

K₂S₃ Structure:

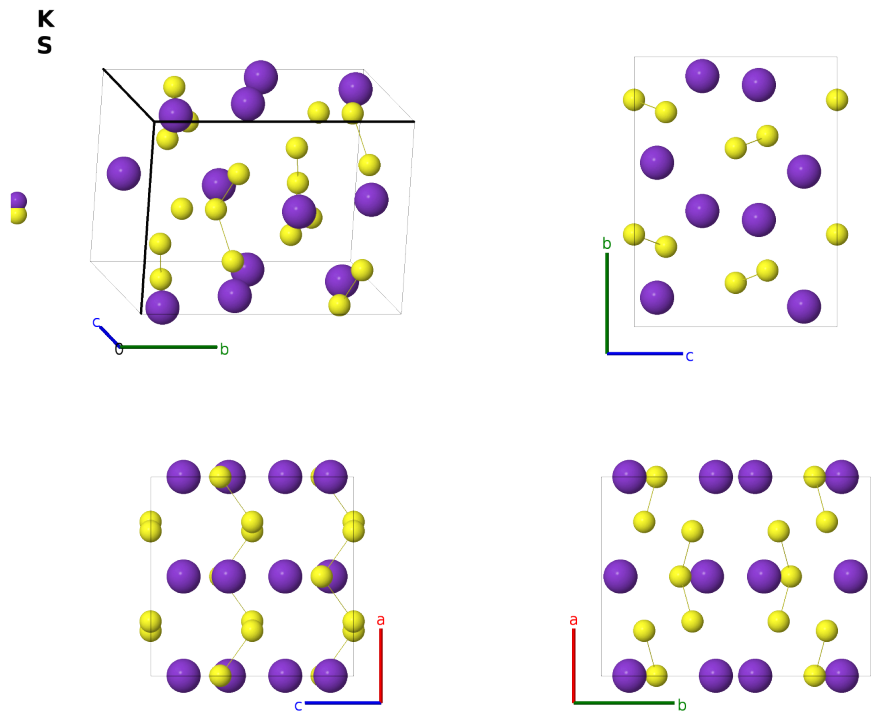
A2B3_oC20_36_2a_ab-001

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<https://aflow.org/prototype-encyclopedia/36FH>

https://aflow.org/prototype-encyclopedia/A2B3_oC20_36_2a_ab-001



Prototype	K ₂ S ₃
AFLOW prototype label	A2B3_oC20_36_2a_ab-001
ICSD	1263
CCDC	1591416
Pearson symbol	oC20
Space group number	36
Space group symbol	<i>Cmc</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=A2B3_oC20_36_2a_ab-001</code> <code>--params=a,b/a,c/a,y₁,z₁,y₂,z₂,y₃,z₃,x₄,y₄,z₄</code>

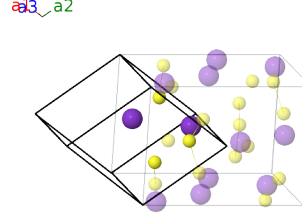
Other compounds with this structure

Cs₂S₃, Cs₂Se₃, Cs₂Te₃, K₂Se₃, Rb₂S₃, Rb₂Se₃

- Space group $Cmc2_1$ allows an arbitrary placement of the origin of the z -axis. Here we follow (Böttcher, 1977) and set $z_4 = 0$.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	K I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	K I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	K II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	K II
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B}_7$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8b)	S II
$\mathbf{B}_8$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	S II
$\mathbf{B}_9$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	S II
$\mathbf{B}_{10}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8b)	S II

References

- [1] J. Böttcher, *Die Kristallstruktur von K_2S_3 und K_2Se_3* , Z. Anorganische und Allgemeine Chemie **432**, 167–172 (1977), doi:10.1002/zaac.19774320122.

Found in

- [1] P. Böttcher, *Synthesis and crystal structure of Rb_2Te_3 and Cs_2Te_3* , J. Less-Common Met. **70**, 263–271 (1980), doi:10.1016/0022-5088(80)90235-0.

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