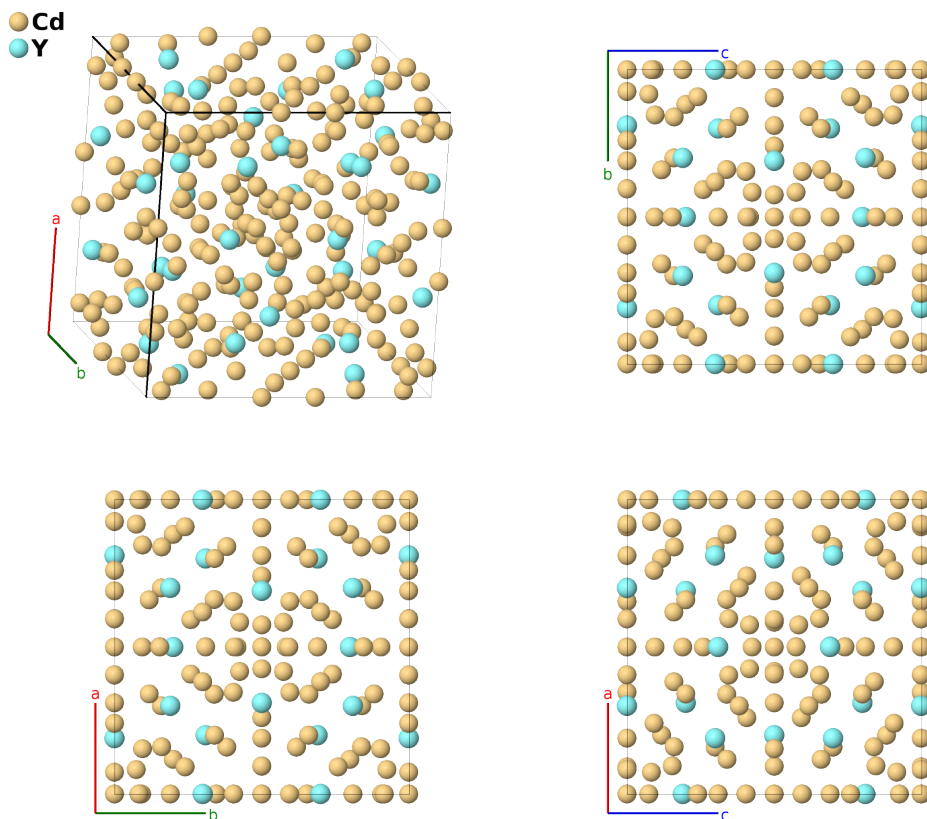


YCd₆ Structure: A20B3_cI184_204_def3gh_g-001

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

https://aflow.org/p/A20B3_cI184_204_def3gh_g-001



Prototype	Cd ₆ Y
AFLOW prototype label	A20B3_cI184_204_def3gh_g-001
ICSD	9148
Pearson symbol	cI184
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	<code>aflow --proto=A20B3_cI184_204_def3gh_g-001</code> <code>--params=a, x₁, x₂, x₃, y₄, z₄, y₅, z₅, y₆, z₆, y₇, z₇, x₈, y₈, z₈</code>

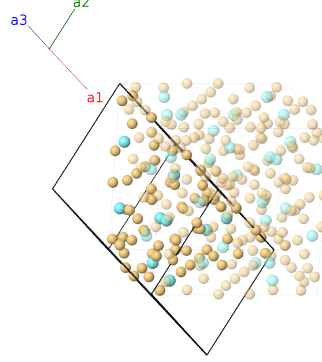
Other compounds with this structure

CeCd₆, DyCd₆, ErCd₆, EuCd₆, GdCd₆, HoCd₆, LuCd₆, NdCd₆, PrCd₆, PuCd₆, SmCd₆, TbCd₆, TmCd₆

- The site we label Cd-VI is occupied only 33.1% of the time. Removing this atom transforms this to the $\text{Ru}_3\text{Be}_{17}$ structure.
- (Armbrüster, 2000) found that what had previously been thought to be CeCd_6 was actually $\text{Ce}_6\text{Cd}_{37}$. This suggests that other XCd_6 structures may actually have different compositions.
- (Armbrüster, 2000) also give a structure for CeCd_6 which differs slightly from the one presented here.

