KSO_3 ($K1_1$) Structure: AB3C_hP30_150_ef_3g_c2d-001

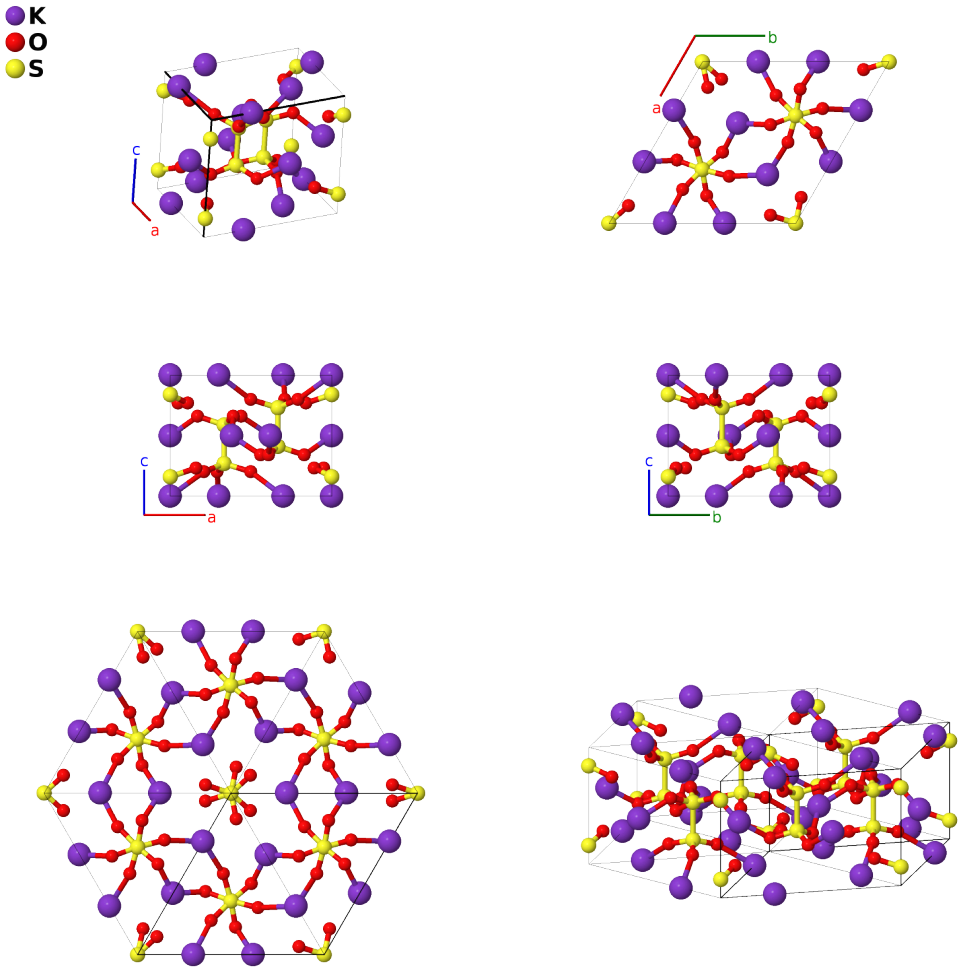
This structure originally had the label `AB3C_hP30_150_ef_3g_c2d`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/p/YVPA

https://aflow.org/p/AB3C_hP30_150_ef_3g_c2d-001



Prototype	KO_3S
AFLOW prototype label	AB3C_hP30_150_ef_3g_c2d-001
***Strukturbericht* designation**	$K1_1$
ICSD	27580
Pearson symbol	hP30
Space group number	150
Space group symbol	$P321$

AFLOW prototype command `aflow --proto=AB3C_hP30_150_ef_3g_c2d-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, x_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

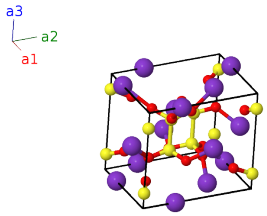
Other compounds with this structure

$RbSO_3$

- The ICSD entry differs from the published version of (Huggins, 1931) by using somewhat different lattice constants and switching the x coordinates of the potassium atoms. We will use the published results here.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	S II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	S II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	S III
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	S III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3e)	K I
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3e)	K I
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(3e)	K I
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	K II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	K II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	K II
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{14}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{15}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{16}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{17}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{19}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{20}}$	=	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{21}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{22}}$	=	$y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{23}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6g)	O II

$\mathbf{B_{24}}$	=	$-x_7\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{25}}$	=	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{26}}$	=	$-y_8\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{27}}$	=	$-(x_8-y_8)\,\mathbf{a}_1-x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{28}}$	=	$y_8\,\mathbf{a}_1+x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{29}}$	=	$(x_8-y_8)\,\mathbf{a}_1-y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{30}}$	=	$-x_8\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(6g)	O III

References

[1] M. L. Huggins and G. O. Frank, *The crystal structure of potassium dithionate, $K_2S_2O_6$*, Am. Mineral. **16**, 580–591 (1931).

Found in

[1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).