

V₅S₈ Structure:

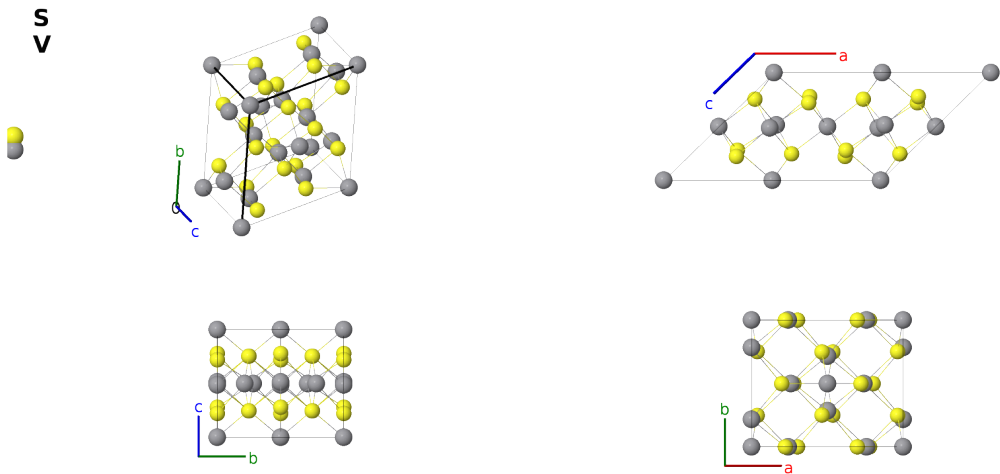
A8B5_mC26_12_2ij_ahi-001

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<https://aflow.org/prototype-encyclopedia/ZQW6>

https://aflow.org/prototype-encyclopedia/A8B5_mC26_12_2ij_ahi-001



Prototype	S_8V_5
AFLOW prototype label	A8B5_mC26_12_2ij_ahi-001
ICSD	42040
CCDC	1611754
Pearson symbol	mC26
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A8B5_mC26_12_2ij_ahi-001 --params=a, b/a, c/a, β, y_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6</pre>

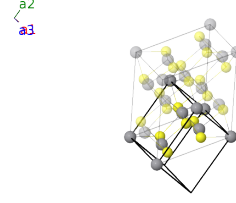
Other compounds with this structure

Cr₅Se₈, Ti₅Se₈, V₅Se₈, V₅Te₈

- (Kawada, 1975) give the structural information in setting $F2/m$ of space group #12. We used FINDSYM to transform this into the standard $C2/m$ setting. This involves a considerable shuffling of the primitive vectors.

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) V I
$\mathbf{B}_2$	=	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h) V II
$\mathbf{B}_3$	=	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h) V 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 I
$\mathbf{B}_5$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) S I
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) S II
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) S II
$\mathbf{B}_8$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) V III
$\mathbf{B}_9$	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) V III
$\mathbf{B}_{10}$	=	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) S III
$\mathbf{B}_{11}$	=	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) S III
$\mathbf{B}_{12}$	=	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) S III
$\mathbf{B}_{13}$	=	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) S III

References

- [1] I. Kawada, M. Nakano-Onoda, M. Ishii, M. Saeki, and M. Nakahira, *Crystal structures of V_3S_4 and V_5S_8* , J. Solid State Chem. **15**, 246–252 (1975), doi:10.1016/0022-4596(75)90209-1.

Found in

- [1] W. Bensch and J. Koy, *The single crystal structure of V_5S_8 determined at two different temperatures: anisotropic changes of the metal atom network*, Inorg. Chim. Acta **206**, 221–223 (1993), doi:10.1016/S0020-1693(00)82870-4.

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