

Cs₆W₁₁O₃₆ Structure:

A6B36C11_hR106_167_3c_6f_cef-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/0MQ1>

https://aflow.org/prototype-encyclopedia/A6B36C11_hR106_167_3c_6f_cef-001

Prototype	Cs ₆ O ₃₆ W ₁₁
AFLOW prototype label	A6B36C11_hR106_167_3c_6f_cef-001
ICSD	80133
CCDC	1640359
Pearson symbol	hR106
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	<pre>aflow --proto=A6B36C11_hR106_167_3c_6f_cef-001 --params=a, c/a, x₁, x₂, x₃, x₄, x₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂</pre>

- (Okada, 1978) placed this in the monoclinic space group Cc #9. (Marsh, 1995) determined that their data fit in space group $R\bar{3}c$ #167, and we show that refinement here.
- The original orientation may be found here.

Rhombohedral primitive vectors

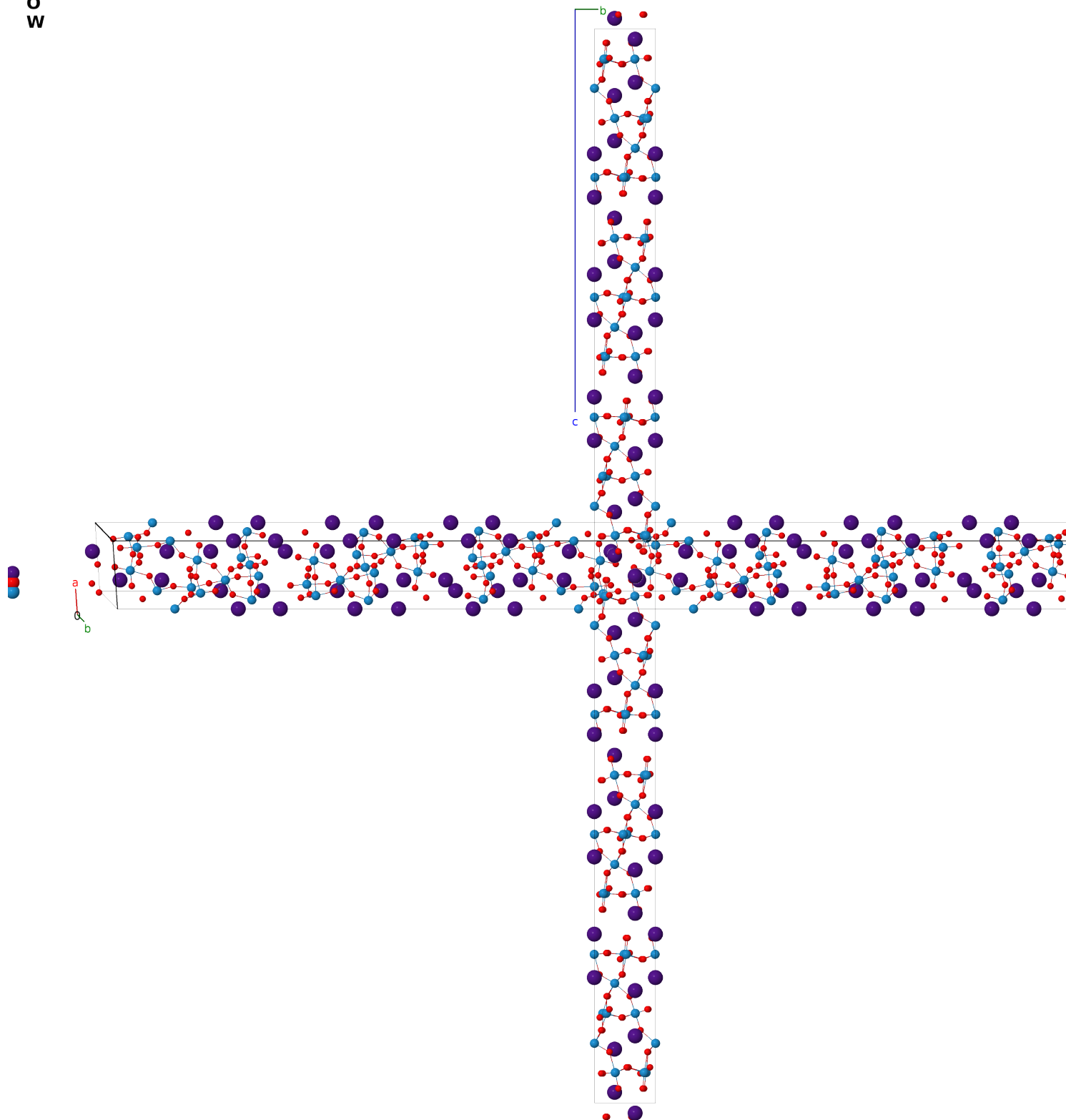
$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$$



