$Be[BH_4]_2$ Structure: A2BC8_tI176_110_2b_b_8b-001

This structure originally had the label `A2BC8_tI176_110_2b_b_8b`. Calls to that address will be redirected here.

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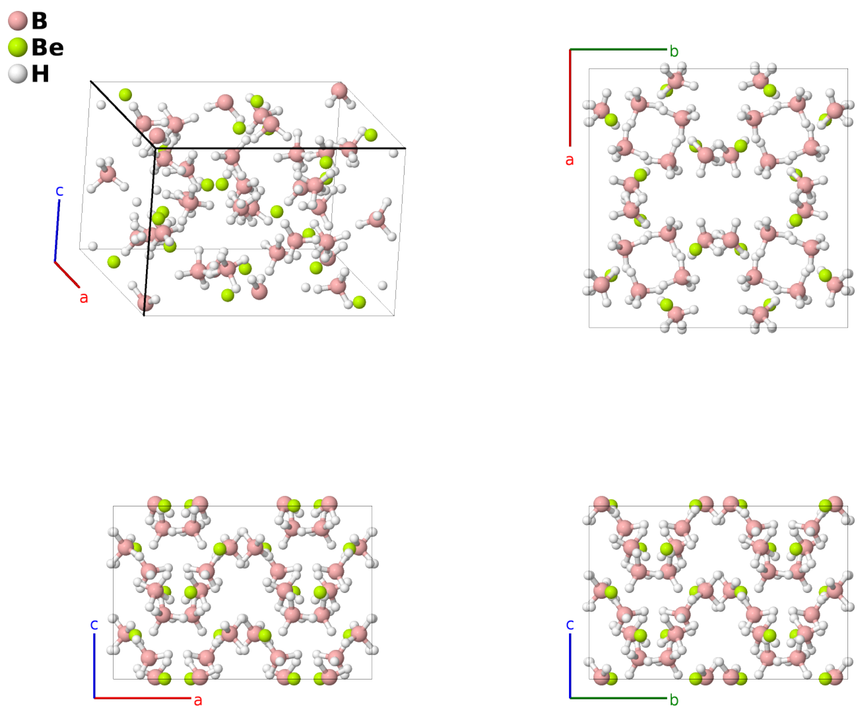
https://aflow.org/p/29CG

