$Na_5Co_{15.5}Te_6O_{36}$ (NCTO) Structure: A7B5C18D3_hP66_176_ci_bef_2h2i_h-001

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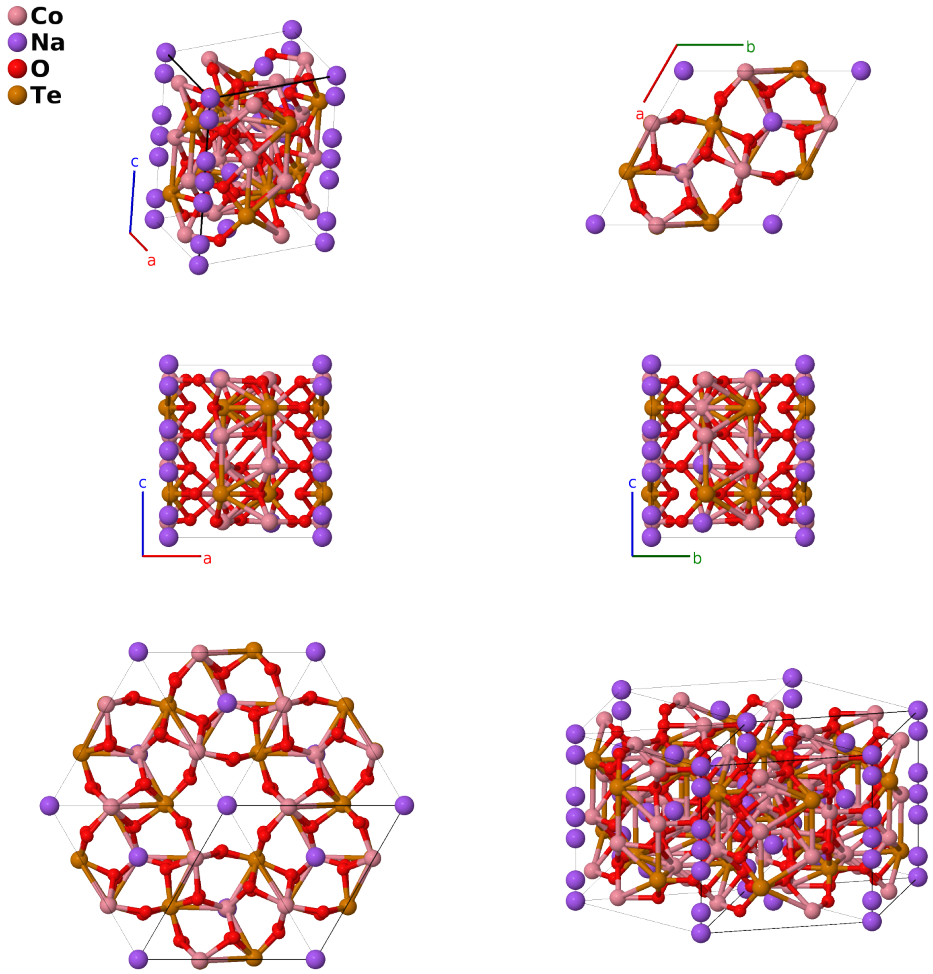
https://aflow.org/p/KL15

https://aflow.org/p/A7B5C18D3_hP66_176_ci_bef_2h2i_h-001

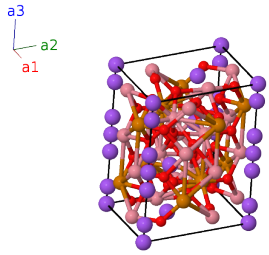


Prototype	$Co_{15.5}Na_5O_{36}Te_6$
AFLOW prototype label	A7B5C18D3_hP66_176_ci_bef_2h2i_h-001
Mineral name	NCTO
ICSD	none
Pearson symbol	hP66
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	`aflow --proto=A7B5C18D3_hP66_176_ci_bef_2h2i_h-001 --params=`$a, c/a, z_3, z_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- (Saha, 2021) set the z-coordinate of the tellurium atom to zero, but this is not consistent with the stoichiometry of the system. We set $z = 1/4$, putting the tellurium atom on a (6h) site.
- Several sites have only partial or mixed occupations: The Na-I (2b) site is 30% occupied. The Na-II (4e) site is 50% occupied. The Na-III (4f) site is 63% sodium and 37% cobalt, which we show as pure sodium.
- FINDSYM rotated the system so that the Co-I atom is on the (2c) Wyckoff position rather than the (2d) position given by (Saha, 2021).

