

KSO₃ (*K*1₁) Structure: AB3C_hP30_150_ef_3g_c2d-001

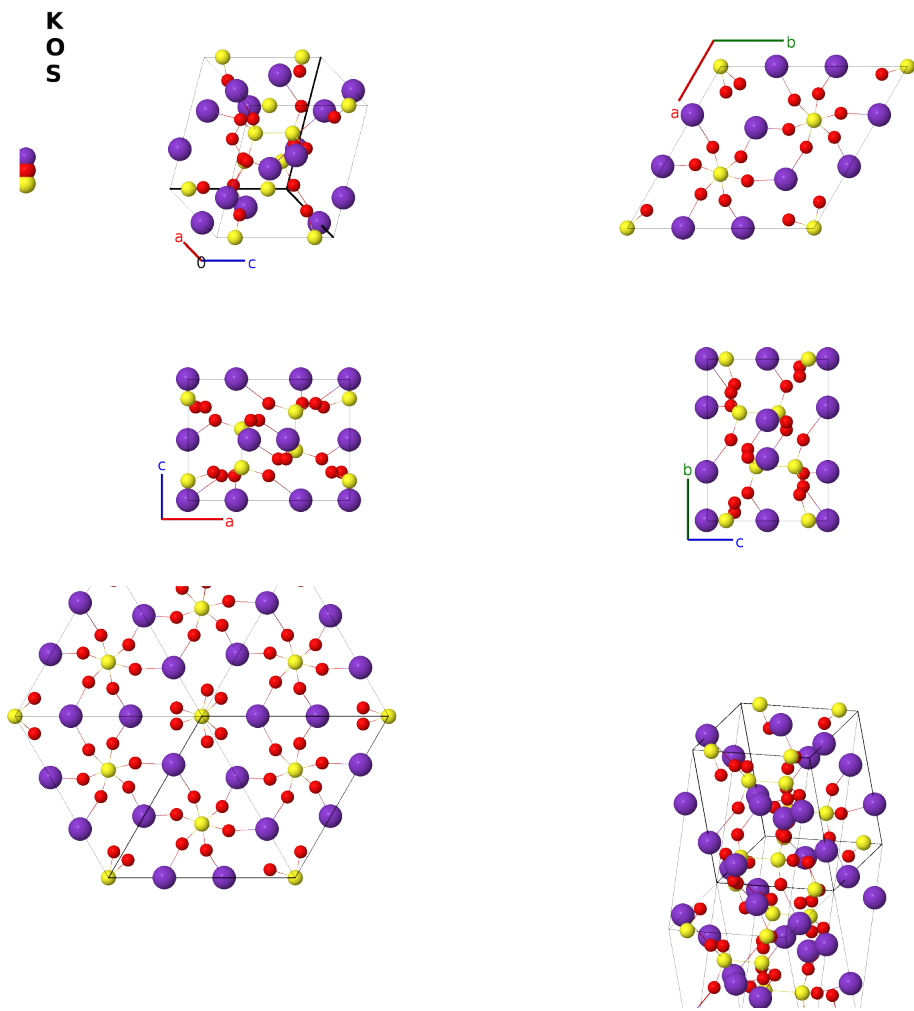
This structure previously used the label(s) **AB3C_hP30_150_ef_3g_c2d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/YVPA>

https://aflow.org/prototype-encyclopedia/AB3C_hP30_150_ef_3g_c2d-001



Prototype	KO ₃ S
AFLOW prototype label	AB3C_hP30_150_ef_3g_c2d-001
<i>Strukturbericht</i> designation	<i>K</i> 1 ₁
ICSD	27580
CCDC	1602837

Pearson symbol	hP30
Space group number	150
Space group symbol	$P\bar{3}21$
AFLOW prototype command	aflow --proto=AB3C_hP30_150_ef_3g_c2d-001 --params= $a, c/a, z_1, z_2, z_3, x_4, x_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

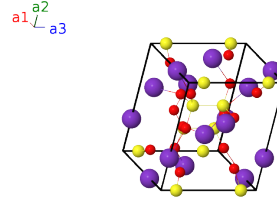
Other compounds with this structure

RbSO₃

- 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

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B}_2$	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2d)	S II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(2d)	S II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2d)	S III
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(2d)	S III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1$	$=$	$\frac{1}{2}a x_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}}$	(3e)	K I
$\mathbf{B}_8$	$= x_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a x_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_4 \hat{\mathbf{y}}$	(3e)	K I
$\mathbf{B}_9$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-a x_4 \hat{\mathbf{x}}$	(3e)	K I
$\mathbf{B}_{10}$	$= x_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	K II
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	K II
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f)	K II
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{14}$	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{15}$	$= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{16}$	$= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}} - c z_6 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{17}$	$= (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} - c z_6 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a y_6 \hat{\mathbf{y}} - c z_6 \hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B}_{19}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_7 - y_7) \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(6g)	O II

$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{O III}
\end{aligned}$$

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).

First cited in

- 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.