https://aflow.org/p/A2BC8_tI176_110_2b_b_8b-001

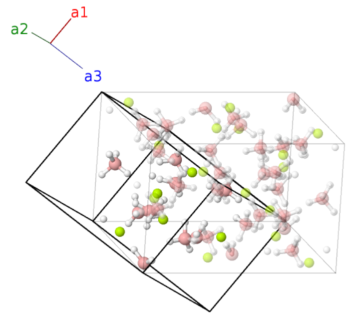


Prototype	B_2BeH_8
AFLOW prototype label	A2BC8_tI176_110_2b_b_8b-001
ICSD	10315
Pearson symbol	tI176
Space group number	110
Space group symbol	$I4_1cd$
AFLOW prototype command	`aflow --proto=A2BC8_tI176_110_2b_b_8b-001` `--params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- Space group $I4_1cd$ #110 allows an arbitary placement of the z-axis origin, and we put a beryllium atom there by setting $z_3 = 0$.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(y_1+z_1)\,\mathbf{a_1} + (x_1+z_1)\,\mathbf{a_2} + (x_1+y_1)\,\mathbf{a_3}$	=	$ax_1\,\mathbf{\hat{x}} + ay_1\,\mathbf{\hat{y}} + cz_1\,\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_2}$	=	$-(y_1-z_1)\,\mathbf{a_1} - (x_1-z_1)\,\mathbf{a_2} - (x_1+y_1)\,\mathbf{a_3}$	=	$-ax_1\,\mathbf{\hat{x}} - ay_1\,\mathbf{\hat{y}} + cz_1\,\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_3}$	=	$\left(x_1+z_1+\frac{3}{4}\right)\mathbf{a_1} + \left(-y_1+z_1+\frac{1}{4}\right)\mathbf{a_2} + \left(x_1-y_1+\frac{1}{2}\right)\mathbf{a_3}$	=	$-ay_1\,\mathbf{\hat{x}} + a\left(x_1+\frac{1}{2}\right)\mathbf{\hat{y}} + c\left(z_1+\frac{1}{4}\right)\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_4}$	=	$\left(-x_1+z_1+\frac{3}{4}\right)\mathbf{a_1} + \left(y_1+z_1+\frac{1}{4}\right)\mathbf{a_2} + \left(-x_1+y_1+\frac{1}{2}\right)\mathbf{a_3}$	=	$ay_1\,\mathbf{\hat{x}} - a\left(x_1-\frac{1}{2}\right)\mathbf{\hat{y}} + c\left(z_1+\frac{1}{4}\right)\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_5}$	=	$\left(-y_1+z_1+\frac{1}{2}\right)\mathbf{a_1} + \left(x_1+z_1+\frac{1}{2}\right)\mathbf{a_2} + (x_1-y_1)\,\mathbf{a_3}$	=	$ax_1\,\mathbf{\hat{x}} - ay_1\,\mathbf{\hat{y}} + c\left(z_1+\frac{1}{2}\right)\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_6}$	=	$\left(y_1+z_1+\frac{1}{2}\right)\mathbf{a_1} + \left(-x_1+z_1+\frac{1}{2}\right)\mathbf{a_2} - (x_1-y_1)\,\mathbf{a_3}$	=	