CsB_4O_6F Structure: A4BCD6_oP48_33_4a_a_a_6a-001

This structure previously used the label(s) `A4BCD6_oP48_33_4a_a_a_6a`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

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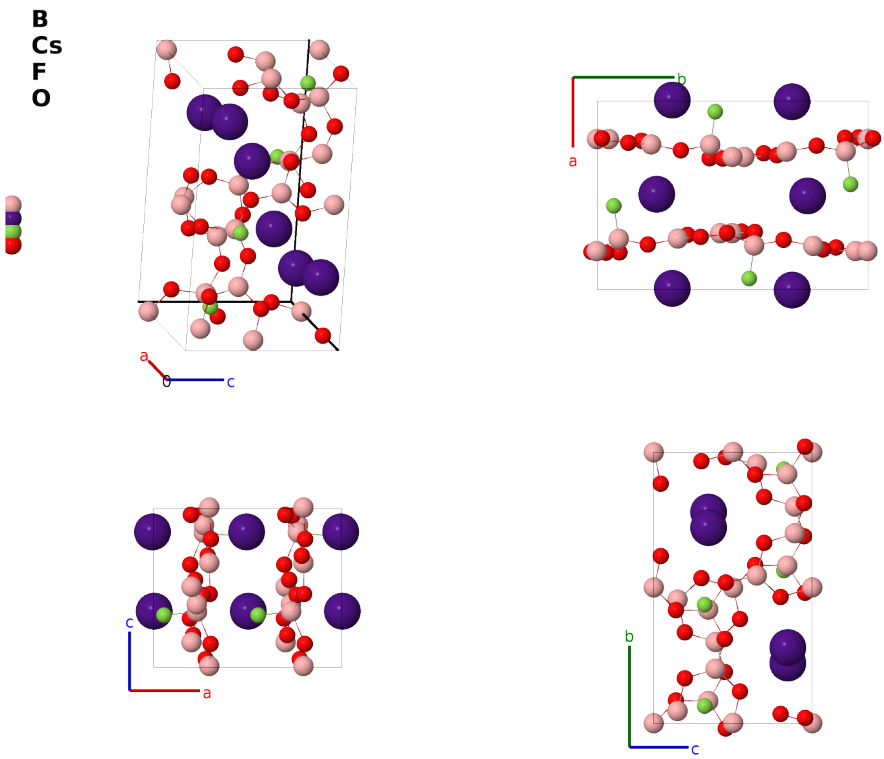
https://aflow.org/prototype-encyclopedia/Z0HT

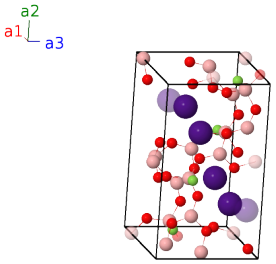
https://aflow.org/prototype-encyclopedia/A4BCD6_oP48_33_4a_a_a_6a-001



Prototype	B_4CsFO_6
AFLOW prototype label	A4BCD6_oP48_33_4a_a_a_6a-001
CCDC	1551261
Pearson symbol	oP48
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	`aflow --proto=A4BCD6_oP48_33_4a_a_a_6a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_3}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_4}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_7}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_8}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{11}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{12}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{15}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{16}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Cs I
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Cs I
$\mathbf{B_{19}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Cs I
$\mathbf{B_{20}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Cs I
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	F I
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	F I
$\mathbf{B_{23}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	F I

$$
\begin{array}{rcccccc}
\mathbf{B_{24}} & = & -\left(x_6-\frac{1}{2}\right)\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_6-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_6+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{F I} \\
\mathbf{B_{25}} & = & x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(4a)} & \text{O I} \\
\mathbf{B_{26}} & = & -x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3 & = & -ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O I} \\
\mathbf{B_{27}} & = & \left(x_7+\frac{1}{2}\right)\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\mathbf{a}_2+z_7\,\mathbf{a}_3 & = & a\left(x_7+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} & \text{(4a)} & \text{O I} \\
\mathbf{B_{28}} & = & -\left(x_7-\frac{1}{2}\right)\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_7-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O I} \\
\mathbf{B_{29}} & = & x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(4a)} & \text{O II} \\
\mathbf{B_{30}} & = & -x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3 & = & -ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O II} \\
\mathbf{B_{31}} & = & \left(x_8+\frac{1}{2}\right)\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(4a)} & \text{O II} \\
\mathbf{B_{32}} & = & -\left(x_8-\frac{1}{2}\right)\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O II} \\
\mathbf{B_{33}} & = & x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(4a)} & \text{O III} \\
\mathbf{B_{34}} & = & -x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O III} \\
\mathbf{B_{35}} & = & \left(x_9+\frac{1}{2}\right)\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & a\left(x_9+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(4a)} & \text{O III} \\
\mathbf{B_{36}} & = & -\left(x_9-\frac{1}{2}\right)\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_9-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O III} \\
\mathbf{B_{37}} & = & x_{10}\,\mathbf{a}_1+y_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IV} \\
\mathbf{B_{38}} & = & -x_{10}\,\mathbf{a}_1-y_{10}\,\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O IV} \\
\mathbf{B_{39}} & = & \left(x_{10}+\frac{1}{2}\right)\mathbf{a}_1-\left(y_{10}-\frac{1}{2}\right)\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & a\left(x_{10}+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IV} \\
\mathbf{B_{40}} & = & -\left(x_{10}-\frac{1}{2}\right)\mathbf{a}_1+\left(y_{10}+\frac{1}{2}\right)\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_{10}-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O IV} \\
\mathbf{B_{41}} & = & x_{11}\,\mathbf{a}_1+y_{11}\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O V} \\
\mathbf{B_{42}} & = & -x_{11}\,\mathbf{a}_1-y_{11}\,\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O V} \\
\mathbf{B_{43}} & = & \left(x_{11}+\frac{1}{2}\right)\mathbf{a}_1-\left(y_{11}-\frac{1}{2}\right)\mathbf{a}_2+z_{11}\,\mathbf{a}_3 & = & a\left(x_{11}+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_{11}-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O V} \\
\mathbf{B_{44}} & = & -\left(x_{11}-\frac{1}{2}\right)\mathbf{a}_1+\left(y_{11}+\frac{1}{2}\right)\mathbf{a}_2+\left(z_{11}+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_{11}-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_{11}+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_{11}+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O V} \\
\mathbf{B_{45}} & = & x_{12}\,\mathbf{a}_1+y_{12}\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3 & = & ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{46}} & = & -x_{12}\,\mathbf{a}_1-y_{12}\,\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\mathbf{a}_3 & = & -ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{47}} & = & \left(x_{12}+\frac{1}{2}\right)\mathbf{a}_1-\left(y_{12}-\frac{1}{2}\right)\mathbf{a}_2+z_{12}\,\mathbf{a}_3 & = & a\left(x_{12}+\frac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_{12}-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{48}} & = & -\left(x_{12}-\frac{1}{2}\right)\mathbf{a}_1+\left(y_{12}+\frac{1}{2}\right)\mathbf{a}_2+\left(z_{12}+\frac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_{12}-\frac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_{12}+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_{12}+\frac{1}{2}\right)\hat{\mathbf{z}} & \text{(4a)} & \text{O VI}
\end{array}
$$

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[1] X. Wang, Y. Wang, B. Zhang, F. Zhang, Z. Yang, and S. Pan, *CsB_4O_6F: A Congruent-Melting Deep-Ultraviolet Nonlinear Optical Material by Combining Superior Functional Units*, Angew. Chem. Int. Ed. **56**, 13901–14314 (2017), doi:10.1002/anie.201708231.

First cited in

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