K_2S_3 Structure: A2B3_oC20_36_2a_ab-001

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https://aflow.org/p/36FH

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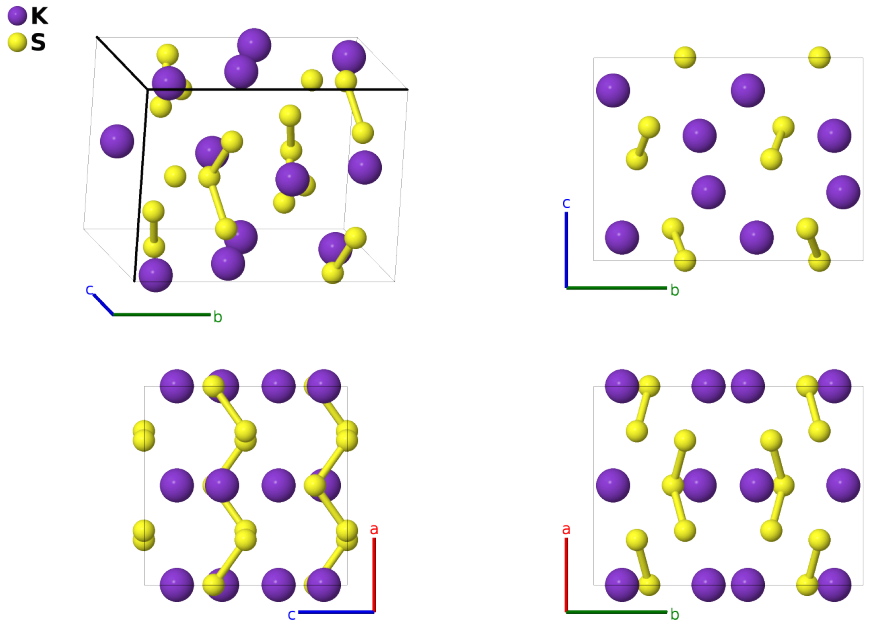


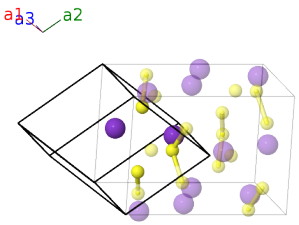
Prototype	K_2S_3
AFLOW prototype label	A2B3_oC20_36_2a_ab-001
ICSD	1263
Pearson symbol	oC20
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=A2B3_oC20_36_2a_ab-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, x_4, y_4, z_4$

Other compounds with this structure
Cs_2S_3, Cs_2Se_3, Cs_2Te_3, K_2Se_3, Rb_2S_3, Rb_2Se_3

- 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

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



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
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	S II
$\mathbf{B_9}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.