$-ax_1\,\mathbf{\hat{x}} + ay_1\,\mathbf{\hat{y}} + c\left(z_1+\frac{1}{2}\right)\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_7}$	=	$\left(-x_1+z_1+\frac{1}{4}\right)\mathbf{a_1} + \left(-y_1+z_1+\frac{3}{4}\right)\mathbf{a_2} - \left(x_1+y_1-\frac{1}{2}\right)\mathbf{a_3}$	=	$-a\left(y_1-\frac{1}{2}\right)\mathbf{\hat{x}} - ax_1\,\mathbf{\hat{y}} + c\left(z_1+\frac{1}{4}\right)\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_8}$	=	$\left(x_1+z_1+\frac{1}{4}\right)\mathbf{a_1} + \left(y_1+z_1+\frac{3}{4}\right)\mathbf{a_2} + \left(x_1+y_1+\frac{1}{2}\right)\mathbf{a_3}$	=	$a\left(y_1+\frac{1}{2}\right)\mathbf{\hat{x}} + ax_1\,\mathbf{\hat{y}} + c\left(z_1+\frac{1}{4}\right)\mathbf{\hat{z}}$	(16b)	B I
$\mathbf{B_9}$	=	$(y_2+z_2)\,\mathbf{a_1} + (x_2+z_2)\,\mathbf{a_2} + (x_2+y_2)\,\mathbf{a_3}$	=	$ax_2\,\mathbf{\hat{x}} + ay_2\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(16b)	B II
$\mathbf{B_{10}}$	=	$-(y_2-z_2)\,\mathbf{a_1} - (x_2-z_2)\,\mathbf{a_2} - (x_2+y_2)\,\mathbf{a_3}$	=	$-ax_2\,\mathbf{\hat{x}} - ay_2\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(16b)	B II
$\mathbf{B_{11}}$	=	$\left(x_2+z_2+\frac{3}{4}\right)\mathbf{a_1} + \left(-y_2+z_2+\frac{1}{4}\right)\mathbf{a_2} + \left(x_2-y_2+\frac{1}{2}\right)\mathbf{a_3}$	=	$-ay_2\,\mathbf{\hat{x}} + a\left(x_2+\frac{1}{2}\right)\mathbf{\hat{y}} + c\left(z_2+\frac{1}{4}\right)\mathbf{\hat{z}}$	(16b)	B II
$\mathbf{B_{12}}$	=	$\left(-x_2+z_2+\frac{3}{4}\right)\mathbf{a_1} + \left(y_2+z_2+\frac{1}{4}\right)\mathbf{a_2} + \left(-x_2+y_2+\frac{1}{2}\right)\mathbf{a_3}$	=	$ay_2\,\mathbf{\hat{x}} - a\left(x_2-\frac{1}{2}\right)\mathbf{\hat{y}} + c\left(z_2+\frac{1}{4}\right)\mathbf{\hat{z}}$	(16b)	B II
$\mathbf{B_{13}}$	=	$\left(-y_2+z_2+\frac{1}{2}\right)\mathbf{a_1} + \left(x_2+z_2+\frac{1}{2}\right)\mathbf{a_2} + (x_2-y_2)\,\mathbf{a_3}$	=	$ax_2\,\mathbf{\hat{x}} - ay_2\,\mathbf{\hat{y}} + c\left(z_2+\frac{1}{2}\right)\mathbf{\hat{z}}$	(16b)	B II

