Tutton salt [$Cu(NH_4)_2(SO_4)_2{\cdot}H_2O$, $H4_4$] Structure: AB20C2D14E2_mP78_14_a_10e_e_7e_e-001

This structure originally had the label `AB20C2D14E2_mP78_14_a_10e_e_7e_e`. Calls to that address will be redirected here.

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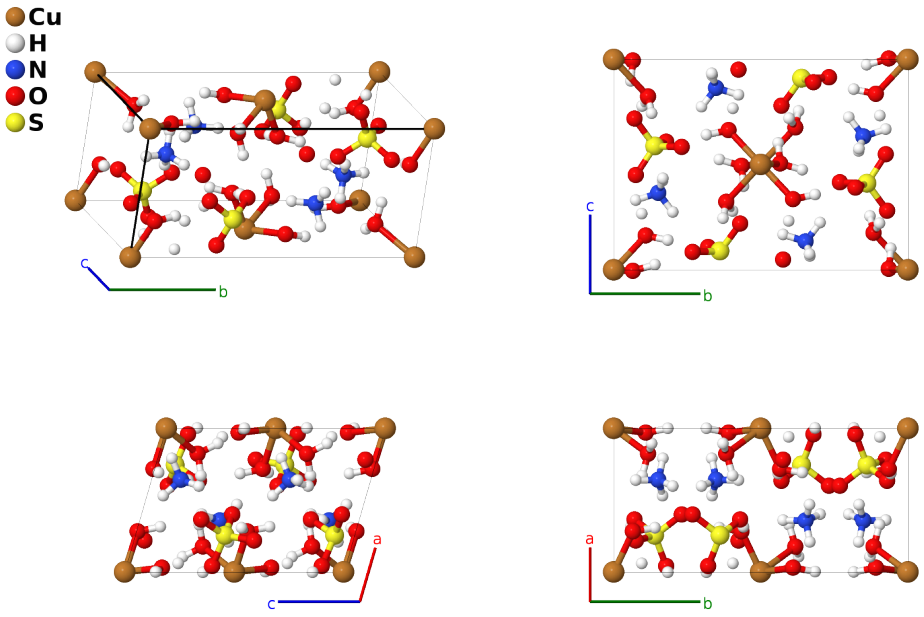
https://aflow.org/p/KT73

https://aflow.org/p/AB20C2D14E2_mP78_14_a_10e_e_7e_e-001



Prototype	$CuH_{20}N_2O_{14}S$
AFLOW prototype label	AB20C2D14E2_mP78_14_a_10e_e_7e_e-001
***Strukturbericht* designation**	$H4_4$
Mineral name	tutton salt
ICSD	23187
Pearson symbol	mP78
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=AB20C2D14E2_mP78_14_a_10e_e_7e_e-001 --params=`$a, b/a, c/a, \beta, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}$

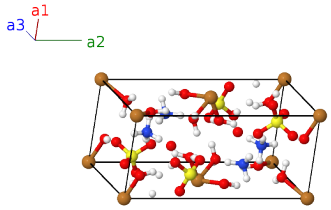
Other compounds with this structure

$Cd(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Co(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Fe(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Mg(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Mn(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Ni(NH_4)_2(S$
$V(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Zn(NH_4)_2(SO_4)_2{\cdot}6H_2O$, $Mg(NH_4)_2(SeO_4)_2{\cdot}6H_2O$, $Co(KSO_4)_2{\cdot}6H_2O$, $Cu(KSeO_4)_2{\cdot}6H_2O$, $Cu(KSO_4)_2{\cdot}6H_2O$,
$Mg(KSO_4)_2{\cdot}6H_2O$, $Mg(TlSO_4)_2{\cdot}6H_2O$, $Ni(KSO_4)_2{\cdot}6H_2O$

- Tutton Salts have the form $AB_2(SO_4)_2{\cdot}6H_2O$, where A is a divalent ion and B is a monovalent ion. (Hermann, 1937) formally lists $Mg(NH_4)_2(SO_4)_2{\cdot}6H_2O$ as the prototype, but notes that one may have "other monovalent metals in place of NH_4 and divalent [metals] in place of Mg." We choose the $Cu(NH_4)_2(SO_4)_2{\cdot}H_2O$ as the prototype because (Brown, 1969) were able to locate all of the hydrogen ions in agreement with expectation, *i.e.*, H_2O molecules have properly bent H-O bonds, and the hydrogen atoms in the ammonium ion form a tetrahedron around the nitrogen atom.
- The atomic positions were originally given in the $P2_1/a$ setting of space group #14. We used FINDSYM to convert this to the standard $P2_1/c$ setting. This resulted in the a and c axes being swapped.

