α-Sm ($C19$) Structure: A_hR3_166_ac-001

This structure originally had the label `A_hR3_166_ac`. Calls to that address will be redirected here.

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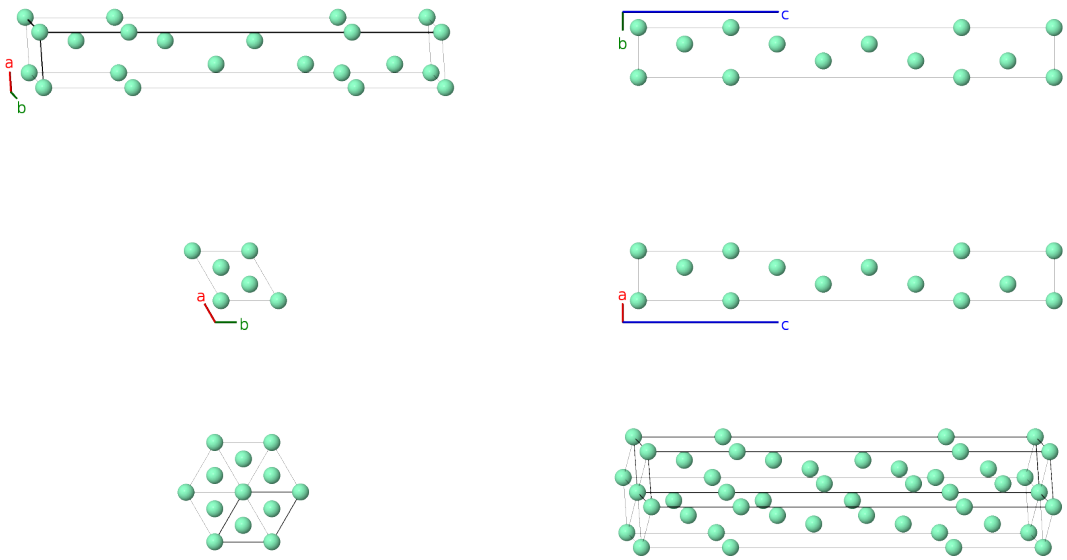
https://aflow.org/p/MPB6

https://aflow.org/p/A_hR3_166_ac-001

Sm



Prototype	Sm
AFLOW prototype label	A_hR3_166_ac-001
***Strukturbericht* designation**	$C19$
ICSD	76031
Pearson symbol	hR3
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A_hR3_166_ac-001 --params=`$a, c/a, x_2$

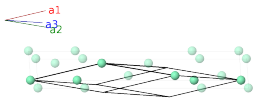
Other compounds with this structure
Li, Gd

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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.