$\mathbf{B_{14}}$	=	$\left(y_2+z_2+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_2+z_2+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_2-y_2\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}+ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	B II
$\mathbf{B_{15}}$	=	$\left(-x_2+z_2+\frac{1}{4}\right)\,\mathbf{a}_1+\left(-y_2+z_2+\frac{3}{4}\right)\,\mathbf{a}_2-\left(x_2+y_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	B II
$\mathbf{B_{16}}$	=	$\left(x_2+z_2+\frac{1}{4}\right)\,\mathbf{a}_1+\left(y_2+z_2+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_2+y_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	B II
$\mathbf{B_{17}}$	=	$\left(y_3+z_3\right)\,\mathbf{a}_1+\left(x_3+z_3\right)\,\mathbf{a}_2+\left(x_3+y_3\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{18}}$	=	$-\left(y_3-z_3\right)\,\mathbf{a}_1-\left(x_3-z_3\right)\,\mathbf{a}_2-\left(x_3+y_3\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{19}}$	=	$\left(x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{20}}$	=	$\left(-x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{21}}$	=	$\left(-y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_3-y_3\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{22}}$	=	$\left(y_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_3-y_3\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{23}}$	=	$\left(-x_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_1+\left(-y_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_2-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{24}}$	=	$\left(x_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_1+\left(y_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Be I
$\mathbf{B_{25}}$	=	$\left(y_4+z_4\right)\,\mathbf{a}_1+\left(x_4+z_4\right)\,\mathbf{a}_2+\left(x_4+y_4\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{26}}$	=	$-\left(y_4-z_4\right)\,\mathbf{a}_1-\left(x_4-z_4\right)\,\mathbf{a}_2-\left(x_4+y_4\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{27}}$	=	$\left(x_4+z_4+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_4-y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{28}}$	=	$\left(-x_4+z_4+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{29}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_4-y_4\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{30}}$	=	$\left(y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_4-y_4\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{31}}$	=	$\left(-x_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_1+\left(-y_4+z_4+\frac{3}{4}\right)\,\mathbf{a}_2-\left(x_4+y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H I
$\mathbf{B_{32}}$	=	$\left(x_4+z_4+\frac{1}{4}\right)\,\mathbf{a}_1+\left(y_4+z_4+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_4+y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H I

$\mathbf{B_{33}}$	=	$\left(y_5+z_5\right)\,\mathbf{a}_1+\left(x_5+z_5\right)\,\mathbf{a}_2+\left(x_5+y_5\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{34}}$	=	$-\left(y_5-z_5\right)\,\mathbf{a}_1-\left(x_5-z_5\right)\,\mathbf{a}_2-\left(x_5+y_5\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{35}}$	=	$\left(x_5+z_5+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_5-y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{36}}$	=	$\left(-x_5+z_5+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_5+y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{37}}$	=	$\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_5-y_5\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{38}}$	=	$\left(y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-y_5\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{39}}$	=	$\left(-x_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_1+\left(-y_5+z_5+\frac{3}{4}\right)\,\mathbf{a}_2-\left(x_5+y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{40}}$	=	$\left(x_5+z_5+\frac{1}{4}\right)\,\mathbf{a}_1+\left(y_5+z_5+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_5+y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H II
$\mathbf{B_{41}}$	=	$\left(y_6+z_6\right)\,\mathbf{a}_1+\left(x_6+z_6\right)\,\mathbf{a}_2+\left(x_6+y_6\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{42}}$	=	$-\left(y_6-z_6\right)\,\mathbf{a}_1-\left(x_6-z_6\right)\,\mathbf{a}_2-\left(x_6+y_6\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{43}}$	=	$\left(x_6+z_6+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_6+z_6+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_6-y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{44}}$	=	$\left(-x_6+z_6+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_6+z_6+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_6+y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{45}}$	=	$\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_6-y_6\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{46}}$	=	$\left(y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_6-y_6\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{47}}$	=	$\left(-x_6+z_6+\frac{1}{4}\right)\,\mathbf{a}_1+\left(-y_6+z_6+\frac{3}{4}\right)\,\mathbf{a}_2-\left(x_6+y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{48}}$	=	$\left(x_6+z_6+\frac{1}{4}\right)\,\mathbf{a}_1+\left(y_6+z_6+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_6+y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H III
$\mathbf{B_{49}}$	=	$\left(y_7+z_7\right)\,\mathbf{a}_1+\left(x_7+z_7\right)\,\mathbf{a}_2+\left(x_7+y_7\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(16b)	H IV
$\mathbf{B_{50}}$	=	$-\left(y_7-z_7\right)\,\mathbf{a}_1-\left(x_7-z_7\right)\,\mathbf{a}_2-\left(x_7+y_7\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(16b)	H IV
$\mathbf{B_{51}}$	=	$\left(x_7+z_7+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_7+z_7+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_7-y_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	H IV

