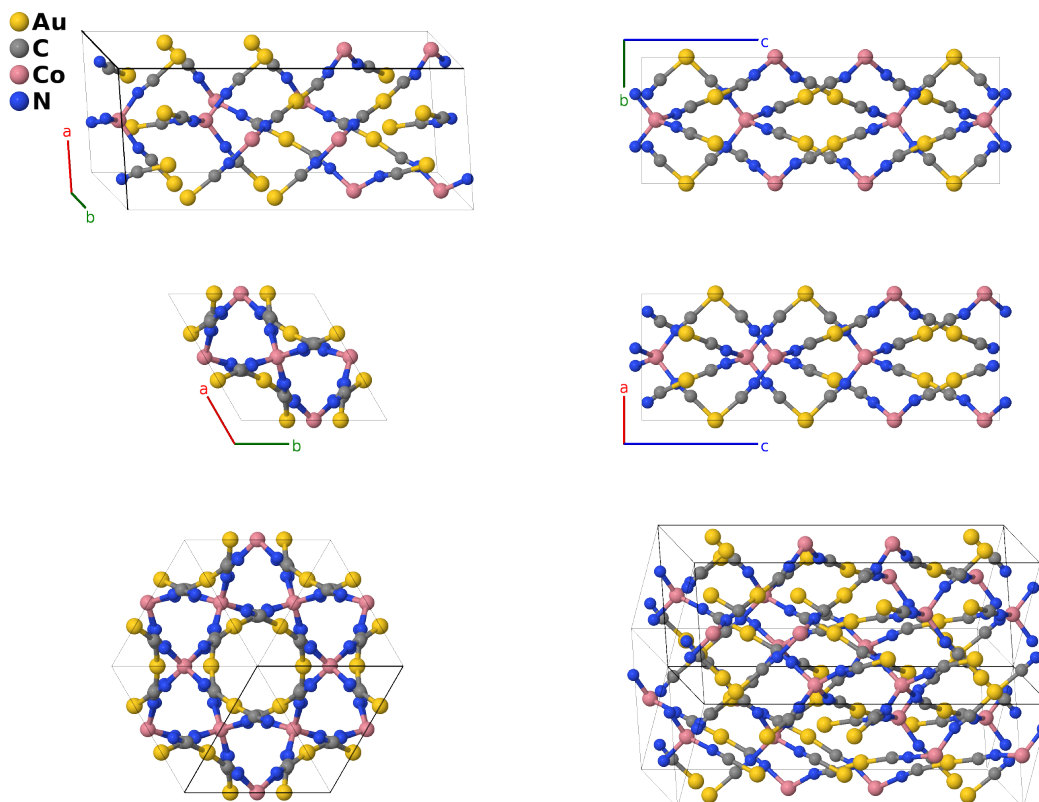


Co[Au(CN)₂]₂ Structure: A2B4CD4_hP66_181_k_2k_f_2k-001

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<https://aflow.org/p/R3D2>

https://aflow.org/p/A2B4CD4_hP66_181_k_2k_f_2k-001

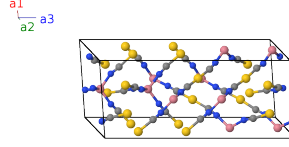


Prototype	Au ₂ C ₄ CoN ₄
AFLOW prototype label	A2B4CD4_hP66_181_k_2k_f_2k-001
ICSD	41197
Pearson symbol	hP66
Space group number	181
Space group symbol	<i>P</i> 6 ₄ 22
AFLOW prototype command	<code>aflow --proto=A2B4CD4_hP66_181_k_2k_f_2k-001 --params=a, c/a, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

- We follow (Abrahams, 1982) and put this structure in space group *P*6₄22 #181. (Villars, 2006) give the structure in the enantiomorphic space group *P*6₂22 #180. The latter paper uses 0.0058 instead of 0.00058 for one of the coordinates of the gold atoms. This change does not affect the distances between atoms published in (Abrahams, 1982), so we do not know which is correct. We use 0.00058.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6f)	Co I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{3}) \hat{\mathbf{z}}$	(6f)	Co I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{3}c(3z_1 + 2) \hat{\mathbf{z}}$	(6f)	Co I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_2 - (z_1 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} - c(z_1 - \frac{1}{3}) \hat{\mathbf{z}}$	(6f)	Co I
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_1 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(6f)	Co I
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_1 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{3}c(3z_1 - 2) \hat{\mathbf{z}}$	(6f)	Co I
\mathbf{B}_7	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_8	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_9	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{10}	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{11}	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{12}	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{13}	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - (z_2 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} - c(z_2 - \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{14}	$= (x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{15}	$= -x_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} - \frac{1}{3}c(3z_2 - 2) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{16}	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - (z_2 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} - c(z_2 - \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{17}	$= -(x_2 - y_2) \mathbf{a}_1 + y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{18}	$= x_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} - \frac{1}{3}c(3z_2 - 2) \hat{\mathbf{z}}$	(12k)	Au I
\mathbf{B}_{19}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{20}	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{21}	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{22}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{23}	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{24}	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{25}	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	C I
\mathbf{B}_{26}	$= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(12k)	C I

$$\begin{aligned}
\mathbf{B}_{27} &= -x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - \frac{1}{3}c(3z_3 - 2) \mathbf{a}_3 = -\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}} & (12k) & \text{C I} \\
\mathbf{B}_{28} &= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{C I} \\
\mathbf{B}_{29} &= -(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = \frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (12k) & \text{C I} \\
\mathbf{B}_{30} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}} & (12k) & \text{C I} \\
\mathbf{B}_{31} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{32} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{33} &= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{34} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{35} &= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{36} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{37} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{38} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{39} &= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{2}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{40} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{41} &= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{42} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} & (12k) & \text{C II} \\
\mathbf{B}_{43} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{44} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{45} &= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{46} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{47} &= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{48} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{49} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (z_5 - \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - c(z_5 - \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{50} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{51} &= -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{2}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{52} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - c(z_5 - \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{53} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{54} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}} & (12k) & \text{N I} \\
\mathbf{B}_{55} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (12k) & \text{N II} \\
\mathbf{B}_{56} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}} & (12k) & \text{N II} \\
\mathbf{B}_{57} &= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}} & (12k) & \text{N II}
\end{aligned}$$

$$\mathbf{B}_{58} = -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{59} = y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{60} = (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{61} = y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (z_6 - \frac{1}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - c(z_6 - \frac{1}{3}) \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{62} = (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{63} = -x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{2}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - \frac{1}{3}c(3z_6 - 2) \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{64} = -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - c(z_6 - \frac{1}{3}) \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{65} = -(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

$$\mathbf{B}_{66} = x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - \frac{1}{3}c(3z_6 - 2) \hat{\mathbf{z}} \quad (12k) \quad \text{N II}$$

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