

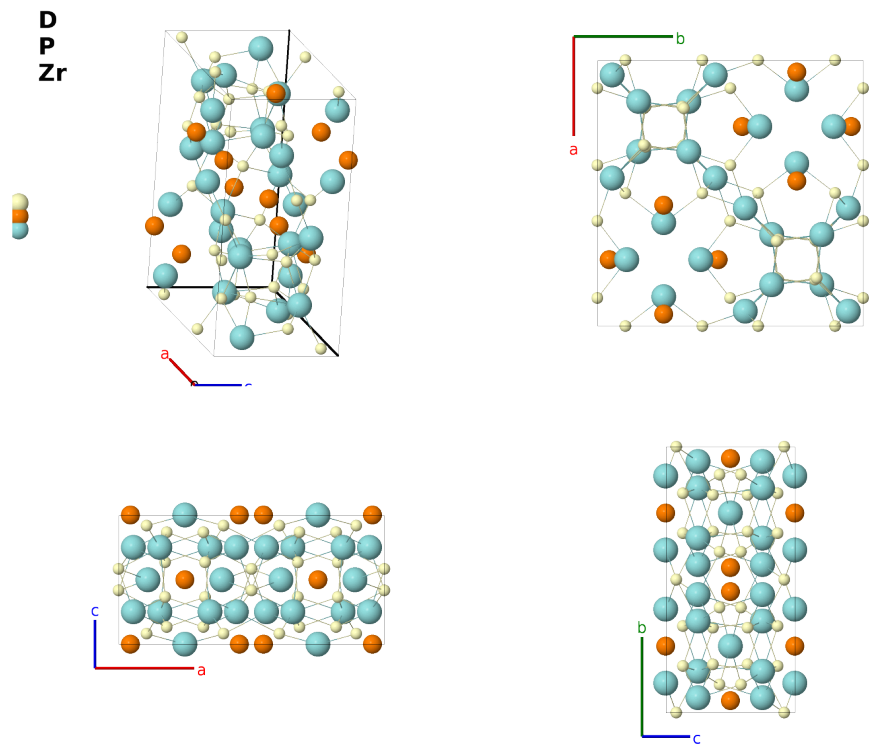
Zr₃PD₃ Structure: A4BC3_tP64_133_2k_h_i2j-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/XBGP>

https://aflow.org/prototype-encyclopedia/A4BC3_tP64_133_2k_h_i2j-001



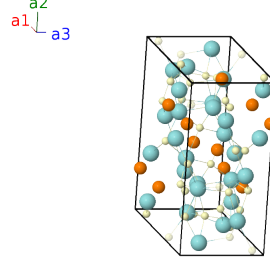
Prototype	H ₃ PZr ₃
AFLOW prototype label	A4BC3_tP64_133_2k_h_i2j-001
ICSD	68531
CCDC	1630449
Pearson symbol	tP64
Space group number	133
Space group symbol	$P4_2/nbc$
AFLOW prototype command	<pre>aflow --proto=A4BC3_tP64_133_2k_h_i2j-001 --params=a, c/a, x₁, x₂, x₃, x₄, x₅, y₅, z₅, x₆, y₆, z₆</pre>

Other compounds with this structure
Ti₃PD₃

- The D-I (16k) site has a small number of vacancies (0.4%).
- The D-II (16k) site is 44.7% occupied.
- Removing all of the deuterium atoms makes this isostructural with β -V₃S.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_6$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	P I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{10}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{14}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	Zr I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	Zr I
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{18}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{19}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{20}$	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{22}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{23}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II
$\mathbf{B}_{24}$	$= -x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	Zr II

$\mathbf{B}_{25} =$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{26} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{27} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{28} =$	$x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{29} =$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{30} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{31} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{32} =$	$-x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	Zr III
$\mathbf{B}_{33} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{34} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{35} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{36} =$	$y_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{37} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{38} =$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{39} =$	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{40} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{41} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{42} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{43} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{44} =$	$-y_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{45} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{46} =$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{47} =$	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{48} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D I
$\mathbf{B}_{49} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{50} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{51} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{52} =$	$y_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{53} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{54} =$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{55} =$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{56} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{57} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16k)	D II
$\mathbf{B}_{58} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(16k)	D II

$$\begin{aligned}
\mathbf{B}_{59} &= (y_6 + \tfrac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \tfrac{1}{2}) \mathbf{a}_3 = a (y_6 + \tfrac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - c (z_6 - \tfrac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{D II} \\
\mathbf{B}_{60} &= -y_6 \mathbf{a}_1 + (x_6 + \tfrac{1}{2}) \mathbf{a}_2 - (z_6 - \tfrac{1}{2}) \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} + a (x_6 + \tfrac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \tfrac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{D II} \\
\mathbf{B}_{61} &= (x_6 + \tfrac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = a (x_6 + \tfrac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16k) & \text{D II} \\
\mathbf{B}_{62} &= -x_6 \mathbf{a}_1 + (y_6 + \tfrac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} + a (y_6 + \tfrac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16k) & \text{D II} \\
\mathbf{B}_{63} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \tfrac{1}{2}) \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + c (z_6 + \tfrac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{D II} \\
\mathbf{B}_{64} &= (y_6 + \tfrac{1}{2}) \mathbf{a}_1 + (x_6 + \tfrac{1}{2}) \mathbf{a}_2 + (z_6 + \tfrac{1}{2}) \mathbf{a}_3 = a (y_6 + \tfrac{1}{2}) \hat{\mathbf{x}} + a (x_6 + \tfrac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \tfrac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{D II}
\end{aligned}$$

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