Steklite [$KAl(SO_4)_2$, $H3_2$] Structure: ABC8D2_hP12_150_a_b_dg_d-001

This structure originally had the label `ABC8D2_hP12_150_b_a_dg_d`. Calls to that address will be redirected here.

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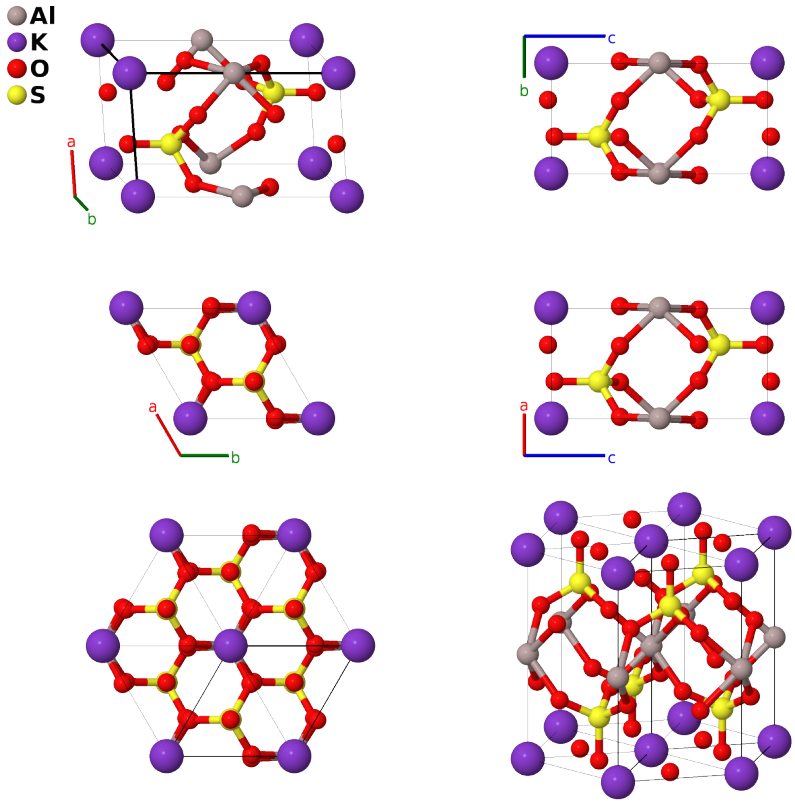
https://aflow.org/p/SDL2

https://aflow.org/p/ABC8D2_hP12_150_a_b_dg_d-001



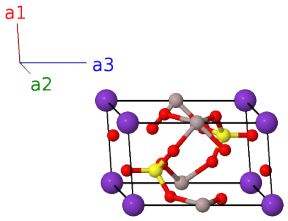
Prototype	$AlKO_8S_2$
AFLOW prototype label	ABC8D2_hP12_150_a_b_dg_d-001
***Strukturbericht* designation**	$H3_2$
Mineral name	steklite
ICSD	60170
Pearson symbol	hP12
Space group number	150
Space group symbol	$P321$
AFLOW prototype command	`aflow --proto=ABC8D2_hP12_150_a_b_dg_d-001 --params=`$a, c/a, z_3, z_4, x_5, y_5, z_5$

Other compounds with this structure
$NH_4(Al, Fe)(SO_4)_2$ (godovikovite), $KCr(SO_4)_2$, $RbCr(SO_4)_2$

- This has been a rather difficult structure to follow through the literature. (Villars, 2016) quotes the structure given by (Manoli, 1970), but gives the space group as $P\bar{3}$ #147. (Murashko, 2013) lists the space group as both $P312$ #149 and $P321$ #150, as well as listing obviously incorrect Wyckoff positions.
- (West, 2008) states that the simple structure is in $P\bar{3}$ but that it may be doubled along the c axis and be in space group $P321$.
- After correcting Murashko's results, we find that all of these interpretations yield essentially the same structure in a given layer, and only differ as the structure is reflected through the $z = 0$ plane. As it is not clear which structure is correct, we will use the original $H3_2$ structure given by (Hermann, 1937).
- Steklite is the name of the mineral form of this compound (Murashko, 2013). (Hermann, 1937) simply calls it *Wasserfreier Alaun* (anhydrous alum). For hydrated alum, $KAl(SO_4)_2{\cdot}12H_2O$, see the $H4_{13}$ structure.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	K I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	S I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	S I
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_8}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_9}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{10}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{11}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6g)	O II

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