$Nb_7Rh_6B_8$ Structure: A8B7C6_hP126_176_2h3i_acd6h_3i-001

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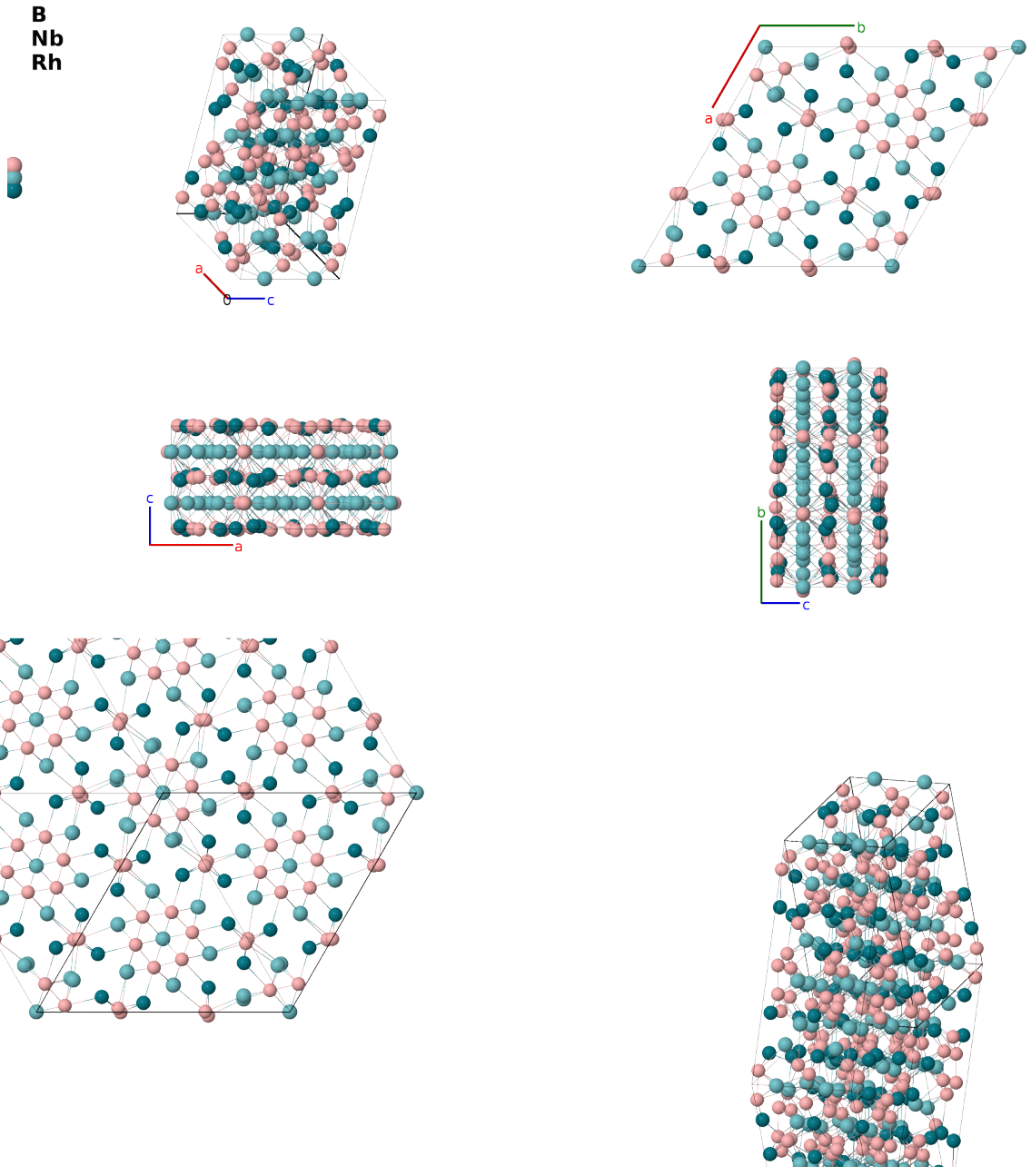
https://aflow.org/prototype-encyclopedia/01SA

https://aflow.org/prototype-encyclopedia/A8B7C6_hP126_176_2h3i_acd6h_3i-001



Prototype $B_8Nb_7Rh_6$

AFLOW prototype label	A8B7C6_hP126_176_2h3i_acd6h_3i-001
ICSD	263043
CCDC	1720600
Pearson symbol	hP126
Space group number	176
Space group symbol	$P6_3/m$
AFLOW prototype command	`aflow --proto=A8B7C6_hP126_176_2h3i_acd6h_3i-001 --params=`$a, c/a, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9, x_{10}, y_{10}, x_{11}, y_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}$

