$LiOH{\cdot}H_2O$ ($B36$) Structure: A3BC2_mC24_12_ij_g_hi-001

This structure originally had the label `A3BC2_mC24_12_ij_h_gi`. Calls to that address will be redirected here.

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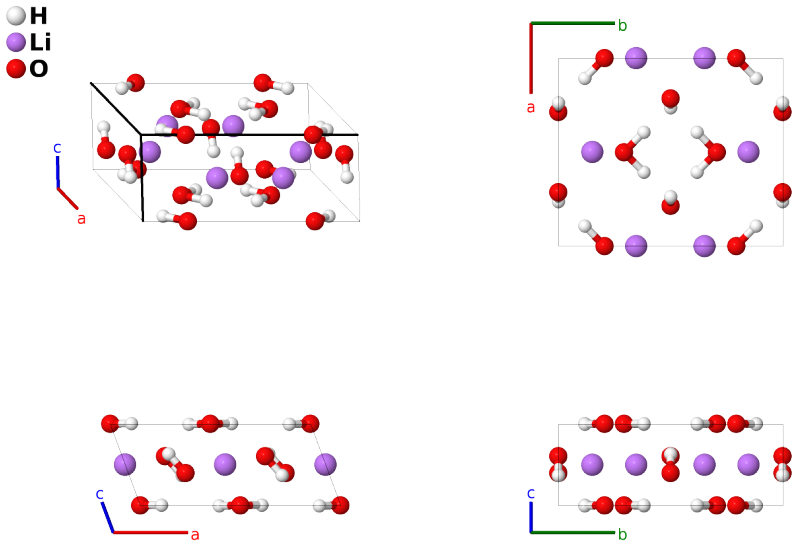
https://aflow.org/p/T76D

https://aflow.org/p/A3BC2_mC24_12_ij_g_hi-001

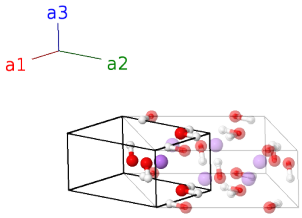


Prototype	H_3LiO_2
AFLOW prototype label	A3BC2_mC24_12_ij_g_hi-001
***Strukturbericht* designation**	$B36$
ICSD	9138
Pearson symbol	mC24
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A3BC2_mC24_12_ij_g_hi-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

- The structure given in *Strukturbericht* (Herrmann, 1943) does not list the hydrogen positions, instead giving positions for Li, OH and H_2O. (Alcock, 1971) found the hydrogen positions.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(4g)	Li I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2$	=	$-by_1\,\hat{\mathbf{y}}$	(4g)	Li I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	O I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	H I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	H I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_9}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	H II
$\mathbf{B_{10}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	H II
$\mathbf{B_{11}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	H II
$\mathbf{B_{12}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8j)	H II

References

[1] N. W. Alcock, *Refinement of the crystal structure of lithium hydroxide monohydrate*, Acta Crystallogr. Sect. B **27**, 1682–1683 (1971), doi:10.1107/S056774087100459X.

[2] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).