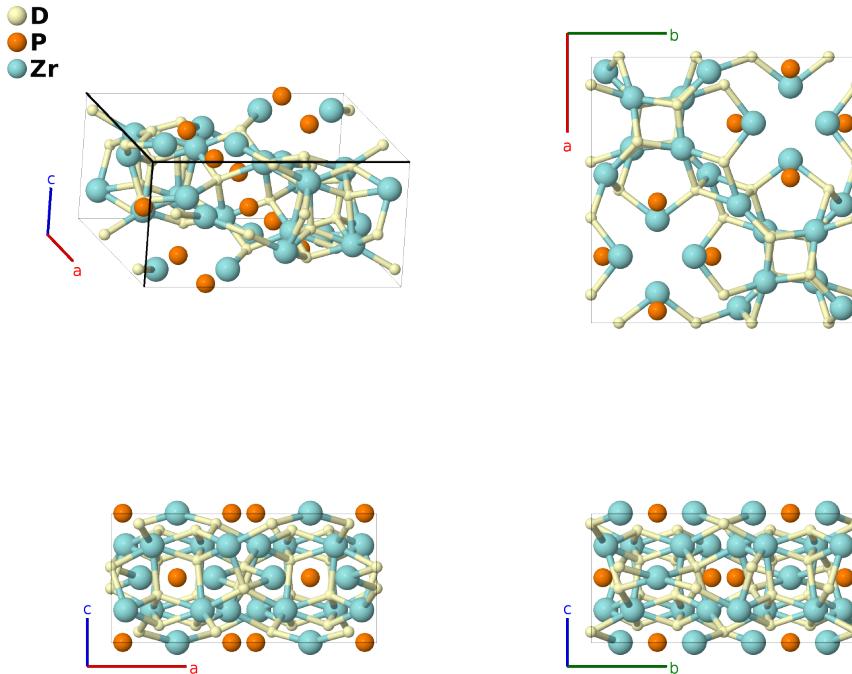


Zr₃PD₃ Structure: A4BC3_tP64_133_2k_h_i2j-001

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<https://aflow.org/p/XBGP>

https://aflow.org/p/A4BC3_tP64_133_2k_h_i2j-001



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

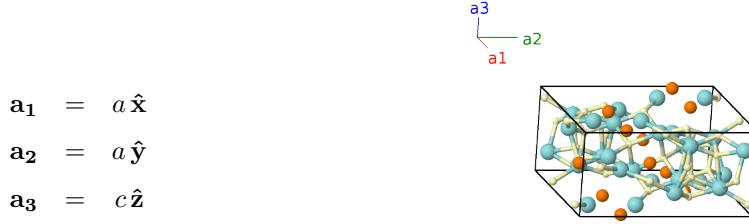
Other compounds with this structure

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



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$a x_1 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(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	$\frac{1}{4} \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{1}{4} a \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$-a x_1 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(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	$\frac{3}{4} \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$\frac{3}{4} a \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$a x_2 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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}	$\frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$\frac{1}{4} a \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(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}	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$-a x_2 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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}	$\frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$\frac{3}{4} a \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}}$	(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}	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(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}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	Zr II
\mathbf{B}_{20}	$x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$a x_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8j)	Zr II
\mathbf{B}_{21}	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(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}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	Zr II
\mathbf{B}_{24}	$-x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$-a x_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8j)	Zr II
\mathbf{B}_{25}	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(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
\mathbf{B}_{59}	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D II
\mathbf{B}_{60}	$-y_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	D II

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

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