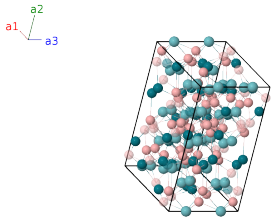
Other compounds with this structure

$Ta_7Rh_6B_8$

- (Zheng, 2012) place the Nb-I (their Nb3) atom on the (2b) Wyckoff position, but give the coordinates for the (2a) position. We assume that the coordinates are correct. This assessment agrees with the ICSD entry.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Nb 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)	Nb II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Nb II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2d)	Nb III
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2d)	Nb III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_9}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{11}}$	=	$y_4\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_4 + 2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{12}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{14}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{15}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	B II

$\mathbf{B_{16}}$	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_5+y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5-y_5)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{17}}$	$y_5\,\mathbf{a}_1 - (x_5-y_5)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_5+2y_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{18}}$	$(x_5-y_5)\;\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_5-y_5)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{19}}$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IV
$\mathbf{B_{20}}$	$-y_6\,\mathbf{a}_1 + (x_6-y_6)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6-2y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IV
$\mathbf{B_{21}}$	$-(x_6-y_6)\;\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IV
$\mathbf{B_{22}}$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IV
$\mathbf{B_{23}}$	$y_6\,\mathbf{a}_1 - (x_6-y_6)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_6+2y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IV
$\mathbf{B_{24}}$	$(x_6-y_6)\;\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IV
$\mathbf{B_{25}}$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb V
$\mathbf{B_{26}}$	$-y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb V
$\mathbf{B_{27}}$	$-(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb V
$\mathbf{B_{28}}$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb V
$\mathbf{B_{29}}$	$y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb V
$\mathbf{B_{30}}$	$(x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb V
$\mathbf{B_{31}}$	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VI
$\mathbf{B_{32}}$	$-y_8\,\mathbf{a}_1 + (x_8-y_8)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8-2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VI
$\mathbf{B_{33}}$	$-(x_8-y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VI
$\mathbf{B_{34}}$	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VI
$\mathbf{B_{35}}$	$y_8\,\mathbf{a}_1 - (x_8-y_8)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_8+2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VI
$\mathbf{B_{36}}$	$(x_8-y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VI
$\mathbf{B_{37}}$	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VII
$\mathbf{B_{38}}$	$-y_9\,\mathbf{a}_1 + (x_9-y_9)\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9-2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VII
$\mathbf{B_{39}}$	$-(x_9-y_9)\;\mathbf{a}_1 - x_9\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VII
$\mathbf{B_{40}}$	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VII
$\mathbf{B_{41}}$	$y_9\,\mathbf{a}_1 - (x_9-y_9)\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_9+2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VII
$\mathbf{B_{42}}$	$(x_9-y_9)\;\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VII
$\mathbf{B_{43}}$	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_{10}+y_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VIII
$\mathbf{B_{44}}$	$-y_{10}\,\mathbf{a}_1 + (x_{10}-y_{10})\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_{10}-2y_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VIII
$\mathbf{B_{45}}$	$-(x_{10}-y_{10})\;\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_{10}-y_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VIII
$\mathbf{B_{46}}$	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_{10}+y_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VIII
$\mathbf{B_{47}}$	$y_{10}\,\mathbf{a}_1 - (x_{10}-y_{10})\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_{10}+2y_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VIII
$\mathbf{B_{48}}$	$(x_{10}-y_{10})\;\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_{10}-y_{10})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb VIII
$\mathbf{B_{49}}$	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_{11}+y_{11})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{11}-y_{11})\;\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IX
$\mathbf{B_{50}}$	$-y_{11}\,\mathbf{a}_1 + (x_{11}-y_{11})\;\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_{11}-2y_{11})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IX
$\mathbf{B_{51}}$	$-(x_{11}-y_{11})\;\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_{11}-y_{11})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IX
$\mathbf{B_{52}}$	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_{11}+y_{11})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_{11}-y_{11})\;\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IX
$\mathbf{B_{53}}$	$y_{11}\,\mathbf{a}_1 - (x_{11}-y_{11})\;\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_{11}+2y_{11})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IX
$\mathbf{B_{54}}$	$(x_{11}-y_{11})\;\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_{11}-y_{11})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb IX

