$BaCaSiO_4$ Structure: ABC4D_hP56_186_bc_ac_b3cd_bc-001

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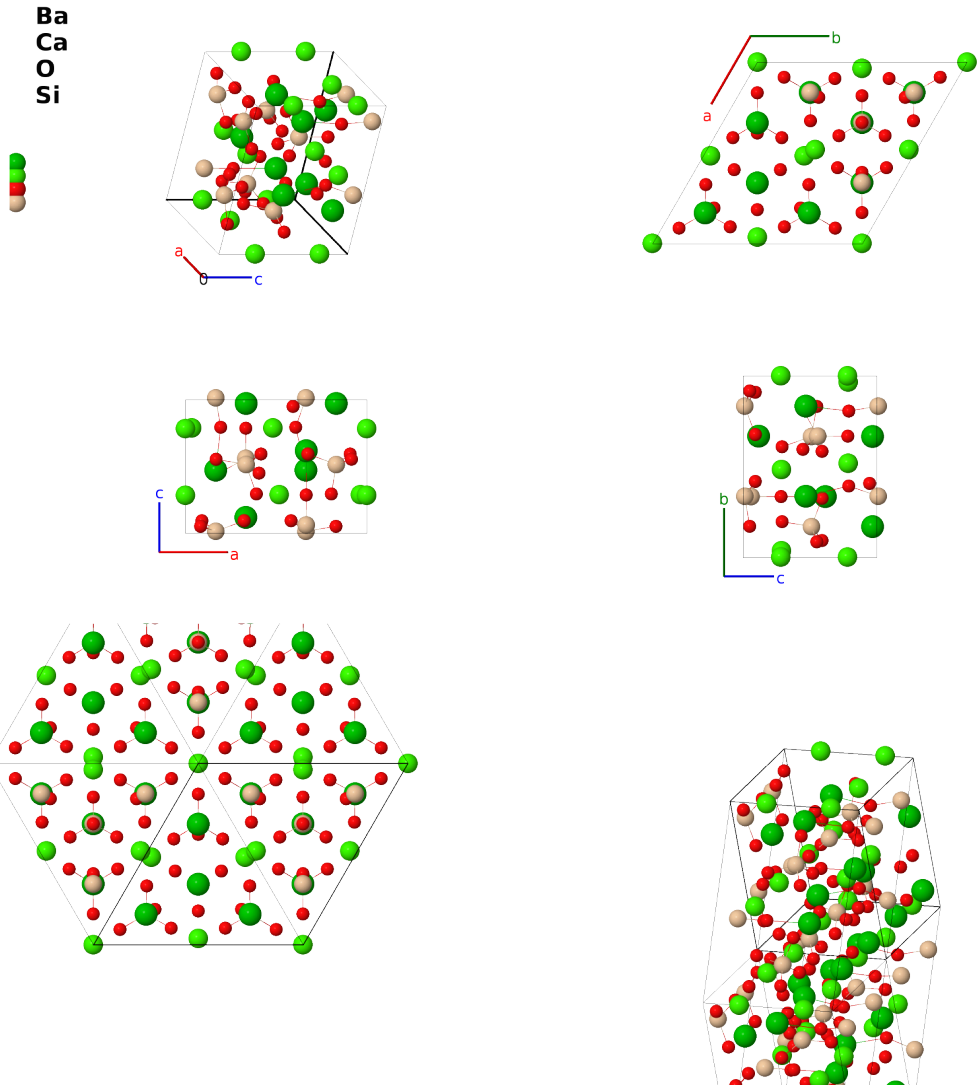
https://aflow.org/prototype-encyclopedia/LE9C

https://aflow.org/prototype-encyclopedia/ABC4D_hP56_186_bc_ac_b3cd_bc-001

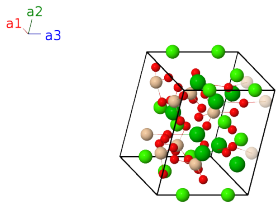


Prototype	$BaCaO_4Si$
AFLOW prototype label	ABC4D_hP56_186_bc_ac_b3cd_bc-001
ICSD	67092
CCDC	1629131
Pearson symbol	hP56

Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=ABC4D_hP56_186_bc_ac_b3cd_bc-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ba I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(2b)	Si I
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Si I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Ba II
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1+2x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Ba II
$\mathbf{B_{11}}$	=	$-2x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Ba II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Ba II
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1-2x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Ba II
$\mathbf{B_{14}}$	=	$2x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Ba II
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	Ca II
$\mathbf{B_{16}}$	=	$x_6\,\mathbf{a}_1+2x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	Ca II
$\mathbf{B_{17}}$	=	$-2x_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(6c)	Ca II
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Ca II
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1-2x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Ca II
$\mathbf{B_{20}}$	=	$2x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Ca II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-\sqrt{3}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{22}}$	=	$x_7\,\mathbf{a}_1+2x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{23}}$	=	$-2x_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{24}}$	=	$-x_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{25}}$	=	$-x_7\,\mathbf{a}_1-2x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II

$\mathbf{B_{26}}$	$=$	$2x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{27}}$	$=$	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$-\sqrt{3}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{28}}$	$=$	$x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{29}}$	$=$	$-2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{30}}$	$=$	$-x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\sqrt{3}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{31}}$	$=$	$-x_8\,\mathbf{a}_1 - 2x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{32}}$	$=$	$2x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O III
$\mathbf{B_{33}}$	$=$	$x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$-\sqrt{3}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{34}}$	$=$	$x_9\,\mathbf{a}_1 + 2x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_9\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{35}}$	$=$	$-2x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_9\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{36}}$	$=$	$-x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\sqrt{3}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{37}}$	$=$	$-x_9\,\mathbf{a}_1 - 2x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_9\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{38}}$	$=$	$2x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_9\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O IV
$\mathbf{B_{39}}$	$=$	$x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	$=$	$-\sqrt{3}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(6c)	Si II
$\mathbf{B_{40}}$	$=$	$x_{10}\,\mathbf{a}_1 + 2x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(6c)	Si II
$\mathbf{B_{41}}$	$=$	$-2x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(6c)	Si II
$\mathbf{B_{42}}$	$=$	$-x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\sqrt{3}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Si II
$\mathbf{B_{43}}$	$=$	$-x_{10}\,\mathbf{a}_1 - 2x_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_{10}\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Si II
$\mathbf{B_{44}}$	$=$	$2x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{3}{2}ax_{10}\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Si II
$\mathbf{B_{45}}$	$=$	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_{11} + y_{11}\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_{11} - y_{11}\right)\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{46}}$	$=$	$-y_{11}\,\mathbf{a}_1 + \left(x_{11} - y_{11}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_{11} - 2y_{11}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{47}}$	$=$	$-\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(2x_{11} - y_{11}\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{48}}$	$=$	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_{11} + y_{11}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_{11} - y_{11}\right)\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{49}}$	$=$	$y_{11}\,\mathbf{a}_1 - \left(x_{11} - y_{11}\right)\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(-x_{11} + 2y_{11}\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{50}}$	$=$	$\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(2x_{11} - y_{11}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{51}}$	$=$	$-y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(x_{11} + y_{11}\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_{11} - y_{11}\right)\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{52}}$	$=$	$-\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(-x_{11} + 2y_{11}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{53}}$	$=$	$x_{11}\,\mathbf{a}_1 + \left(x_{11} - y_{11}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(2x_{11} - y_{11}\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{54}}$	$=$	$y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_{11} + y_{11}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_{11} - y_{11}\right)\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{55}}$	$=$	$\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\left(x_{11} - 2y_{11}\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O V
$\mathbf{B_{56}}$	$=$	$-x_{11}\,\mathbf{a}_1 - \left(x_{11} - y_{11}\right)\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\left(2x_{11} - y_{11}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O V

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