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
$\mathbf{B_1}$	=	0	=	0	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\left(ax_3 + cz_3\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	H III
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H III
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	H III
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H III
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	H IV
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H IV
$\mathbf{B_{17}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	H IV
$\mathbf{B_{18}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	H IV

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\begin{array}{lcccccc}
\mathbf{B_{19}} & = & 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}} & \text{(4e)} & \text{H V} \\
\mathbf{B_{20}} & = & -x_6\,\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H V} \\
\mathbf{B_{21}} & = & -x_6\,\mathbf{a}_1 - y_6\,\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}} & \text{(4e)} & \text{H V} \\
\mathbf{B_{22}} & = & x_6\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H V} \\
\mathbf{B_{23}} & = & 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}} & \text{(4e)} & \text{H VI} \\
\mathbf{B_{24}} & = & -x_7\,\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_7 + c\left(z_7 - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H VI} \\
\mathbf{B_{25}} & = & -x_7\,\mathbf{a}_1 - y_7\,\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}} & \text{(4e)} & \text{H VI} \\
\mathbf{B_{26}} & = & x_7\,\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_7 + c\left(z_7 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H VI} \\
\mathbf{B_{27}} & = & 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}} & \text{(4e)} & \text{H VII} \\
\mathbf{B_{28}} & = & -x_8\,\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_8 + c\left(z_8 - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_8 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H VII} \\
\mathbf{B_{29}} & = & -x_8\,\mathbf{a}_1 - y_8\,\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}} & \text{(4e)} & \text{H VII} \\
\mathbf{B_{30}} & = & x_8\,\mathbf{a}_1 - \left(y_8 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_8 + c\left(z_8 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_8 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H VII} \\
\mathbf{B_{31}} & = & 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}} & \text{(4e)} & \text{H VIII} \\
\mathbf{B_{32}} & = & -x_9\,\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_9 + c\left(z_9 - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_9 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H VIII} \\
\mathbf{B_{33}} & = & -x_9\,\mathbf{a}_1 - y_9\,\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}} & \text{(4e)} & \text{H VIII} \\
\mathbf{B_{34}} & = & x_9\,\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_9 + c\left(z_9 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_9 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H VIII} \\
\mathbf{B_{35}} & = & 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}} & \text{(4e)} & \text{H IX} \\
\mathbf{B_{36}} & = & -x_{10}\,\mathbf{a}_1 + \left(y_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{10} + c\left(z_{10} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H IX} \\
\mathbf{B_{37}} & = & -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & -\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H IX} \\
\mathbf{B_{38}} & = & x_{10}\,\mathbf{a}_1 - \left(y_{10} - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{10} + c\left(z_{10} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{10} - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H IX} \\
\mathbf{B_{39}} & = & x_{11}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{H X} \\
\mathbf{B_{40}} & = & -x_{11}\,\mathbf{a}_1 + \left(y_{11} + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{11} - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{11} + c\left(z_{11} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{11} + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{11} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H X} \\
\mathbf{B_{41}} & = & -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & -\left(ax_{11} + cz_{11}\cos\beta\right)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H X} \\
\mathbf{B_{42}} & = & x_{11}\,\mathbf{a}_1 - \left(y_{11} - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{11} + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{11} + c\left(z_{11} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{11} - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{11} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{H X} \\
\mathbf{B_{43}} & = & x_{12}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{N I} \\
\mathbf{B_{44}} & = & -x_{12}\,\mathbf{a}_1 + \left(y_{12} + \tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{12} - \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{12} + c\left(z_{12} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{12} + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{12} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{N I} \\
\mathbf{B_{45}} & = & -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 & = & -\left(ax_{12} + cz_{12}\cos\beta\right)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{N I} \\
\mathbf{B_{46}} & = & x_{12}\,\mathbf{a}_1 - \left(y_{12} - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{12} + \tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{12} + c\left(z_{12} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{12} - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{N I}
\end{array}
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\begin{array}{lcccccc}
\mathbf{B_{47}} & = & x_{13}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O I} \\
\mathbf{B_{48}} & = & -x_{13}\,\mathbf{a}_1 + \left(y_{13}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{13}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{13} + c\left(z_{13}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{13}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{13}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O I} \\
\mathbf{B_{49}} & = & -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 & = & -\left(ax_{13} + cz_{13}\cos\beta\right)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O I} \\
\mathbf{B_{50}} & = & x_{13}\,\mathbf{a}_1 - \left(y_{13}-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{13}+\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{13} + c\left(z_{13}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{13}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O I} \\
\mathbf{B_{51}} & = & x_{14}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O II} \\
\mathbf{B_{52}} & = & -x_{14}\,\mathbf{a}_1 + \left(y_{14}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{14}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{14} + c\left(z_{14}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{14}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{14}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O II} \\
\mathbf{B_{53}} & = & -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 & = & -\left(ax_{14} + cz_{14}\cos\beta\right)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O II} \\
\mathbf{B_{54}} & = & x_{14}\,\mathbf{a}_1 - \left(y_{14}-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{14} + c\left(z_{14}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{14}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O II} \\
\mathbf{B_{55}} & = & x_{15}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O III} \\
\mathbf{B_{56}} & = & -x_{15}\,\mathbf{a}_1 + \left(y_{15}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{15}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{15} + c\left(z_{15}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{15}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{15}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O III} \\
\mathbf{B_{57}} & = & -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 & = & -\left(ax_{15} + cz_{15}\cos\beta\right)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O III} \\
\mathbf{B_{58}} & = & x_{15}\,\mathbf{a}_1 - \left(y_{15}-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{15} + c\left(z_{15}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{15}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O III} \\
\mathbf{B_{59}} & = & x_{16}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O IV} \\
\mathbf{B_{60}} & = & -x_{16}\,\mathbf{a}_1 + \left(y_{16}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{16}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{16} + c\left(z_{16}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{16}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{16}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O IV} \\
\mathbf{B_{61}} & = & -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 & = & -\left(ax_{16} + cz_{16}\cos\beta\right)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O IV} \\
\mathbf{B_{62}} & = & x_{16}\,\mathbf{a}_1 - \left(y_{16}-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{16} + c\left(z_{16}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{16}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O IV} \\
\mathbf{B_{63}} & = & x_{17}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O V} \\
\mathbf{B_{64}} & = & -x_{17}\,\mathbf{a}_1 + \left(y_{17}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{17}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{17} + c\left(z_{17}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{17}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{17}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O V} \\
\mathbf{B_{65}} & = & -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 & = & -\left(ax_{17} + cz_{17}\cos\beta\right)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O V} \\
\mathbf{B_{66}} & = & x_{17}\,\mathbf{a}_1 - \left(y_{17}-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{17}+\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{17} + c\left(z_{17}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{17}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{17}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O V} \\
\mathbf{B_{67}} & = & x_{18}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O VI} \\
\mathbf{B_{68}} & = & -x_{18}\,\mathbf{a}_1 + \left(y_{18}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{18}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{18} + c\left(z_{18}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{18}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{18}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O VI} \\
\mathbf{B_{69}} & = & -x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 & = & -\left(ax_{18} + cz_{18}\cos\beta\right)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O VI} \\
\mathbf{B_{70}} & = & x_{18}\,\mathbf{a}_1 - \left(y_{18}-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{18}+\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & \left(ax_{18} + c\left(z_{18}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{18}-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{18}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O VI} \\
\mathbf{B_{71}} & = & x_{19}\,\mathbf{a}_1 + 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}} & \text{(4e)} & \text{O VII} \\
\mathbf{B_{72}} & = & -x_{19}\,\mathbf{a}_1 + \left(y_{19}+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{19}-\tfrac{1}{2}\right)\,\mathbf{a}_3 & = & -\left(ax_{19} + c\left(z_{19}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{19}+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{19}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} & \text{(4e)} & \text{O VII}
\end{array}
$$