$$\mathbf{B_{55}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12}+y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{12}-y_{12})\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{56}} = -y_{12}\,\mathbf{a}_1 + (x_{12}-y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12}-2y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{57}} = -(x_{12}-y_{12})\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{12}-y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{58}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{12}+y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{12}-y_{12})\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{59}} = y_{12}\,\mathbf{a}_1 - (x_{12}-y_{12})\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{12}+2y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{60}} = (x_{12}-y_{12})\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{12}-y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{61}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{12}+y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{12}-y_{12})\,\hat{\mathbf{y}} - cz_{12}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{62}} = y_{12}\,\mathbf{a}_1 - (x_{12}-y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{12}+2y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} - cz_{12}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{63}} = (x_{12}-y_{12})\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{12}-y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} - cz_{12}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{64}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 - \left(z_{12}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12}+y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{12}-y_{12})\,\hat{\mathbf{y}} - c\left(z_{12}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{65}} = -y_{12}\,\mathbf{a}_1 + (x_{12}-y_{12})\,\mathbf{a}_2 - \left(z_{12}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12}-2y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} - c\left(z_{12}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{66}} = -(x_{12}-y_{12})\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 - \left(z_{12}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{12}-y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} - c\left(z_{12}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B III}$$

$$\mathbf{B_{67}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{13}+y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{13}-y_{13})\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{68}} = -y_{13}\,\mathbf{a}_1 + (x_{13}-y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{13}-2y_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{69}} = -(x_{13}-y_{13})\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{13}-y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{70}} = -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{13}+y_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{13}-y_{13})\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{71}} = y_{13}\,\mathbf{a}_1 - (x_{13}-y_{13})\,\mathbf{a}_2 + \left(z_{13}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{13}+2y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{72}} = (x_{13}-y_{13})\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + \left(z_{13}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{13}-y_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{73}} = -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{13}+y_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{13}-y_{13})\,\hat{\mathbf{y}} - cz_{13}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{74}} = y_{13}\,\mathbf{a}_1 - (x_{13}-y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{13}+2y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{13}\,\hat{\mathbf{y}} - cz_{13}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{75}} = (x_{13}-y_{13})\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{13}-y_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{13}\,\hat{\mathbf{y}} - cz_{13}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{76}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 - \left(z_{13}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{13}+y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{13}-y_{13})\,\hat{\mathbf{y}} - c\left(z_{13}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{77}} = -y_{13}\,\mathbf{a}_1 + (x_{13}-y_{13})\,\mathbf{a}_2 - \left(z_{13}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{13}-2y_{13})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{13}\,\hat{\mathbf{y}} - c\left(z_{13}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{78}} = -(x_{13}-y_{13})\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 - \left(z_{13}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{13}-y_{13})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{13}\,\hat{\mathbf{y}} - c\left(z_{13}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B IV}$$

$$\mathbf{B_{79}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{14}+y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{14}-y_{14})\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{80}} = -y_{14}\,\mathbf{a}_1 + (x_{14}-y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{14}-2y_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{81}} = -(x_{14}-y_{14})\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{14}-y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{82}} = -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{14}+y_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{14}-y_{14})\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{83}} = y_{14}\,\mathbf{a}_1 - (x_{14}-y_{14})\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{14}+2y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{84}} = (x_{14}-y_{14})\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{14}-y_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{85}} = -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{14}+y_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{14}-y_{14})\,\hat{\mathbf{y}} - cz_{14}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{86}} = y_{14}\,\mathbf{a}_1 - (x_{14}-y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{14}+2y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{14}\,\hat{\mathbf{y}} - cz_{14}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{87}} = (x_{14}-y_{14})\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{14}-y_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{14}\,\hat{\mathbf{y}} - cz_{14}\,\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{88}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 - \left(z_{14}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{14}+y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{14}-y_{14})\,\hat{\mathbf{y}} - c\left(z_{14}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{89}} = -y_{14}\,\mathbf{a}_1 + (x_{14}-y_{14})\,\mathbf{a}_2 - \left(z_{14}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{14}-2y_{14})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{14}\,\hat{\mathbf{y}} - c\left(z_{14}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{90}} = -(x_{14}-y_{14})\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 - \left(z_{14}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{14}-y_{14})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{14}\,\hat{\mathbf{y}} - c\left(z_{14}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{B V}$$

$$\mathbf{B_{91}} = x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{15}+y_{15})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{15}-y_{15})\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{92}} = -y_{15}\,\mathbf{a}_1 + (x_{15}-y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{15}-2y_{15})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{93}} = -(x_{15}-y_{15})\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{15}-y_{15})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{94}} = -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{15}+y_{15})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{15}-y_{15})\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{95}} = y_{15}\,\mathbf{a}_1 - (x_{15}-y_{15})\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{15}+2y_{15})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{96}} = (x_{15}-y_{15})\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{15}-y_{15})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{97}} = -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{15}+y_{15})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{15}-y_{15})\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{98}} = y_{15}\,\mathbf{a}_1 - (x_{15}-y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{15}+2y_{15})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{15}\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{99}} = (x_{15}-y_{15})\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{15}-y_{15})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{15}\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{100}} = x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 - \left(z_{15}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{15}+y_{15})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{15}-y_{15})\,\hat{\mathbf{y}} - c\left(z_{15}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{101}} = -y_{15}\,\mathbf{a}_1 + (x_{15}-y_{15})\,\mathbf{a}_2 - \left(z_{15}-\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{15}-2y_{15})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{15}\,\hat{\mathbf{y}} - c\left(z_{15}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{102}} = -(x_{15}-y_{15})\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 - \left(z_{15}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{15}-y_{15})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{15}\,\hat{\mathbf{y}} - c\left(z_{15}-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh I}$$

