

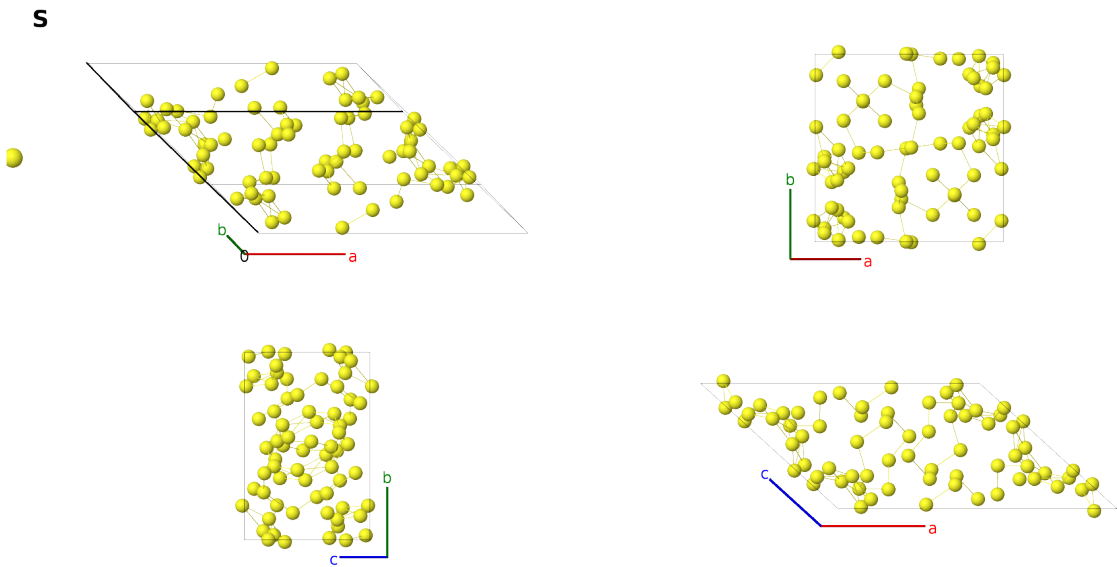
β -monoclinic Sulfur Structure: A_mP64_14_16e-002

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/AYZW>

https://aflow.org/prototype-encyclopedia/A_mP64_14_16e-002



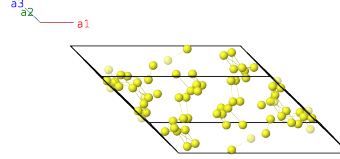
Prototype	S
AFLOW prototype label	A_mP64_14_16e-002
ICSD	870
CCDC	1591114
Pearson symbol	mP64
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A_mP64_14_16e-002 --params=a,b/a,c/a,β,$x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3,x_4,y_4,z_4,x_5,y_5,z_5,x_6,y_6,z_6,x_7,y_7,z_7,x_8,y_8,z_8,x_9,y_9,z_9,x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},z_{15},x_{16},y_{16},z_{16}$</pre>

- We take the name of this structure from (Donohue, 1976). This is the high temperature phase of sulfur, stable from 95°C to the melting point at 115°C, although it can be kept at room temperatures for some time. (Templeton, 1976)
- This is a refinement of the original structure found by (Sands, 1965). There are two types of sulfur atoms in this sample:

- atoms S-I through S-VIII form stable sulfur rings with all the sites fully occupied, just as in the ground state α -S (A16).
- Atoms S-IX through S-XVI form a ring with one of two orientations, randomly chosen.
- The S-IX through S-XVI sites are thus half occupied, so there are only 48 atoms and six sulfur rings in any unit cell. Contrast this with A_k selenium, which has eight complete rings in the unit cell.
- Both A_k selenium and β -monoclinic sulfur have the same AFLOW prototype label, A_mP64_14_16e. They are generated by the same symmetry operations with different sets of parameters (**--params**) specified in their corresponding CIF files.

