Bassanite [$CaSO_4(H_2O)_{0.5}$, $H4_7$] Structure: A2B2C9D2_mC90_5_ab2c_3c_a13c_3c-001

This structure originally had the label `A2B2C9D2_mC90_5_ab2c_3c_b13c_3c`. Calls to that address will be redirected here.

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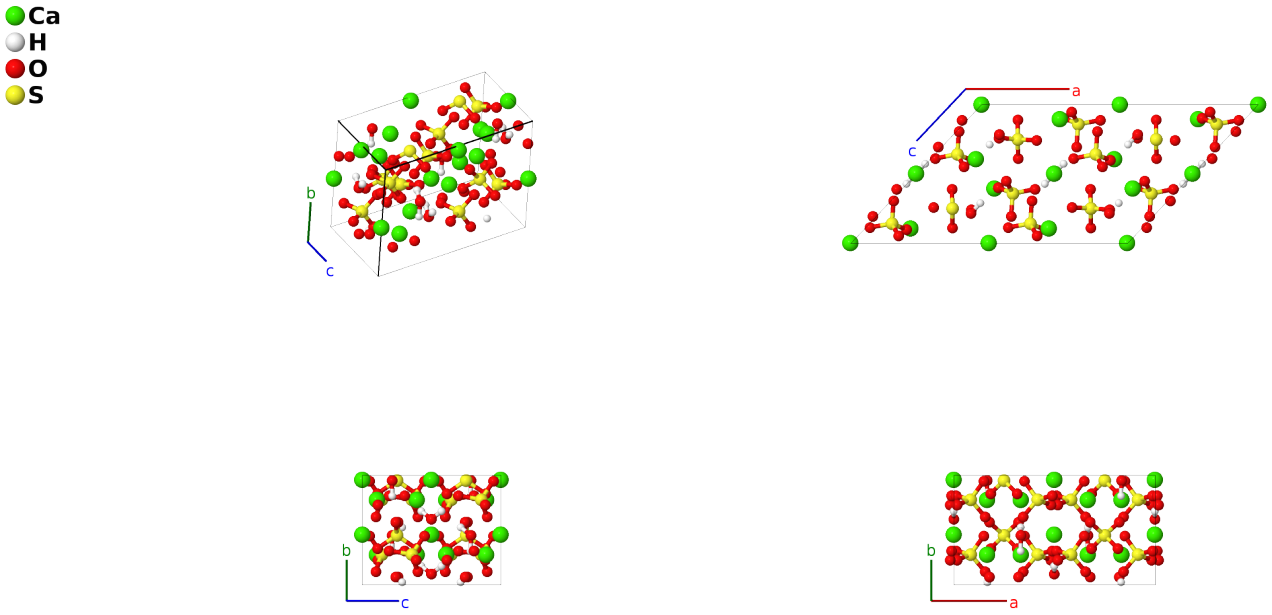
https://aflow.org/p/Q14S

https://aflow.org/p/A2B2C9D2_mC90_5_ab2c_3c_a13c_3c-001

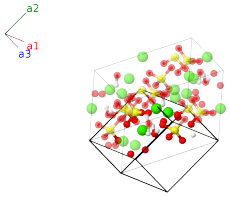


Prototype	$Ca(H_2O)_{0.5}O_4S$
AFLOW prototype label	A2B2C9D2_mC90_5_ab2c_3c_a13c_3c-001
***Strukturbericht* designation**	$H4_7$
Mineral name	bassanite
ICSD	73262
Pearson symbol	mC90
Space group number	5
Space group symbol	$C2$
AFLOW prototype command	`aflow --proto=A2B2C9D2_mC90_5_ab2c_3c_a13c_3c-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, y_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}, x_{23}, y_{23}, z_{23}, x_{24}, y_{24}, z_{24}$

