

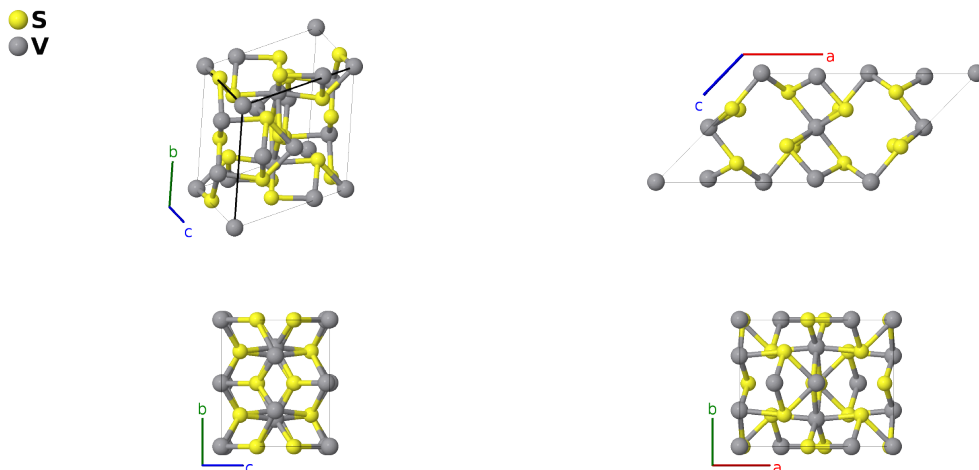
# V<sub>5</sub>S<sub>8</sub> Structure:

## A8B5\_mC26\_12\_2ij\_ahi-001

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<https://aflow.org/p/ZQW6>

[https://aflow.org/p/A8B5\\_mC26\\_12\\_2ij\\_ahi-001](https://aflow.org/p/A8B5_mC26_12_2ij_ahi-001)



Prototype	S <sub>8</sub> V <sub>5</sub>
AFLOW prototype label	A8B5_mC26_12_2ij_ahi-001
ICSD	42040
Pearson symbol	mC26
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	aflow --proto=A8B5_mC26_12_2ij_ahi-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , $\beta$ , <i>y</i> <sub>2</sub> , <i>x</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>x</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>x</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>x</i> <sub>6</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub>

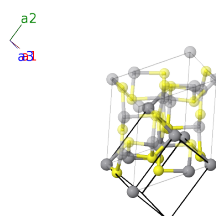
### Other compounds with this structure

Cr<sub>5</sub>Se<sub>8</sub>, Ti<sub>5</sub>Se<sub>8</sub>, V<sub>5</sub>Se<sub>8</sub>, V<sub>5</sub>Te<sub>8</sub>

- (Kawada, 1975) give the structural information in setting *F*2/*m* of space group #12. We used FINDSYM to transform this into the standard *C*2/*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.