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
$\mathbf{B_1}$	=	0	=	0	(2b)	Na I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_6}$	=	$\left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_8}$	=	$-\left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B_{11}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B_{12}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{14}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{15}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{17}}$	=	$y_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{18}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{20}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{21}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{23}}$	=	$y_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O II

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\begin{array}{lcccccc}
\mathbf{B_{24}} & = & (x_6-y_6)\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{O II}\\
\mathbf{B_{25}} & = & x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{Te I}\\
\mathbf{B_{26}} & = & -y_7\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_7-2y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{Te I}\\
\mathbf{B_{27}} & = & -(x_7-y_7)\,\mathbf{a}_1-x_7\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{Te I}\\
\mathbf{B_{28}} & = & -x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{Te I}\\
\mathbf{B_{29}} & = & y_7\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_7+2y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{Te I}\\
\mathbf{B_{30}} & = & (x_7-y_7)\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}} & \text{(6h)} & \text{Te I}\\
\mathbf{B_{31}} & = & x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{32}} & = & -y_8\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{33}} & = & -(x_8-y_8)\,\mathbf{a}_1-x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{34}} & = & -x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{35}} & = & y_8\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_8+2y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{36}} & = & (x_8-y_8)\,\mathbf{a}_1+x_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{37}} & = & -x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{38}} & = & y_8\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_8+2y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{39}} & = & (x_8-y_8)\,\mathbf{a}_1+x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{40}} & = & x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{41}} & = & -y_8\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{42}} & = & -(x_8-y_8)\,\mathbf{a}_1-x_8\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{Co II}\\
\mathbf{B_{43}} & = & x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{44}} & = & -y_9\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9-2y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{45}} & = & -(x_9-y_9)\,\mathbf{a}_1-x_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{46}} & = & -x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{47}} & = & y_9\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_9+2y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{48}} & = & (x_9-y_9)\,\mathbf{a}_1+x_9\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{49}} & = & -x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{50}} & = & y_9\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_9+2y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{51}} & = & (x_9-y_9)\,\mathbf{a}_1+x_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{52}} & = & x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{53}} & = & -y_9\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_9-2y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{54}} & = & -(x_9-y_9)\,\mathbf{a}_1-x_9\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12i)} & \text{O III}\\
\mathbf{B_{55}} & = & x_{10}\,\mathbf{a}_1+y_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(12i)} & \text{O IV}\\
\mathbf{B_{56}} & = & -y_{10}\,\mathbf{a}_1+(x_{10}-y_{10})\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_{10}-2y_{10})\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(12i)} & \text{O IV}\\
\mathbf{B_{57}} & = & -(x_{10}-y_{10})\,\mathbf{a}_1-x_{10}\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_{10}-y_{10})\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} & \text{(12i)} & \text{O IV}
\end{array}
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$\mathbf{B_{58}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{59}}$	=	$y_{10}\,\mathbf{a}_1 - (x_{10}-y_{10})\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_{10}+2y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{60}}$	=	$(x_{10}-y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_{10}-y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{61}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{62}}$	=	$y_{10}\,\mathbf{a}_1 - (x_{10}-y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_{10}+2y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{63}}$	=	$(x_{10}-y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_{10}-y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{64}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - \left(z_{10}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{10}+y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\,\hat{\mathbf{y}} - c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{65}}$	=	$-y_{10}\,\mathbf{a}_1 + (x_{10}-y_{10})\,\mathbf{a}_2 - \left(z_{10}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_{10}-2y_{10})\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV
$\mathbf{B_{66}}$	=	$-(x_{10}-y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - \left(z_{10}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_{10}-y_{10})\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} - c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	O IV

References

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