SrN Structure:
AB_mC16_12_2i_2i-001

https://aflow.org/p/ASFW

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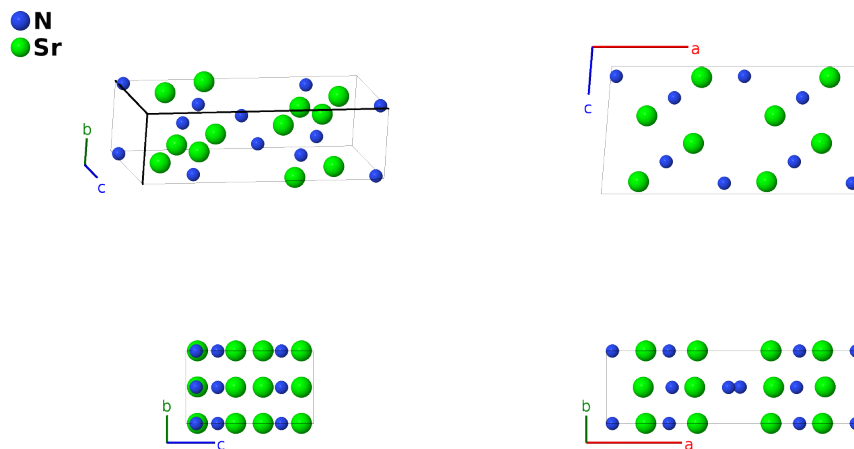
Prototype	NSr
AFLOW prototype label	AB_mC16_12_2i_2i-001
ICSD	411555
Pearson symbol	mC16
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	aflow --proto=AB_mC16_12_2i_2i-001
	--params=$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- SrN was prepared starting with Sr_2N at 920K and 40 MPa. The measurements were taken at 298K.

- SrN, β-BiI, and γ-BiI share the same AFLOW prototype label, AB_mC16_12_2i_2i. The structures are generated by the same symmetry operations with different sets of parameters (--params) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
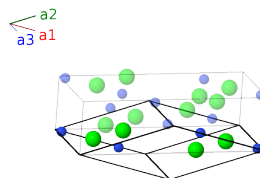
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	$=$	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	N I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	$=$	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	N I
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	N II
$\mathbf{B_4}$	$=$	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	N II
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sr I
$\mathbf{B_6}$	$=$	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sr I
$\mathbf{B_7}$	$=$	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sr II
$\mathbf{B_8}$	$=$	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sr II

References

[1] G. Auffermann, Y. Prots, and R. Kniep, *SrN and SrN₂: Diazenides by Synthesis under High N₂-Pressure*, angchemint **40**, 547–549 (2001), doi:10.1002/1521-3773(20010202)40:3<547::AID-ANIE547>3.0.CO;2-X.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 411555 (SrN).