$Li_2SO_4{\cdot}H_2O$ ($H4_8$) Structure: A2B2C5D_mP20_4_2a_2a_5a_a-001

This structure originally had the label `A2B2C5D_mP20_4_2a_2a_5a_a`. Calls to that address will be redirected here.

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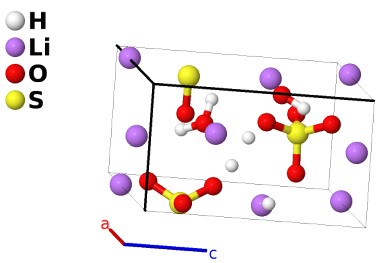
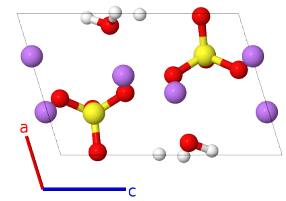
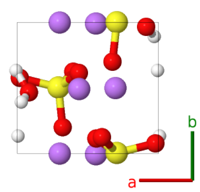
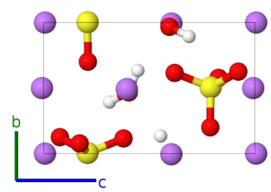
https://aflow.org/p/674K

https://aflow.org/p/A2B2C5D_mP20_4_2a_2a_5a_a-001







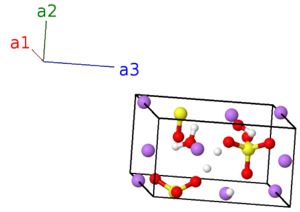


Prototype	$H_2Li_2O_5S$
AFLOW prototype label	A2B2C5D_mP20_4_2a_2a_5a_a-001
***Strukturbericht* designation**	$H4_8$
ICSD	201532
Pearson symbol	mP20
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	`aflow --proto=A2B2C5D_mP20_4_2a_2a_5a_a-001` `--params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- We use the data from (Lundgren, 1984) at 20K, including the positions of the hydrogen atoms not found in the original $H4_8$ structure in (Gottfried, 1937).
- Space group $P2_1$ #4 allows the y coordinates to have an arbitrary origin. We follow (Lundgren, 1984) and set the y coordinate of the sulfur atom, y_{10}, to zero.

Simple Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	H I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	H II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	H II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	Li II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2a)	S I
$\mathbf{B_{20}}$	=	$-x_{10}\,\mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2a)	S I

References

[1] J.-O. Lundgren, Å. Kvick, M. Karppinen, R. Liminga, and S. C. Abrahams, *Neutron diffraction structural study of pyroelectric $Li_2SO_4{\cdot}H_2O$ at 293, 80, and 20 K*, J. Chem. Phys. **80**, 423–430 (1984), doi:10.1063/1.446465.

[2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).