- (Gottfried, 1937) gave this the *Strukturbericht* designation $H4_7$. They listed the system as monoclinic, with space group $C2$ #5, but noted that it was pseudo-hexagonal and gave the coordinates for the all of the atoms except the water molecules in terms of the trigonal space group $P3_121$ #152. (Abriel, 1993) found a complete determination of the structure in space group $I2$ #5, which we have converted to the standard $C2$ setting. The structure of this system seems to depend on the actual amount of water and the preparation mechanism, as there are both α- and β- forms which have different strengths but similar crystal structures (Singh, 2007).
- The $P3_121$ structure can be obtained from these positions by removing all of the water molecules (the hydrogen atoms plus O-I and O-XIV, and allowing for a small uncertainty in the positions of the remaining atoms.
- The ICSD entry only describes the $P3_121$ structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(2a)	Ca I
$\mathbf{B_2}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$by_2\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_3}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2b)	Ca II
$\mathbf{B_4}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4c)	Ca III
$\mathbf{B_5}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4c)	Ca III
$\mathbf{B_6}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4c)	Ca IV
$\mathbf{B_7}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4c)	Ca IV
$\mathbf{B_8}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_9}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4c)	H I
$\mathbf{B_{10}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{11}}$	=	$-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4c)	H II
$\mathbf{B_{12}}$	=	$(x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B_{13}}$	=	$-(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4c)	H III
$\mathbf{B_{14}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{15}}$	=	$-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4c)	O II

$$\mathbf{B_{16}} = (x_{10}-y_{10})\,\mathbf{a}_1 + (x_{10}+y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = (ax_{10}+cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O III}$$

$$\mathbf{B_{17}} = -(x_{10}+y_{10})\,\mathbf{a}_1 - (x_{10}-y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -(ax_{10}+cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O III}$$

$$\mathbf{B_{18}} = (x_{11}-y_{11})\,\mathbf{a}_1 + (x_{11}+y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = (ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O IV}$$

$$\mathbf{B_{19}} = -(x_{11}+y_{11})\,\mathbf{a}_1 - (x_{11}-y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O IV}$$

$$\mathbf{B_{20}} = (x_{12}-y_{12})\,\mathbf{a}_1 + (x_{12}+y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = (ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O V}$$

$$\mathbf{B_{21}} = -(x_{12}+y_{12})\,\mathbf{a}_1 - (x_{12}-y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O V}$$

$$\mathbf{B_{22}} = (x_{13}-y_{13})\,\mathbf{a}_1 + (x_{13}+y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = (ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O VI}$$

$$\mathbf{B_{23}} = -(x_{13}+y_{13})\,\mathbf{a}_1 - (x_{13}-y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -(ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O VI}$$

$$\mathbf{B_{24}} = (x_{14}-y_{14})\,\mathbf{a}_1 + (x_{14}+y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = (ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O VII}$$

$$\mathbf{B_{25}} = -(x_{14}+y_{14})\,\mathbf{a}_1 - (x_{14}-y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -(ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O VII}$$

$$\mathbf{B_{26}} = (x_{15}-y_{15})\,\mathbf{a}_1 + (x_{15}+y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O VIII}$$

$$\mathbf{B_{27}} = -(x_{15}+y_{15})\,\mathbf{a}_1 - (x_{15}-y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O VIII}$$

$$\mathbf{B_{28}} = (x_{16}-y_{16})\,\mathbf{a}_1 + (x_{16}+y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O IX}$$

$$\mathbf{B_{29}} = -(x_{16}+y_{16})\,\mathbf{a}_1 - (x_{16}-y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O IX}$$

$$\mathbf{B_{30}} = (x_{17}-y_{17})\,\mathbf{a}_1 + (x_{17}+y_{17})\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = (ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} + cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O X}$$

$$\mathbf{B_{31}} = -(x_{17}+y_{17})\,\mathbf{a}_1 - (x_{17}-y_{17})\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O X}$$

$$\mathbf{B_{32}} = (x_{18}-y_{18})\,\mathbf{a}_1 + (x_{18}+y_{18})\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = (ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} + cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XI}$$

$$\mathbf{B_{33}} = -(x_{18}+y_{18})\,\mathbf{a}_1 - (x_{18}-y_{18})\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 = -(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XI}$$

$$\mathbf{B_{34}} = (x_{19}-y_{19})\,\mathbf{a}_1 + (x_{19}+y_{19})\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = (ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} + cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XII}$$

$$\mathbf{B_{35}} = -(x_{19}+y_{19})\,\mathbf{a}_1 - (x_{19}-y_{19})\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3 = -(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} - cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XII}$$

$$\mathbf{B_{36}} = (x_{20}-y_{20})\,\mathbf{a}_1 + (x_{20}+y_{20})\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 = (ax_{20}+cz_{20}\cos\beta)\,\hat{\mathbf{x}} + by_{20}\,\hat{\mathbf{y}} + cz_{20}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XIII}$$

