

SrH₂ (*C*29) Structure: A2B_oP12_62_2c_c-004

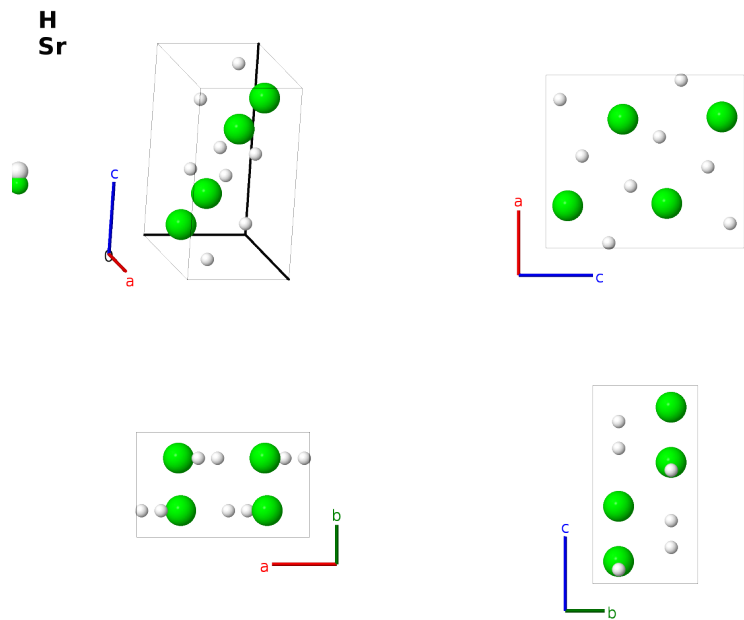
This structure previously used the label(s) **A2B_oP12_62_2c_c.SrH2**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/4GNV>

https://aflow.org/prototype-encyclopedia/A2B_oP12_62_2c_c-004



Prototype	H ₂ Sr
AFLOW prototype label	A2B_oP12_62_2c_c-004
<i>Strukturbericht</i> designation	<i>C</i> 29
ICSD	69077
CCDC	1630963
Pearson symbol	oP12
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=A2B_oP12_62_2c_c-004</code> <code>--params=a,b/a,c/a,x₁,z₁,x₂,z₂,x₃,z₃</code>

Other compounds with this structure

CaH₂, EuD₂, YbH₂

- We use this SrH_2 as the prototype for the hydrides with this structure.
- The ternary form of this structure is MnCuP . See that structure for similar ternary compounds.
- PbCl_2 (*C*23), HgCl_2 (*C*25), SrH_2 (*C*29), Co_2Si (*C*37), and SrBr_2 (*C*53) all share the same AFLOW label, A2B_oP12_62.2c.c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We have updated the reported structure from (Roop, 2013) to use the actual structure from (Brese, 1990). The sample studied used deuterium.

Simple Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_2$	$=$	$-\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_3$	$=$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_4$	$=$	$\left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B}_6$	$=$	$-\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B}_7$	$=$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B}_8$	$=$	$\left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_{10}$	$=$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_{12}$	$=$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Sr I

References

- [1] N. E. Brese, M. O’Keeffe, and R. B. von Dreele, *Synthesis and crystal structure of SrD_2 and SrND and bond valence parameters for hydrides*, J. Solid State Chem. **88**, 571–576 (1990), doi:10.1016/0022-4596(90)90255-V.
- [2] R. C. Ropp, *Encyclopedia of the Alkaline Earth Compounds* (Elsevier, Oxford, 2013), chap. 2, pp. 30–31.

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