Body-centered Cubic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}a \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}}$	(12d)	Cd I
\mathbf{B}_2	$= -x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}}$	(12d)	Cd I
\mathbf{B}_3	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{y}}$	(12d)	Cd I
\mathbf{B}_4	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{y}}$	(12d)	Cd I
\mathbf{B}_5	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{z}}$	(12d)	Cd I
\mathbf{B}_6	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{z}}$	(12d)	Cd I
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	Cd II
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	Cd II
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(12e)	Cd II
\mathbf{B}_{10}	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(12e)	Cd II
\mathbf{B}_{11}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(12e)	Cd II
\mathbf{B}_{12}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(12e)	Cd II
\mathbf{B}_{13}	$= 2x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{14}	$= -2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{15}	$= -2x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{16}	$= -2x_3 \mathbf{a}_1$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{17}	$= -2x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{18}	$= 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{19}	$= 2x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{20}	$= 2x_3 \mathbf{a}_1$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Cd III
\mathbf{B}_{21}	$= (y_4 + z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24g)	Cd IV
\mathbf{B}_{22}	$= -(y_4 - z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24g)	Cd IV
\mathbf{B}_{23}	$= (y_4 - z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24g)	Cd IV

$\mathbf{B}_{24} =$	$-(y_4 + z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24g)	Cd IV
$\mathbf{B}_{25} =$	$y_4 \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(24g)	Cd IV
$\mathbf{B}_{26} =$	$-y_4 \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(24g)	Cd IV
$\mathbf{B}_{27} =$	$y_4 \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(24g)	Cd IV
$\mathbf{B}_{28} =$	$-y_4 \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(24g)	Cd IV
$\mathbf{B}_{29} =$	$z_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}}$	(24g)	Cd IV
$\mathbf{B}_{30} =$	$z_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}}$	(24g)	Cd IV
$\mathbf{B}_{31} =$	$-z_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}}$	(24g)	Cd IV
$\mathbf{B}_{32} =$	$-z_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}}$	(24g)	Cd IV
$\mathbf{B}_{33} =$	$(y_5 + z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{34} =$	$-(y_5 - z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{35} =$	$(y_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{36} =$	$-(y_5 + z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{37} =$	$y_5 \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{38} =$	$-y_5 \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{39} =$	$y_5 \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{40} =$	$-y_5 \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$	(24g)	Cd V
$\mathbf{B}_{41} =$	$z_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + (y_5 + z_5) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}}$	(24g)	Cd V
$\mathbf{B}_{42} =$	$z_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - (y_5 - z_5) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}}$	(24g)	Cd V
$\mathbf{B}_{43} =$	$-z_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + (y_5 - z_5) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}}$	(24g)	Cd V
$\mathbf{B}_{44} =$	$-z_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - (y_5 + z_5) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}}$	(24g)	Cd V
$\mathbf{B}_{45} =$	$(y_6 + z_6) \mathbf{a}_1 + z_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{46} =$	$-(y_6 - z_6) \mathbf{a}_1 + z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{47} =$	$(y_6 - z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{48} =$	$-(y_6 + z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{49} =$	$y_6 \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{50} =$	$-y_6 \mathbf{a}_1 - (y_6 - z_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{51} =$	$y_6 \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{52} =$	$-y_6 \mathbf{a}_1 - (y_6 + z_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{z}}$	(24g)	Cd VI
$\mathbf{B}_{53} =$	$z_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + (y_6 + z_6) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}}$	(24g)	Cd VI
$\mathbf{B}_{54} =$	$z_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - (y_6 - z_6) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}}$	(24g)	Cd VI
$\mathbf{B}_{55} =$	$-z_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + (y_6 - z_6) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}}$	(24g)	Cd VI
$\mathbf{B}_{56} =$	$-z_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - (y_6 + z_6) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}}$	(24g)	Cd VI
$\mathbf{B}_{57} =$	$(y_7 + z_7) \mathbf{a}_1 + z_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{58} =$	$-(y_7 - z_7) \mathbf{a}_1 + z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{59} =$	$(y_7 - z_7) \mathbf{a}_1 - z_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{60} =$	$-(y_7 + z_7) \mathbf{a}_1 - z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{61} =$	$y_7 \mathbf{a}_1 + (y_7 + z_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{62} =$	$-y_7 \mathbf{a}_1 - (y_7 - z_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{63} =$	$y_7 \mathbf{a}_1 + (y_7 - z_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{z}}$	(24g)	Y I
$\mathbf{B}_{64} =$	$-y_7 \mathbf{a}_1 - (y_7 + z_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{z}}$	(24g)	Y I

$$\mathbf{B}_{90} = \begin{matrix} (x_8 - z_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + \\ (y_8 - z_8) \mathbf{a}_3 \end{matrix} = ay_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} \quad (48h) \quad \text{Cd VII}$$

$$\mathbf{B}_{91} = \begin{matrix} (x_8 + z_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - \\ (y_8 - z_8) \mathbf{a}_3 \end{matrix} = -ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} \quad (48h) \quad \text{Cd VII}$$

$$\mathbf{B}_{92} = \begin{matrix} -(x_8 - z_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 + \\ (y_8 + z_8) \mathbf{a}_3 \end{matrix} = ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} \quad (48h) \quad \text{Cd VII}$$

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