

Ho₂S₃ Structure:

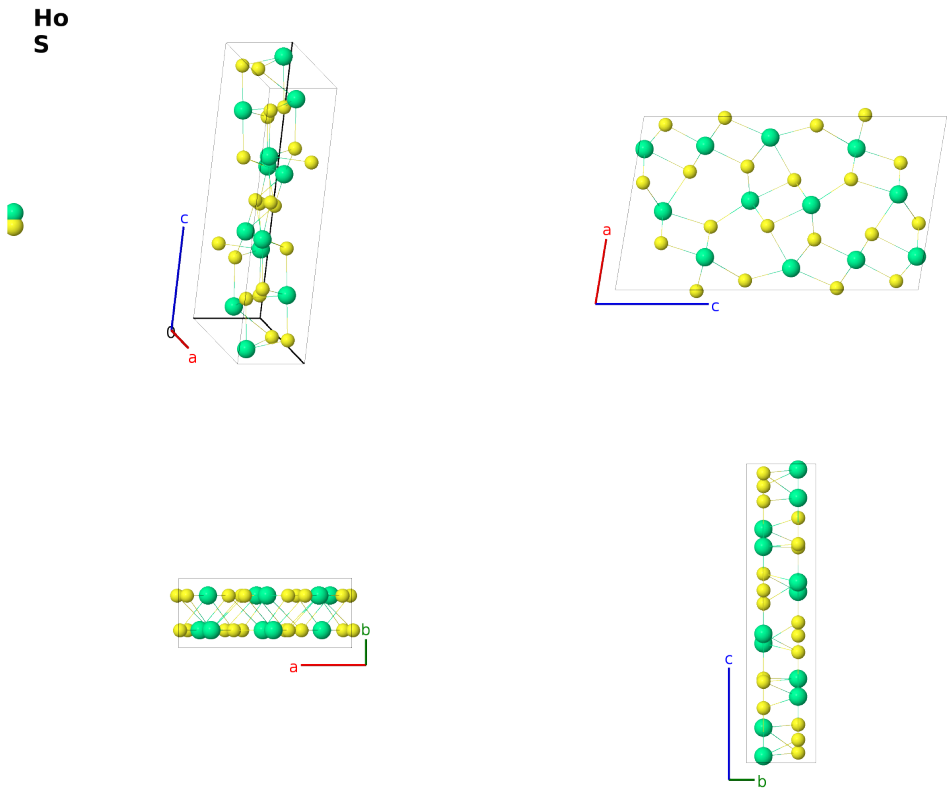
A2B3_mP30_11_6e_9e-001

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/TWS9>

https://aflow.org/prototype-encyclopedia/A2B3_mP30_11_6e_9e-001

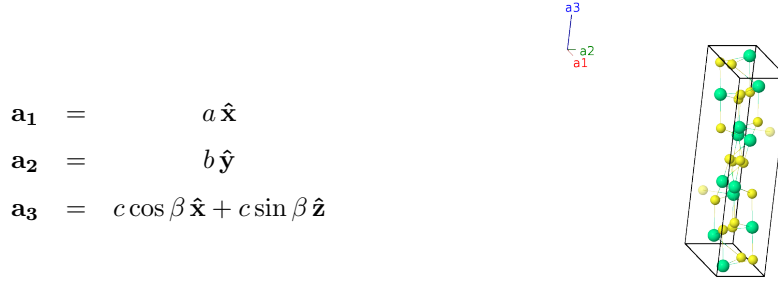


Prototype	Ho ₂ S ₃
AFLOW prototype label	A2B3_mP30_11_6e_9e-001
ICSD	22252
CCDC	1599026
Pearson symbol	mP30
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	<pre>aflow --proto=A2B3_mP30_11_6e_9e-001 --params=a,b/a,c/a,β,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀, z₁₀,x₁₁,z₁₁,x₁₂,z₁₂,x₁₃,z₁₃,x₁₄,z₁₄,x₁₅,z₁₅</pre>

Other compounds with this structure

Dy₂S₃, Er₂S₃, Tm₂S₃, Y₂S₃, δ -Yb₂S₃

Simple Monoclinic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho IV
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho V
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho V
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho VI
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Ho VI
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	S I
$\mathbf{B}_{14}$	$= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	S I
$\mathbf{B}_{15}$	$= x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	S II
$\mathbf{B}_{16}$	$= -x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	S II
$\mathbf{B}_{17}$	$= x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2e)	S III
$\mathbf{B}_{18}$	$= -x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2e)	S III
$\mathbf{B}_{19}$	$= x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2e)	S IV
$\mathbf{B}_{20}$	$= -x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(2e)	S IV
$\mathbf{B}_{21}$	$= x_{11} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(2e)	S V
$\mathbf{B}_{22}$	$= -x_{11} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(2e)	S V
$\mathbf{B}_{23}$	$= x_{12} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(2e)	S VI
$\mathbf{B}_{24}$	$= -x_{12} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(2e)	S VI
$\mathbf{B}_{25}$	$= x_{13} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(2e)	S VII
$\mathbf{B}_{26}$	$= -x_{13} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}}$	(2e)	S VII

$$\begin{aligned}
\mathbf{B}_{27} &= x_{14} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} &(2e) &\text{S VIII} \\
\mathbf{B}_{28} &= -x_{14} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= -(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{14} \sin \beta \hat{\mathbf{z}} &(2e) &\text{S VIII} \\
\mathbf{B}_{29} &= x_{15} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= (ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}} &(2e) &\text{S IX} \\
\mathbf{B}_{30} &= -x_{15} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{15} \mathbf{a}_3 &= -(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{15} \sin \beta \hat{\mathbf{z}} &(2e) &\text{S IX}
\end{aligned}$$

References

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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.