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
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_4$	$x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_8$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	S IV
$\mathbf{B}_{14}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S IV
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	S IV
$\mathbf{B}_{16}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S IV
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	S V

$\mathbf{B}_{18} =$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S V
$\mathbf{B}_{19} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	S V
$\mathbf{B}_{20} =$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S V
$\mathbf{B}_{21} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	S VI
$\mathbf{B}_{22} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S VI
$\mathbf{B}_{23} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	S VI
$\mathbf{B}_{24} =$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S VI
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4e)	S VII
$\mathbf{B}_{26} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S VII
$\mathbf{B}_{27} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4e)	S VII
$\mathbf{B}_{28} =$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S VII
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4e)	S VIII
$\mathbf{B}_{30} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S VIII
$\mathbf{B}_{31} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4e)	S VIII
$\mathbf{B}_{32} =$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S VIII
$\mathbf{B}_{33} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4e)	S IX
$\mathbf{B}_{34} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S IX
$\mathbf{B}_{35} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4e)	S IX
$\mathbf{B}_{36} =$	$x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S IX
$\mathbf{B}_{37} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4e)	S X
$\mathbf{B}_{38} =$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{10} + c(z_{10} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S X
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4e)	S X
$\mathbf{B}_{40} =$	$x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S X
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4e)	S XI
$\mathbf{B}_{42} =$	$-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_{11} + c(z_{11} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S XI
$\mathbf{B}_{43} =$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4e)	S XI
$\mathbf{B}_{44} =$	$x_{11} \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	S XI
$\mathbf{B}_{45} =$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4e)	S XII

$$\begin{aligned}
\mathbf{B}_{46} &= -x_{12} \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{12} + c\left(z_{12} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XII} \\
\mathbf{B}_{47} &= -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}} &(4e) &\text{S XII} \\
\mathbf{B}_{48} &= x_{12} \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{12} + c\left(z_{12} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XII} \\
\mathbf{B}_{49} &= 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}} &(4e) &\text{S XIII} \\
\mathbf{B}_{50} &= -x_{13} \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{13} + c\left(z_{13} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XIII} \\
\mathbf{B}_{51} &= -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}} &(4e) &\text{S XIII} \\
\mathbf{B}_{52} &= x_{13} \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{13} + c\left(z_{13} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XIII} \\
\mathbf{B}_{53} &= 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}} &(4e) &\text{S XIV} \\
\mathbf{B}_{54} &= -x_{14} \mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{14} + c\left(z_{14} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XIV} \\
\mathbf{B}_{55} &= -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}} &(4e) &\text{S XIV} \\
\mathbf{B}_{56} &= x_{14} \mathbf{a}_1 - \left(y_{14} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{14} + c\left(z_{14} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XIV} \\
\mathbf{B}_{57} &= 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}} &(4e) &\text{S XV} \\
\mathbf{B}_{58} &= -x_{15} \mathbf{a}_1 + \left(y_{15} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{15} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{15} + c\left(z_{15} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{15} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{15} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XV} \\
\mathbf{B}_{59} &= -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}} &(4e) &\text{S XV} \\
\mathbf{B}_{60} &= x_{15} \mathbf{a}_1 - \left(y_{15} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{15} + c\left(z_{15} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{15} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{15} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XV} \\
\mathbf{B}_{61} &= 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}} &(4e) &\text{S XVI} \\
\mathbf{B}_{62} &= -x_{16} \mathbf{a}_1 + \left(y_{16} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{16} - \frac{1}{2}\right) \mathbf{a}_3 &= -\left(ax_{16} + c\left(z_{16} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{16} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{16} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XVI} \\
\mathbf{B}_{63} &= -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}} &(4e) &\text{S XVI} \\
\mathbf{B}_{64} &= x_{16} \mathbf{a}_1 - \left(y_{16} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{16} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{16} + c\left(z_{16} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - b\left(y_{16} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{16} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(4e) &\text{S XVI}
\end{aligned}$$

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