$K_2S_3O_6$ ($K5_1$) Structure: A2B6C3_oP44_62_2c_2c2d_3c-001

This structure originally had the label `A2B6C3_oP44_62_2c_2c2d_3c`. Calls to that address will be redirected here.

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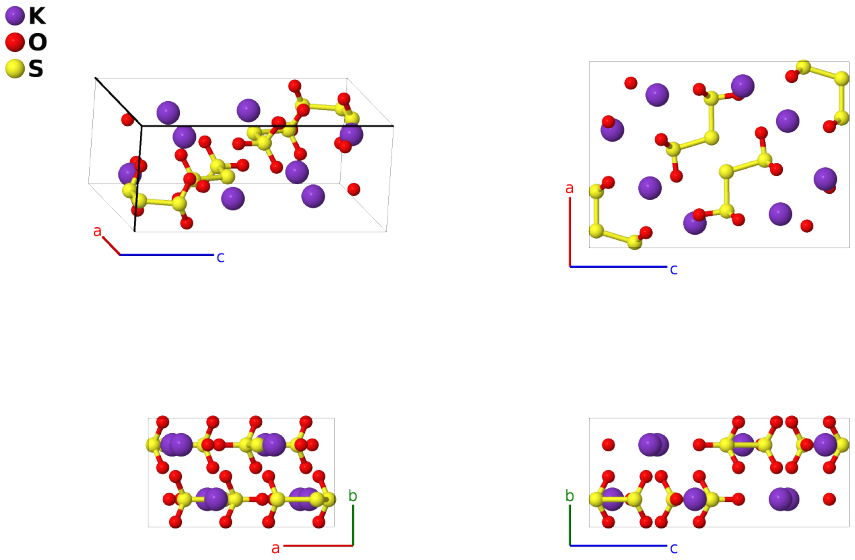
https://aflow.org/p/PD3R

https://aflow.org/p/A2B6C3_oP44_62_2c_2c2d_3c-001



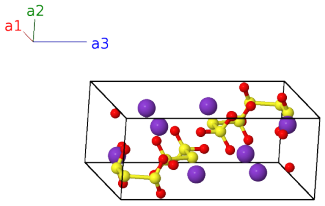
Prototype	$K_2O_6S_3$
AFLOW prototype label	A2B6C3_oP44_62_2c_2c2d_3c-001
***Strukturbericht* designation**	$K5_1$
ICSD	8200
Pearson symbol	oP44
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A2B6C3_oP44_62_2c_2c2d_3c-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

Other compounds with this structure
$Rb_2S_3O_6$

- (Stewart, 1979) give the Wyckoff positions of this structure using the *Pnam* orientation of space group #62. We have used FINDSYM to change this to our standard *Pnma* orientation.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	K II
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	K II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	K II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	K II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B_{22}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B_{24}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4c)	S III

$\mathbf{B_{26}}$	$=$	$-\left(x_7-\frac{1}{2}\right)\mathbf{a}_1+\frac{3}{4}\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_7-\frac{1}{2}\right)\hat{\mathbf{x}}+\frac{3}{4}b\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B_{27}}$	$=$	$-x_7\mathbf{a}_1+\frac{3}{4}\mathbf{a}_2-z_7\mathbf{a}_3$	$=$	$-ax_7\hat{\mathbf{x}}+\frac{3}{4}b\hat{\mathbf{y}}-cz_7\hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B_{28}}$	$=$	$\left(x_7+\frac{1}{2}\right)\mathbf{a}_1+\frac{1}{4}\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_7+\frac{1}{2}\right)\hat{\mathbf{x}}+\frac{1}{4}b\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B_{29}}$	$=$	$x_8\mathbf{a}_1+y_8\mathbf{a}_2+z_8\mathbf{a}_3$	$=$	$ax_8\hat{\mathbf{x}}+by_8\hat{\mathbf{y}}+cz_8\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{30}}$	$=$	$-\left(x_8-\frac{1}{2}\right)\mathbf{a}_1-y_8\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{x}}-by_8\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{31}}$	$=$	$-x_8\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\mathbf{a}_2-z_8\mathbf{a}_3$	$=$	$-ax_8\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_8\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{32}}$	$=$	$\left(x_8+\frac{1}{2}\right)\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{33}}$	$=$	$-x_8\mathbf{a}_1-y_8\mathbf{a}_2-z_8\mathbf{a}_3$	$=$	$-ax_8\hat{\mathbf{x}}-by_8\hat{\mathbf{y}}-cz_8\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{34}}$	$=$	$\left(x_8+\frac{1}{2}\right)\mathbf{a}_1+y_8\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{x}}+by_8\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{35}}$	$=$	$x_8\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\mathbf{a}_2+z_8\mathbf{a}_3$	$=$	$ax_8\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_8\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{36}}$	$=$	$-\left(x_8-\frac{1}{2}\right)\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B_{37}}$	$=$	$x_9\mathbf{a}_1+y_9\mathbf{a}_2+z_9\mathbf{a}_3$	$=$	$ax_9\hat{\mathbf{x}}+by_9\hat{\mathbf{y}}+cz_9\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{38}}$	$=$	$-\left(x_9-\frac{1}{2}\right)\mathbf{a}_1-y_9\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_9-\frac{1}{2}\right)\hat{\mathbf{x}}-by_9\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{39}}$	$=$	$-x_9\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\mathbf{a}_2-z_9\mathbf{a}_3$	$=$	$-ax_9\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_9\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{40}}$	$=$	$\left(x_9+\frac{1}{2}\right)\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_9+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{41}}$	$=$	$-x_9\mathbf{a}_1-y_9\mathbf{a}_2-z_9\mathbf{a}_3$	$=$	$-ax_9\hat{\mathbf{x}}-by_9\hat{\mathbf{y}}-cz_9\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{42}}$	$=$	$\left(x_9+\frac{1}{2}\right)\mathbf{a}_1+y_9\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_9+\frac{1}{2}\right)\hat{\mathbf{x}}+by_9\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{43}}$	$=$	$x_9\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\mathbf{a}_2+z_9\mathbf{a}_3$	$=$	$ax_9\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_9\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{44}}$	$=$	$-\left(x_9-\frac{1}{2}\right)\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_9-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	O IV

References

[1] J. M. Stewart and J. T. Szymański, *A redetermination of the crystal structure of potassium trithionate, $K_2S_3O_6$*, Acta Crystallogr. Sect. B **35**, 1967–1970 (1979), doi:10.1107/S0567740879008268.