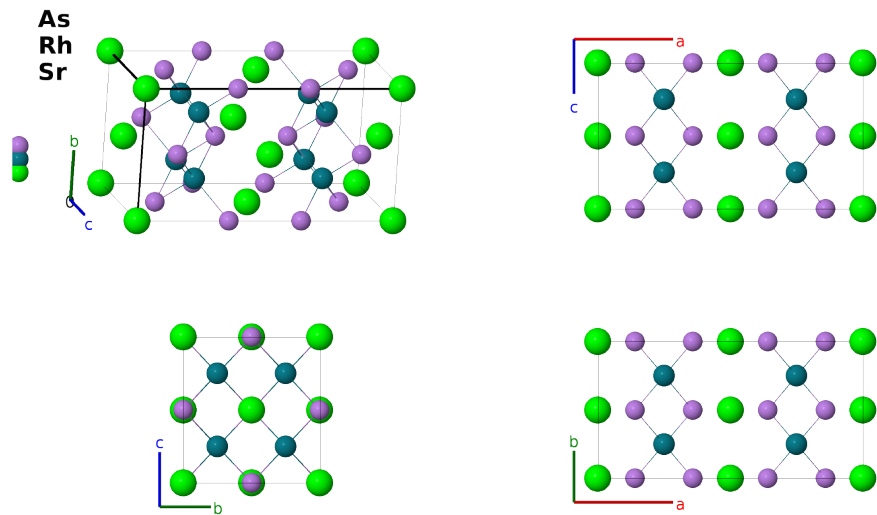
β -SrRh₂As₂ Structure: A2B2C_oF20_69_g_f_a-001

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<https://aflow.org/prototype-encyclopedia/DY16>

https://aflow.org/prototype-encyclopedia/A2B2C_oF20_69_g_f_a-001



Prototype	As ₂ Rh ₂ Sr
AFLOW prototype label	A2B2C_oF20_69_g_f_a-001
ICSD	417001
CCDC	1730533
Pearson symbol	oF20
Space group number	69
Space group symbol	<i>Fmmm</i>
AFLOW prototype command	<code>aflow --proto=A2B2C_oF20_69_g_f_a-001</code> <code>--params=a, b/a, c/a, x₃</code>

Other compounds with this structure

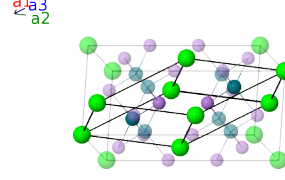
EuRh₂As₂

- SrRh₂As₂ is known to have two temperature-driven structural phase transitions (Zinth, 2012):
 - Below 463K it is in the monoclinic α -SrRh₂As₂ structure.
 - In the range 463-555K it is in this orthorhombic β -SrRh₂As₂ structure.
 - Above 555K γ -SrRh₂As₂ is in the tetragonal ThCr₂Si₂ structure.

- (Zinth, 2012) have incorrect Wyckoff symbols for the structure of β -SrRh₂As₂ 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}}\end{aligned}$$



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 SrRh₂As₂*, 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 ThCr₂Si₂-type or Related Structures: The Compounds ARh₂As₂ (A: Eu, Sr, Ba) and BaZn₂As₂*, Z. Naturforsch. B **62**, 155–161 (2007), doi:10.1515/znb-2007-0203.

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