Cs
O
W



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(4c)	Cs I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cs I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(4c)	Cs I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cs I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(4c)	Cs II
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cs II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(4c)	Cs II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cs II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(4c)	Cs III
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cs III
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(4c)	Cs III
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Cs III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-cx_4 \hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a(4x_5 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a(4x_5 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	W II
$\mathbf{B}_{18}$	$= \frac{1}{4} \mathbf{a}_1 + x_5 \mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{8}a(4x_5 - 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a(4x_5 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	W II
$\mathbf{B}_{19}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6e)	W II
$\mathbf{B}_{20}$	$= -x_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8}a(4x_5 + 3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a(12x_5 + 1) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	W II
$\mathbf{B}_{21}$	$= \frac{3}{4} \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{8}a(4x_5 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a(12x_5 + 5) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	W II
$\mathbf{B}_{22}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6e)	W II
$\mathbf{B}_{23}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B}_{24}$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B}_{25}$	$= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B}_{26}$	$= -\left(z_6 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 - 3) \hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B}_{27}$	$= -\left(y_6 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 - 3) \hat{\mathbf{z}}$	(12f)	O I

$\mathbf{B}_{51}$	$=$	$-\left(y_8 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} - \frac{1}{6}c(2x_8 + 2y_8 + 2z_8 - 3) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{52}$	$=$	$-\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} - \frac{1}{6}c(2x_8 + 2y_8 + 2z_8 - 3) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{53}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{54}$	$=$	$-z_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - y_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{55}$	$=$	$-y_8 \mathbf{a}_1 - z_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{56}$	$=$	$\left(z_8 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} + \frac{1}{6}c(2x_8 + 2y_8 + 2z_8 + 3) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{57}$	$=$	$\left(y_8 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} + \frac{1}{6}c(2x_8 + 2y_8 + 2z_8 + 3) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{58}$	$=$	$\left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} + \frac{1}{6}c(2x_8 + 2y_8 + 2z_8 + 3) \hat{\mathbf{z}}$	(12f)	O III
$\mathbf{B}_{59}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{60}$	$=$	$z_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + y_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{61}$	$=$	$y_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{62}$	$=$	$-\left(z_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} - \frac{1}{6}c(2x_9 + 2y_9 + 2z_9 - 3) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{63}$	$=$	$-\left(y_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} - \frac{1}{6}c(2x_9 + 2y_9 + 2z_9 - 3) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{64}$	$=$	$-\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} - \frac{1}{6}c(2x_9 + 2y_9 + 2z_9 - 3) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{65}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} - \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{66}$	$=$	$-z_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - y_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} - \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{67}$	$=$	$-y_9 \mathbf{a}_1 - z_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} - \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{68}$	$=$	$\left(z_9 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} + \frac{1}{6}c(2x_9 + 2y_9 + 2z_9 + 3) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{69}$	$=$	$\left(y_9 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} + \frac{1}{6}c(2x_9 + 2y_9 + 2z_9 + 3) \hat{\mathbf{z}}$	(12f)	O IV
$\mathbf{B}_{70}$	$=$	$\left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_9 + \frac{1}{$				