$\mathbf{B_{52}}$	=	$\left(-x_{7}+z_{7}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(y_{7}+z_{7}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(-x_{7}+y_{7}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ay_{7}\,\mathbf{\hat{x}}-a\left(x_{7}-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{7}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H IV
$\mathbf{B_{53}}$	=	$\left(-y_{7}+z_{7}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(x_{7}+z_{7}+\frac{1}{2}\right)\,\mathbf{a}_{2}+\left(x_{7}-y_{7}\right)\,\mathbf{a}_{3}$	=	$ax_{7}\,\mathbf{\hat{x}}-ay_{7}\,\mathbf{\hat{y}}+c\left(z_{7}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H IV
$\mathbf{B_{54}}$	=	$\left(y_{7}+z_{7}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(-x_{7}+z_{7}+\frac{1}{2}\right)\,\mathbf{a}_{2}-\left(x_{7}-y_{7}\right)\,\mathbf{a}_{3}$	=	$-ax_{7}\,\mathbf{\hat{x}}+ay_{7}\,\mathbf{\hat{y}}+c\left(z_{7}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H IV
$\mathbf{B_{55}}$	=	$\left(-x_{7}+z_{7}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(-y_{7}+z_{7}+\frac{3}{4}\right)\,\mathbf{a}_{2}-\left(x_{7}+y_{7}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{7}-\frac{1}{2}\right)\,\mathbf{\hat{x}}-ax_{7}\,\mathbf{\hat{y}}+c\left(z_{7}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H IV
$\mathbf{B_{56}}$	=	$\left(x_{7}+z_{7}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(y_{7}+z_{7}+\frac{3}{4}\right)\,\mathbf{a}_{2}+\left(x_{7}+y_{7}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(y_{7}+\frac{1}{2}\right)\,\mathbf{\hat{x}}+ax_{7}\,\mathbf{\hat{y}}+c\left(z_{7}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H IV
$\mathbf{B_{57}}$	=	$\left(y_{8}+z_{8}\right)\,\mathbf{a}_{1}+\left(x_{8}+z_{8}\right)\,\mathbf{a}_{2}+\left(x_{8}+y_{8}\right)\,\mathbf{a}_{3}$	=	$ax_{8}\,\mathbf{\hat{x}}+ay_{8}\,\mathbf{\hat{y}}+cz_{8}\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{58}}$	=	$-\left(y_{8}-z_{8}\right)\,\mathbf{a}_{1}-\left(x_{8}-z_{8}\right)\,\mathbf{a}_{2}-\left(x_{8}+y_{8}\right)\,\mathbf{a}_{3}$	=	$-ax_{8}\,\mathbf{\hat{x}}-ay_{8}\,\mathbf{\hat{y}}+cz_{8}\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{59}}$	=	$\left(x_{8}+z_{8}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(-y_{8}+z_{8}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(x_{8}-y_{8}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ay_{8}\,\mathbf{\hat{x}}+a\left(x_{8}+\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{60}}$	=	$\left(-x_{8}+z_{8}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(y_{8}+z_{8}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(-x_{8}+y_{8}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ay_{8}\,\mathbf{\hat{x}}-a\left(x_{8}-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{61}}$	=	$\left(-y_{8}+z_{8}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(x_{8}+z_{8}+\frac{1}{2}\right)\,\mathbf{a}_{2}+\left(x_{8}-y_{8}\right)\,\mathbf{a}_{3}$	=	$ax_{8}\,\mathbf{\hat{x}}-ay_{8}\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{62}}$	=	$\left(y_{8}+z_{8}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(-x_{8}+z_{8}+\frac{1}{2}\right)\,\mathbf{a}_{2}-\left(x_{8}-y_{8}\right)\,\mathbf{a}_{3}$	=	$-ax_{8}\,\mathbf{\hat{x}}+ay_{8}\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{63}}$	=	$\left(-x_{8}+z_{8}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(-y_{8}+z_{8}+\frac{3}{4}\right)\,\mathbf{a}_{2}-\left(x_{8}+y_{8}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{8}-\frac{1}{2}\right)\,\mathbf{\hat{x}}-ax_{8}\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{64}}$	=	$\left(x_{8}+z_{8}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(y_{8}+z_{8}+\frac{3}{4}\right)\,\mathbf{a}_{2}+\left(x_{8}+y_{8}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(y_{8}+\frac{1}{2}\right)\,\mathbf{\hat{x}}+ax_{8}\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H V
$\mathbf{B_{65}}$	=	$\left(y_{9}+z_{9}\right)\,\mathbf{a}_{1}+\left(x_{9}+z_{9}\right)\,\mathbf{a}_{2}+\left(x_{9}+y_{9}\right)\,\mathbf{a}_{3}$	=	$ax_{9}\,\mathbf{\hat{x}}+ay_{9}\,\mathbf{\hat{y}}+cz_{9}\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{66}}$	=	$-\left(y_{9}-z_{9}\right)\,\mathbf{a}_{1}-\left(x_{9}-z_{9}\right)\,\mathbf{a}_{2}-\left(x_{9}+y_{9}\right)\,\mathbf{a}_{3}$	=	$-ax_{9}\,\mathbf{\hat{x}}-ay_{9}\,\mathbf{\hat{y}}+cz_{9}\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{67}}$	=	$\left(x_{9}+z_{9}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(-y_{9}+z_{9}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(x_{9}-y_{9}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ay_{9}\,\mathbf{\hat{x}}+a\left(x_{9}+\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{68}}$	=	$\left(-x_{9}+z_{9}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(y_{9}+z_{9}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(-x_{9}+y_{9}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ay_{9}\,\mathbf{\hat{x}}-a\left(x_{9}-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{69}}$	=	$\left(-y_{9}+z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(x_{9}+z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{2}+\left(x_{9}-y_{9}\right)\,\mathbf{a}_{3}$	=	$ax_{9}\,\mathbf{\hat{x}}-ay_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{70}}$	=	$\left(y_{9}+z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(-x_{9}+z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{2}-\left(x_{9}-y_{9}\right)\,\mathbf{a}_{3}$	=	$-ax_{9}\,\mathbf{\hat{x}}+ay_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H VI

