

SmSI Structure: ABC_hR6_166_c_c_c-001

This structure previously used the label(s) **ABC_hR6_166_c_c_c**. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/YTD1>

https://aflow.org/prototype-encyclopedia/ABC_hR6_166_c_c_c-001

Prototype	ISSm
AFLOW prototype label	ABC_hR6_166_c_c_c-001
ICSD	59202
CCDC	1623066
Pearson symbol	hR6
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=ABC_hR6_166_c_c_c-001 --params=a, c/a, x₁, x₂, x₃</code>

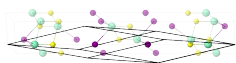
Other compounds with this structure

β -CeSi, DySI, GdSI, HfNBr, HfNCl, HfNI, NdSI, PrSI, TbSI, ZrNBr, ZrNCl, ZrNI

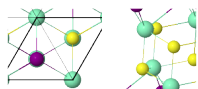
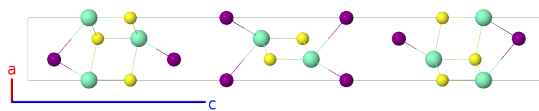
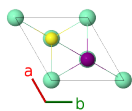
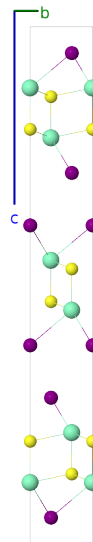
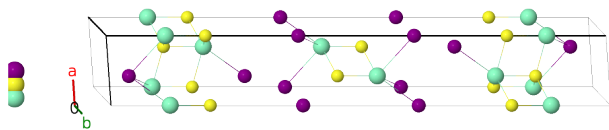
- The published version of this page (Hicks, 2019) has incorrect lattice constants. We have corrected this here.
- Although this has the same crystallographic structure as the *C12* structure, the layering is substantially different.
- SmSI and YOF have the same AFLOW prototype label, ABC_hR6_166_c_c_c. They are generated by the same symmetry operations with different sets of parameters (**--params**) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option **--hex**.

Rhombohedral primitive vectors

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



I
S
Sm



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c) I I
$\mathbf{B}_2$	$=$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c) I I
$\mathbf{B}_3$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c) S I
$\mathbf{B}_4$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c) S I
$\mathbf{B}_5$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c) Sm I
$\mathbf{B}_6$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c) Sm I

References

- [1] H. P. Beck and C. Strobel, *Zur Hochdruckpolymorphie der Seltenerdsulfidiodide $LnSI$* , Z. Anorganische und Allgemeine Chemie **535**, 222–239 (1986), doi:10.1002/zaac.19865350427.
- [2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

- [1] A. M. Fogg, J. S. O. Evens, and D. O’Hare, *Crystal structure of β -MNX ($M = \text{Zr, Hf}$; $X = \text{Cl, Br}$)*, Chem. Comm. **0**, 2269–2270 (1998), doi:10.1039/A806415F.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043