$$\mathbf{B_{37}} = -(x_{20}+y_{20})\,\mathbf{a}_1 - (x_{20}-y_{20})\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3 = -(ax_{20}+cz_{20}\cos\beta)\,\hat{\mathbf{x}} + by_{20}\,\hat{\mathbf{y}} - cz_{20}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XIII}$$

$$\mathbf{B_{38}} = (x_{21}-y_{21})\,\mathbf{a}_1 + (x_{21}+y_{21})\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3 = (ax_{21}+cz_{21}\cos\beta)\,\hat{\mathbf{x}} + by_{21}\,\hat{\mathbf{y}} + cz_{21}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XIV}$$

$$\mathbf{B_{39}} = -(x_{21}+y_{21})\,\mathbf{a}_1 - (x_{21}-y_{21})\,\mathbf{a}_2 - z_{21}\,\mathbf{a}_3 = -(ax_{21}+cz_{21}\cos\beta)\,\hat{\mathbf{x}} + by_{21}\,\hat{\mathbf{y}} - cz_{21}\sin\beta\,\hat{\mathbf{z}} \quad (4c) \quad \text{O XIV}$$

$\mathbf{B_{40}}$	=	$(x_{22} - y_{22})\ \mathbf{a}_1 + (x_{22} + y_{22})\ \mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$(ax_{22} + cz_{22}\cos\beta)\ \hat{\mathbf{x}} + by_{22}\,\hat{\mathbf{y}} + cz_{22}\sin\beta\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{41}}$	=	$-(x_{22} + y_{22})\ \mathbf{a}_1 - (x_{22} - y_{22})\ \mathbf{a}_2 - z_{22}\,\mathbf{a}_3$	=	$-(ax_{22} + cz_{22}\cos\beta)\ \hat{\mathbf{x}} + by_{22}\,\hat{\mathbf{y}} - cz_{22}\sin\beta\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_{42}}$	=	$(x_{23} - y_{23})\ \mathbf{a}_1 + (x_{23} + y_{23})\ \mathbf{a}_2 + z_{23}\,\mathbf{a}_3$	=	$(ax_{23} + cz_{23}\cos\beta)\ \hat{\mathbf{x}} + by_{23}\,\hat{\mathbf{y}} + cz_{23}\sin\beta\,\hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B_{43}}$	=	$-(x_{23} + y_{23})\ \mathbf{a}_1 - (x_{23} - y_{23})\ \mathbf{a}_2 - z_{23}\,\mathbf{a}_3$	=	$-(ax_{23} + cz_{23}\cos\beta)\ \hat{\mathbf{x}} + by_{23}\,\hat{\mathbf{y}} - cz_{23}\sin\beta\,\hat{\mathbf{z}}$	(4c)	S II
$\mathbf{B_{44}}$	=	$(x_{24} - y_{24})\ \mathbf{a}_1 + (x_{24} + y_{24})\ \mathbf{a}_2 + z_{24}\,\mathbf{a}_3$	=	$(ax_{24} + cz_{24}\cos\beta)\ \hat{\mathbf{x}} + by_{24}\,\hat{\mathbf{y}} + cz_{24}\sin\beta\,\hat{\mathbf{z}}$	(4c)	S III
$\mathbf{B_{45}}$	=	$-(x_{24} + y_{24})\ \mathbf{a}_1 - (x_{24} - y_{24})\ \mathbf{a}_2 - z_{24}\,\mathbf{a}_3$	=	$-(ax_{24} + cz_{24}\cos\beta)\ \hat{\mathbf{x}} + by_{24}\,\hat{\mathbf{y}} - cz_{24}\sin\beta\,\hat{\mathbf{z}}$	(4c)	S III

References

[1] W. Abriel and R. Nesper, *Bestimmung der Kristallstruktur von $CaSO_4(H_2O)_{0.5}$ mit Röntgenbeugungsmethoden und mit Potentialprofil-Rechnungen*, Z. Krystallogr. **205**, 99–113 (1993), doi:10.1524/zkri.1993.205.12.99.

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

[3] N. B. Singh and B. Middendorf, *Calcium sulphate hemihydrate hydration leading to gypsum crystallization*, Prog. Cryst. Growth Char. Materials **53**, 57–77 (2007), doi:10.1016/j.pcrysgrow.2007.01.002.

Found in

[1] P. Ballirano, A. Maras, S. Meloni, and R. Caminiti, *The monoclinic I2 structure of bassanite, calcium sulphate hemihydrate ($CaSO_4{\cdot}0.5H_2O$)*, Euro. J. Mineral. **13**, 985–993 (2001).