$\mathbf{B_{73}}$	$=$	$-x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3$	$=$	$-\left(ax_{19} + cz_{19}\cos\beta\right)\,\hat{\mathbf{x}} - by_{19}\,\hat{\mathbf{y}} - cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B_{74}}$	$=$	$x_{19}\,\mathbf{a}_1 - \left(y_{19} - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\left(ax_{19} + c\left(z_{19} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{19} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{19} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B_{75}}$	$=$	$x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	$=$	$\left(ax_{20} + cz_{20}\cos\beta\right)\,\hat{\mathbf{x}} + by_{20}\,\hat{\mathbf{y}} + cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_{76}}$	$=$	$-x_{20}\,\mathbf{a}_1 + \left(y_{20} + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_{20} - \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\left(ax_{20} + c\left(z_{20} - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_{20} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_{20} - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_{77}}$	$=$	$-x_{20}\,\mathbf{a}_1 - y_{20}\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3$	$=$	$-\left(ax_{20} + cz_{20}\cos\beta\right)\,\hat{\mathbf{x}} - by_{20}\,\hat{\mathbf{y}} - cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_{78}}$	$=$	$x_{20}\,\mathbf{a}_1 - \left(y_{20} - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\left(ax_{20} + c\left(z_{20} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_{20} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{20} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I

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