Pyrophyllite [$AlSi_2O_5(OH)$, $S5_6$] Structure: AB5CD2_mC72_15_f_5f_f_2f-001

This structure originally had the label `AB5CD2_mC72_15_f_5f_f_2f`. Calls to that address will be redirected here.

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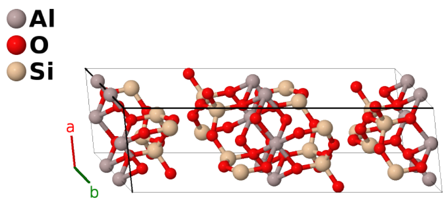
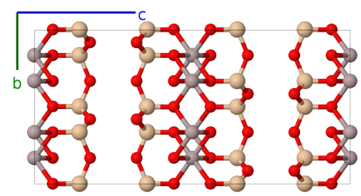
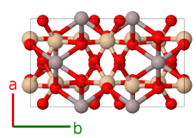
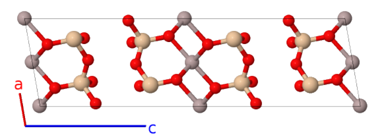
https://aflow.org/p/J4ZX

https://aflow.org/p/AB5CD2_mC72_15_f_5f_f_2f-001









Prototype	$AlHO_6Si_2$
AFLOW prototype label	AB5CD2_mC72_15_f_5f_f_2f-001
***Strukturbericht* designation**	$S5_6$
Mineral name	pyrophyllite
ICSD	26742
Pearson symbol	mC72
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=AB5CD2_mC72_15_f_5f_f_2f-001` `--params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

Other compounds with this structure

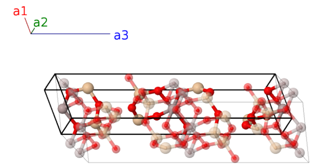
$Mg_3Si_4O_{10}(OH)_2$ (talc)

- This a double-layer version of the pyrophyllite structure. (Brindley, 1259) has shown that some samples have only one layer, with a corresponding reduction in the c lattice vector. Both Brindley and (Lee, 1981) found pyrophyllite samples with space group $P\bar{1}$ #2.

- Talc ($Mg_3Si_4O_{10}(OH)_2$) is isostructural with pyrophyllite, with magnesium replacing aluminum on the (8f) site and the addition of another magnesium atom on the (4a) Wyckoff site.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(x_1 - y_1)\,\mathbf{a}_1 + (x_1 + y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_2}$	=	$-(x_1 + y_1)\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_3}$	=	$-(x_1 - y_1)\,\mathbf{a}_1 - (x_1 + y_1)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_4}$	=	$(x_1 + y_1)\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_5}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_6}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_7}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_8}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_9}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{10}}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{11}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{14}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{15}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{16}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{17}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV

$\mathbf{B_{18}}$	=	$-\left(x_5+y_5\right)\,\mathbf{a}_1-\left(x_5-y_5\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5+c\left(z_5-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{19}}$	=	$-\left(x_5-y_5\right)\,\mathbf{a}_1-\left(x_5+y_5\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-\left(ax_5+cz_5\cos\beta\right)\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}-cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{20}}$	=	$\left(x_5+y_5\right)\,\mathbf{a}_1+\left(x_5-y_5\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5+c\left(z_5+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{21}}$	=	$\left(x_6-y_6\right)\,\mathbf{a}_1+\left(x_6+y_6\right)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\left(ax_6+cz_6\cos\beta\right)\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{22}}$	=	$-\left(x_6+y_6\right)\,\mathbf{a}_1-\left(x_6-y_6\right)\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6+c\left(z_6-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{23}}$	=	$-\left(x_6-y_6\right)\,\mathbf{a}_1-\left(x_6+y_6\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$-\left(ax_6+cz_6\cos\beta\right)\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}-cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{24}}$	=	$\left(x_6+y_6\right)\,\mathbf{a}_1+\left(x_6-y_6\right)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6+c\left(z_6+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{25}}$	=	$\left(x_7-y_7\right)\,\mathbf{a}_1+\left(x_7+y_7\right)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$\left(ax_7+cz_7\cos\beta\right)\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{26}}$	=	$-\left(x_7+y_7\right)\,\mathbf{a}_1-\left(x_7-y_7\right)\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7+c\left(z_7-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{27}}$	=	$-\left(x_7-y_7\right)\,\mathbf{a}_1-\left(x_7+y_7\right)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-\left(ax_7+cz_7\cos\beta\right)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{28}}$	=	$\left(x_7+y_7\right)\,\mathbf{a}_1+\left(x_7-y_7\right)\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7+c\left(z_7+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	OH I
$\mathbf{B_{29}}$	=	$\left(x_8-y_8\right)\,\mathbf{a}_1+\left(x_8+y_8\right)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$\left(ax_8+cz_8\cos\beta\right)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{30}}$	=	$-\left(x_8+y_8\right)\,\mathbf{a}_1-\left(x_8-y_8\right)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8+c\left(z_8-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{31}}$	=	$-\left(x_8-y_8\right)\,\mathbf{a}_1-\left(x_8+y_8\right)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	=	$-\left(ax_8+cz_8\cos\beta\right)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{32}}$	=	$\left(x_8+y_8\right)\,\mathbf{a}_1+\left(x_8-y_8\right)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8+c\left(z_8+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{33}}$	=	$\left(x_9-y_9\right)\,\mathbf{a}_1+\left(x_9+y_9\right)\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$\left(ax_9+cz_9\cos\beta\right)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{34}}$	=	$-\left(x_9+y_9\right)\,\mathbf{a}_1-\left(x_9-y_9\right)\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_9+c\left(z_9-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{35}}$	=	$-\left(x_9-y_9\right)\,\mathbf{a}_1-\left(x_9+y_9\right)\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	=	$-\left(ax_9+cz_9\cos\beta\right)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{36}}$	=	$\left(x_9+y_9\right)\,\mathbf{a}_1+\left(x_9-y_9\right)\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_9+c\left(z_9+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II

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