

α -Sm (*C*19) Structure: A_hR3_166_ac-001

This structure previously used the label(s) **A_hR3_166_ac**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/MPB6>

https://aflow.org/prototype-encyclopedia/A_hR3_166_ac-001

Prototype	Sm
AFLOW prototype label	A_hR3_166_ac-001
<i>Strukturbericht</i> designation	<i>C</i> 19
ICSD	76031
CCDC	1636669
Pearson symbol	hR3
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A_hR3_166_ac-001 --params=$a, c/a, x_2$</code>

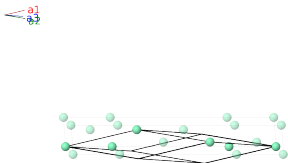
Other compounds with this structure

Li, Gd

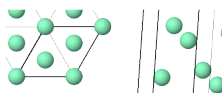
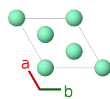
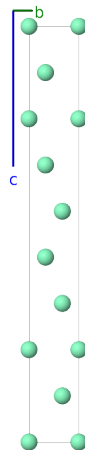
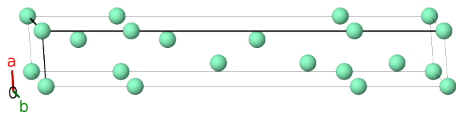
- This is also the proposed ground state of lithium as described in (Overhauser, 1984).
- Binary compounds with this structure are listed using CdCl_2 as the prototype.
- This is a close-packed system, with stacking ABCBCACAB, in contrast to the ABAB stacking of the hexagonal close-packed structure and the ABCABC stacking of the face-centered cubic structure.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Sm



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) Sm I
$\mathbf{B}_2$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$cx_2 \hat{\mathbf{z}}$	(2c) Sm II
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-cx_2 \hat{\mathbf{z}}$	(2c) Sm II

References

- [1] A. H. Daane, R. E. Rundle, H. G. Smith, and F. H. Spedding, *The crystal structure of samarium*, Acta Cryst. **7**, 532–535 (1954), doi:10.1107/S0365110X54001818.
- [2] A. W. Overhauser, *Crystal Structure of Lithium at 4.2 K*, Phys. Rev. Lett. **53**, 64–65 (1984), doi:10.1103/PhysRevLett.53.64.

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M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017