$BeSO_4{\cdot}4H_2O$ ($H4_3$) Structure: AB8C8D_tI72_120_b_2i_2i_c-001

This structure originally had the label `AB8C8D_tI72_120_c_2i_2i_b`. Calls to that address will be redirected here.

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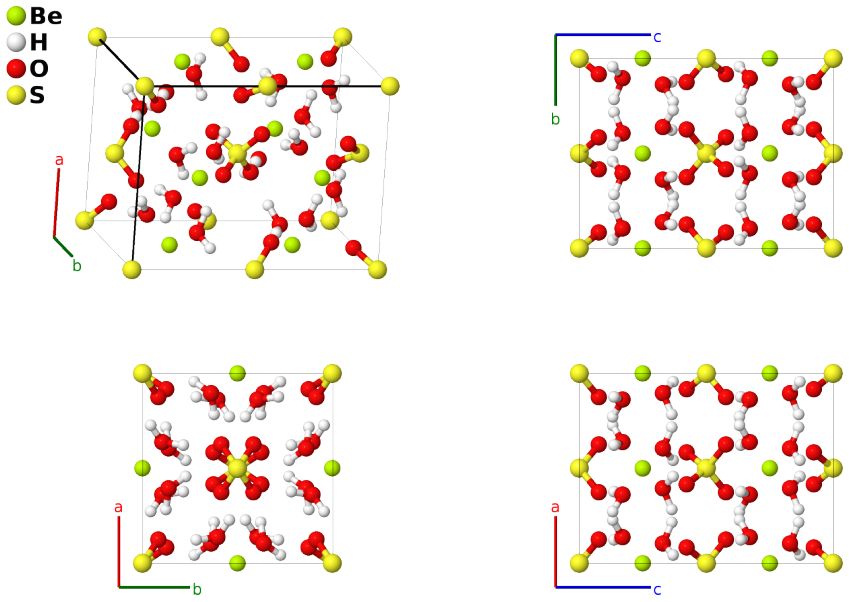
https://aflow.org/p/KR2S

https://aflow.org/p/AB8C8D_tI72_120_b_2i_2i_c-001

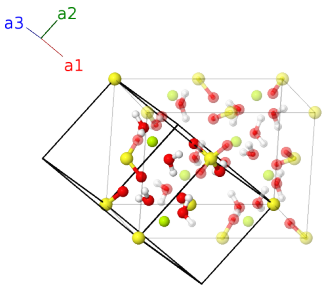


Prototype	BeH_8O_8S
AFLOW prototype label	AB8C8D_tI72_120_b_2i_2i_c-001
***Strukturbericht* designation**	$H4_3$
ICSD	23219
Pearson symbol	tI72
Space group number	120
Space group symbol	$I\bar{4}c2$
AFLOW prototype command	`aflow --proto=AB8C8D_tI72_120_b_2i_2i_c-001 --params=`$a, c/a, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- The original determination of the $H4_3$ structure did not determine the positions of the hydrogen atoms. Since (Sikka, 1969) showed that the placement of they hydrogen atoms did not substantially affect the postions of the other atoms in the primitive cell, nor change the space group, we retain the original *Strukturbericht* designation for the improved structure.

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4b)	Be I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Be I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_5}$	=	$(y_3+z_3)\,\mathbf{a}_1 + (x_3+z_3)\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_6}$	=	$-(y_3-z_3)\,\mathbf{a}_1 - (x_3-z_3)\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_7}$	=	$-(x_3+z_3)\,\mathbf{a}_1 + (y_3-z_3)\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_8}$	=	$(x_3-z_3)\,\mathbf{a}_1 - (y_3+z_3)\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_9}$	=	$\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_{10}}$	=	$\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_{11}}$	=	$\left(x_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_{12}}$	=	$-\left(x_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3+z_3-\frac{1}{2}\right)\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H I
$\mathbf{B_{13}}$	=	$(y_4+z_4)\,\mathbf{a}_1 + (x_4+z_4)\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{14}}$	=	$-(y_4-z_4)\,\mathbf{a}_1 - (x_4-z_4)\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{15}}$	=	$-(x_4+z_4)\,\mathbf{a}_1 + (y_4-z_4)\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{16}}$	=	$(x_4-z_4)\,\mathbf{a}_1 - (y_4+z_4)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{17}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{18}}$	=	$\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H II

$\mathbf{B_{19}}$	=	$\left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{20}}$	=	$-\left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	H II
$\mathbf{B_{21}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{22}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{23}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{24}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{25}}$	=	$\left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{26}}$	=	$\left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{27}}$	=	$\left(x_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{28}}$	=	$-\left(x_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O I
$\mathbf{B_{29}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{30}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{31}}$	=	$-(x_6 + z_6)\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{32}}$	=	$(x_6 - z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{33}}$	=	$\left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{34}}$	=	$\left(y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{35}}$	=	$\left(x_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O II
$\mathbf{B_{36}}$	=	$-\left(x_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	O II

References

[1] S. K. Sikka and R. Chidambaram, *A neutron diffraction determination of the structure of beryllium sulphate tetrahydrate, $BeSO_4 \cdot 4H_2O$*, Acta Crystallogr. Sect. B **25**, 310–315 (1969), doi:10.1107/S0567740869002160.