$$\mathbf{B_{103}} = x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{16}+y_{16})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{16}-y_{16})\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{104}} = -y_{16}\,\mathbf{a}_1 + (x_{16}-y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{16}-2y_{16})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{105}} = -(x_{16}-y_{16})\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{16}-y_{16})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{106}} = -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{16}+y_{16})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{16}-y_{16})\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{107}} = y_{16}\,\mathbf{a}_1 - (x_{16}-y_{16})\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{16}+2y_{16})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{108}} = (x_{16}-y_{16})\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{16}-y_{16})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{109}} = -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{16}+y_{16})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{16}-y_{16})\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{110}} = y_{16}\,\mathbf{a}_1 - (x_{16}-y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{16}+2y_{16})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{16}\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}} \quad (12i) \quad \text{Rh II}$$

$$\mathbf{B_{111}} = (x_{16} - y_{16})\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{16} - y_{16})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{16}\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh II}$$

$$\mathbf{B_{112}} = x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 - \left(z_{16} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{16} + y_{16})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{16} - y_{16})\,\hat{\mathbf{y}} - c\left(z_{16} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh II}$$

$$\mathbf{B_{113}} = -y_{16}\,\mathbf{a}_1 + (x_{16} - y_{16})\,\mathbf{a}_2 - \left(z_{16} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{16} - 2y_{16})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{16}\,\hat{\mathbf{y}} - c\left(z_{16} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh II}$$

$$\mathbf{B_{114}} = -(x_{16} - y_{16})\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 - \left(z_{16} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{16} - y_{16})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{16}\,\hat{\mathbf{y}} - c\left(z_{16} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh II}$$

$$\mathbf{B_{115}} = x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{17} + y_{17})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{17} - y_{17})\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{116}} = -y_{17}\,\mathbf{a}_1 + (x_{17} - y_{17})\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{17} - 2y_{17})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{117}} = -(x_{17} - y_{17})\,\mathbf{a}_1 - x_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{17} - y_{17})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{118}} = -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + \left(z_{17} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{17} + y_{17})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{17} - y_{17})\,\hat{\mathbf{y}} + c\left(z_{17} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{119}} = y_{17}\,\mathbf{a}_1 - (x_{17} - y_{17})\,\mathbf{a}_2 + \left(z_{17} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{17} + 2y_{17})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{17}\,\hat{\mathbf{y}} + c\left(z_{17} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{120}} = (x_{17} - y_{17})\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + \left(z_{17} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{17} - y_{17})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{17}\,\hat{\mathbf{y}} + c\left(z_{17} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{121}} = -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{17} + y_{17})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{17} - y_{17})\,\hat{\mathbf{y}} - cz_{17}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{122}} = y_{17}\,\mathbf{a}_1 - (x_{17} - y_{17})\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{17} + 2y_{17})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{17}\,\hat{\mathbf{y}} - cz_{17}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{123}} = (x_{17} - y_{17})\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{17} - y_{17})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{17}\,\hat{\mathbf{y}} - cz_{17}\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{124}} = x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 - \left(z_{17} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{17} + y_{17})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{17} - y_{17})\,\hat{\mathbf{y}} - c\left(z_{17} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{125}} = -y_{17}\,\mathbf{a}_1 + (x_{17} - y_{17})\,\mathbf{a}_2 - \left(z_{17} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{17} - 2y_{17})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{17}\,\hat{\mathbf{y}} - c\left(z_{17} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

$$\mathbf{B_{126}} = -(x_{17} - y_{17})\,\mathbf{a}_1 - x_{17}\,\mathbf{a}_2 - \left(z_{17} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{17} - y_{17})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{17}\,\hat{\mathbf{y}} - c\left(z_{17} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12i)} \quad \text{Rh III}$$

References

[1] Q. Zheng, M. Kohout, R. Gumeniuk, N. Abramchuk, H. Borrmann, Y. Prots, U. Burkhardt, W. Schnelle, L. Akselrud, H. Gu, A. Leithe-Jasper, and Y. Grin, *$TM_7TM'_6B_8$ (TM = Ta, Nb; TM' = Ru, Rh, Ir): New Compounds with [B_6] Ring Polyanions*, Inorg. Chem. **51**, 7492–7483 (2012), doi:10.1021/ic201978n.

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