$$\begin{aligned}
\mathbf{B}_{73} &= y_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3 = -\frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{74} &= -\left(z_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{75} &= -\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{76} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{77} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -\frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{78} &= -z_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - y_{10} \mathbf{a}_3 = \frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{79} &= -y_{10} \mathbf{a}_1 - z_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3 = \frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{80} &= \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{81} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{82} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{10} + 2y_{10} + 2z_{10} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{O V} \\
\mathbf{B}_{83} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{84} &= z_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + y_{11} \mathbf{a}_3 = -\frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{85} &= y_{11} \mathbf{a}_1 + z_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3 = -\frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{86} &= -\left(z_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{11} + 2y_{11} + 2z_{11} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{87} &= -\left(y_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{11} + 2y_{11} + 2z_{11} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{88} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{11} + 2y_{11} + 2z_{11} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{O VI}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{89} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -\frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{90} &= -z_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - y_{11} \mathbf{a}_3 = \frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{91} &= -y_{11} \mathbf{a}_1 - z_{11} \mathbf{a}_2 - x_{11} \mathbf{a}_3 = \frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{92} &= \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{11} + 2y_{11} + 2z_{11} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{93} &= \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{11} + 2y_{11} + 2z_{11} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{94} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{11} + 2y_{11} + 2z_{11} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{O VI} \\
\mathbf{B}_{95} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(x_{12} - z_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{12} - 2y_{12} + z_{12}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{12} + y_{12} + z_{12}) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{96} &= z_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + y_{12} \mathbf{a}_3 = -\frac{1}{2}a(y_{12} - z_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{12} - y_{12} - z_{12}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{12} + y_{12} + z_{12}) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{97} &= y_{12} \mathbf{a}_1 + z_{12} \mathbf{a}_2 + x_{12} \mathbf{a}_3 = -\frac{1}{2}a(x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{12} + y_{12} - 2z_{12}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{12} + y_{12} + z_{12}) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{98} &= -\left(z_{12} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{12} - z_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{12} - 2y_{12} + z_{12}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{12} + 2y_{12} + 2z_{12} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{99} &= -\left(y_{12} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{12} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(y_{12} - z_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{12} - y_{12} - z_{12}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{12} + 2y_{12} + 2z_{12} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{100} &= -\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_{12} - y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{12} + y_{12} - 2z_{12}) \hat{\mathbf{y}} - \frac{1}{6}c(2x_{12} + 2y_{12} + 2z_{12} - 3) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{101} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 = -\frac{1}{2}a(x_{12} - z_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{12} - 2y_{12} + z_{12}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{12} + y_{12} + z_{12}) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{102} &= -z_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 - y_{12} \mathbf{a}_3 = \frac{1}{2}a(y_{12} - z_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{12} - y_{12} - z_{12}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{12} + y_{12} + z_{12}) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{103} &= -y_{12} \mathbf{a}_1 - z_{12} \mathbf{a}_2 - x_{12} \mathbf{a}_3 = \frac{1}{2}a(x_{12} - y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{12} + y_{12} - 2z_{12}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{12} + y_{12} + z_{12}) \hat{\mathbf{z}} & (12f) & \quad \text{W III} \\
\mathbf{B}_{104} &= \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_{12} + \frac{1}{2}\right) \mathbf{a}_3 = -\frac{1}{2}a(x_{12} - z_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{12} - 2y_{12} + z_{12}) \hat{\mathbf{y}} + \frac{1}{6}c(2x_{12} + 2y_{12} + 2z_{12} + 3) \hat{\mathbf{z}} & (12f) & \quad \text{W III}
\end{aligned}$$

$$\mathbf{B}_{105} = \begin{pmatrix} y_{12} + \frac{1}{2} \\ z_{12} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_{12} + \frac{1}{2} \\ z_{12} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_{12} + \frac{1}{2} \\ z_{12} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2}a(y_{12} - z_{12})\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a(2x_{12} - y_{12} - z_{12})\hat{\mathbf{y}} + \\ \frac{1}{6}c(2x_{12} + 2y_{12} + 2z_{12} + 3)\hat{\mathbf{z}} \end{pmatrix} \quad (12f) \quad \text{W III}$$

$$\mathbf{B}_{106} = \begin{pmatrix} x_{12} + \frac{1}{2} \\ y_{12} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_{12} + \frac{1}{2} \\ y_{12} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_{12} + \frac{1}{2} \\ y_{12} + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = \begin{pmatrix} \frac{1}{2}a(x_{12} - y_{12})\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a(x_{12} + y_{12} - 2z_{12})\hat{\mathbf{y}} + \\ \frac{1}{6}c(2x_{12} + 2y_{12} + 2z_{12} + 3)\hat{\mathbf{z}} \end{pmatrix} \quad (12f) \quad \text{W III}$$

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