

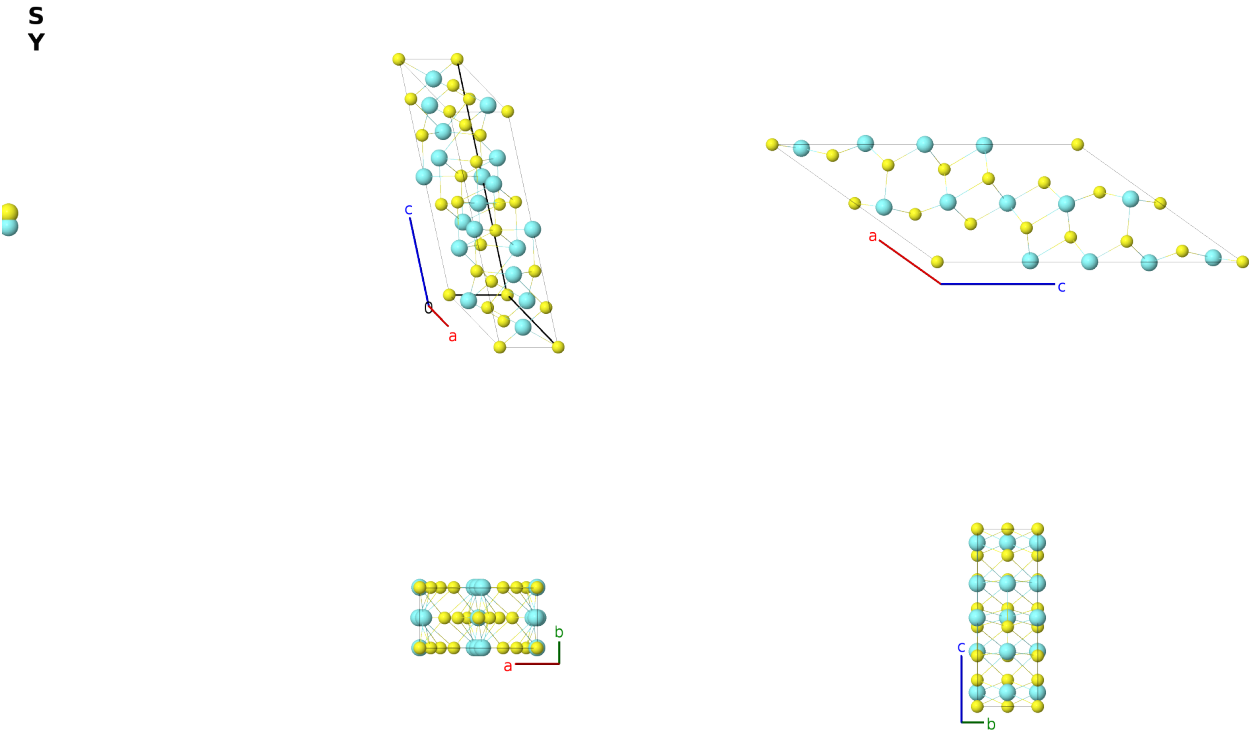
Y₅S₇ Structure: A7B5_mC24_12_a3i_c2i-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/G5Z0>

https://aflow.org/prototype-encyclopedia/A7B5_mC24_12_a3i_c2i-001



Prototype	S ₇ Y ₅
AFLOW prototype label	A7B5_mC24_12_a3i_c2i-001
ICSD	43620
CCDC	1613099
Pearson symbol	mC24
Space group number	12
Space group symbol	C2/m
AFLOW prototype command	<code>aflow --proto=A7B5_mC24_12_a3i_c2i-001</code> <code>--params=a, b/a, c/a, β, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7</code>

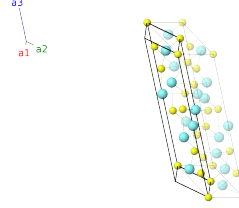
Other compounds with this structure

Dy₅S₇, Er₅S₇, Ho₅S₇, Tm₅S₇, CdY₄S₇, CrY₄S₇, MnDy₄S₇, MnEr₄S₇, MnHo₄S₇, MnTm₄S₇, MnY₄S₇, MnYb₄S₇, FeEr₄S₇, FeHo₄S₇, FeTm₄S₇, FeY₄S₇, FeYb₄S₇

- (Adolphe, 1965) gives the lattice parameters for the ternary versions of this structure, but not the atomic positions. Presumably the third atom species replaces the atom on the (1a) or (1c) site.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	S I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c)	Y I
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	S II
$\mathbf{B}_4$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	S II
$\mathbf{B}_5$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	S III
$\mathbf{B}_6$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	S III
$\mathbf{B}_7$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	S IV
$\mathbf{B}_8$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	S IV
$\mathbf{B}_9$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	Y II
$\mathbf{B}_{10}$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	Y II
$\mathbf{B}_{11}$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	Y III
$\mathbf{B}_{12}$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	Y III

References

- [1] C. Adolphe, *Contribution a l'etude d'un groupe de sulfures isostructuraux de terres rares et d'yttrium de type: Y₅S₇ et FeY₄S₇*, Ann. Chim. (Paris) **10**, 271–297 (1965).

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- [1] C. N. R. Rao and K. P. R. Pisharody, *Transition Metal Sulfides*, Prog. Solid State Chem. **10**, 207–270 (1976), doi:10.1016/0079-6786(76)90009-1.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.