$\mathbf{B_{71}}$	=	$\left(-x_{9}+z_{9}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(-y_{9}+z_{9}+\frac{3}{4}\right)\,\mathbf{a}_{2}-\left(x_{9}+y_{9}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{9}-\frac{1}{2}\right)\,\mathbf{\hat{x}}-ax_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{72}}$	=	$\left(x_{9}+z_{9}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(y_{9}+z_{9}+\frac{3}{4}\right)\,\mathbf{a}_{2}+\left(x_{9}+y_{9}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(y_{9}+\frac{1}{2}\right)\,\mathbf{\hat{x}}+ax_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VI
$\mathbf{B_{73}}$	=	$\left(y_{10}+z_{10}\right)\,\mathbf{a}_{1}+\left(x_{10}+z_{10}\right)\,\mathbf{a}_{2}+\left(x_{10}+y_{10}\right)\,\mathbf{a}_{3}$	=	$ax_{10}\,\mathbf{\hat{x}}+ay_{10}\,\mathbf{\hat{y}}+cz_{10}\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{74}}$	=	$-\left(y_{10}-z_{10}\right)\,\mathbf{a}_{1}-\left(x_{10}-z_{10}\right)\,\mathbf{a}_{2}-\left(x_{10}+y_{10}\right)\,\mathbf{a}_{3}$	=	$-ax_{10}\,\mathbf{\hat{x}}-ay_{10}\,\mathbf{\hat{y}}+cz_{10}\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{75}}$	=	$\left(x_{10}+z_{10}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(-y_{10}+z_{10}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(x_{10}-y_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ay_{10}\,\mathbf{\hat{x}}+a\left(x_{10}+\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{76}}$	=	$\left(-x_{10}+z_{10}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(y_{10}+z_{10}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(-x_{10}+y_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ay_{10}\,\mathbf{\hat{x}}-a\left(x_{10}-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{77}}$	=	$\left(-y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(x_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{2}+\left(x_{10}-y_{10}\right)\,\mathbf{a}_{3}$	=	$ax_{10}\,\mathbf{\hat{x}}-ay_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{78}}$	=	$\left(y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(-x_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{2}-\left(x_{10}-y_{10}\right)\,\mathbf{a}_{3}$	=	$-ax_{10}\,\mathbf{\hat{x}}+ay_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{79}}$	=	$\left(-x_{10}+z_{10}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(-y_{10}+z_{10}+\frac{3}{4}\right)\,\mathbf{a}_{2}-\left(x_{10}+y_{10}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{10}-\frac{1}{2}\right)\,\mathbf{\hat{x}}-ax_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{80}}$	=	$\left(x_{10}+z_{10}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(y_{10}+z_{10}+\frac{3}{4}\right)\,\mathbf{a}_{2}+\left(x_{10}+y_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(y_{10}+\frac{1}{2}\right)\,\mathbf{\hat{x}}+ax_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VII
$\mathbf{B_{81}}$	=	$\left(y_{11}+z_{11}\right)\,\mathbf{a}_{1}+\left(x_{11}+z_{11}\right)\,\mathbf{a}_{2}+\left(x_{11}+y_{11}\right)\,\mathbf{a}_{3}$	=	$ax_{11}\,\mathbf{\hat{x}}+ay_{11}\,\mathbf{\hat{y}}+cz_{11}\,\mathbf{\hat{z}}$	(16b)	H VIII
$\mathbf{B_{82}}$	=	$-\left(y_{11}-z_{11}\right)\,\mathbf{a}_{1}-\left(x_{11}-z_{11}\right)\,\mathbf{a}_{2}-\left(x_{11}+y_{11}\right)\,\mathbf{a}_{3}$	=	$-ax_{11}\,\mathbf{\hat{x}}-ay_{11}\,\mathbf{\hat{y}}+cz_{11}\,\mathbf{\hat{z}}$	(16b)	H VIII
$\mathbf{B_{83}}$	=	$\left(x_{11}+z_{11}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(-y_{11}+z_{11}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(x_{11}-y_{11}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ay_{11}\,\mathbf{\hat{x}}+a\left(x_{11}+\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VIII
$\mathbf{B_{84}}$	=	$\left(-x_{11}+z_{11}+\frac{3}{4}\right)\,\mathbf{a}_{1}+\left(y_{11}+z_{11}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\left(-x_{11}+y_{11}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ay_{11}\,\mathbf{\hat{x}}-a\left(x_{11}-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VIII
$\mathbf{B_{85}}$	=	$\left(-y_{11}+z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(x_{11}+z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{2}+\left(x_{11}-y_{11}\right)\,\mathbf{a}_{3}$	=	$ax_{11}\,\mathbf{\hat{x}}-ay_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H VIII
$\mathbf{B_{86}}$	=	$\left(y_{11}+z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{1}+\left(-x_{11}+z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{2}-\left(x_{11}-y_{11}\right)\,\mathbf{a}_{3}$	=	$-ax_{11}\,\mathbf{\hat{x}}+ay_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(16b)	H VIII
$\mathbf{B_{87}}$	=	$\left(-x_{11}+z_{11}+\frac{1}{4}\right)\,\mathbf{a}_{1}+\left(-y_{11}+z_{11}+\frac{3}{4}\right)\,\mathbf{a}_{2}-\left(x_{11}+y_{11}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{11}-\frac{1}{2}\right)\,\mathbf{\hat{x}}-ax_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16b)	H VIII

$$\mathbf{B_{88}} = \left(x_{11}+z_{11}+\frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_{11}+z_{11}+\frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_{11}+y_{11}+\frac{1}{2}\right)\,\mathbf{a}_3 = a\left(y_{11}+\frac{1}{2}\right)\,\mathbf{\hat{x}} + a x_{11}\,\mathbf{\hat{y}} + c\left(z_{11}+\frac{1}{4}\right)\,\mathbf{\hat{z}} \qquad (16b) \qquad \text{H VIII}$$

References

[1] D. S. Marynick and W. N. Lipscomb, *Crystal Structure of Beryllium Borohydride*, Inorg. Chem. **11**, 820–823 (1972), doi:10.1021/ic50110a033.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.