

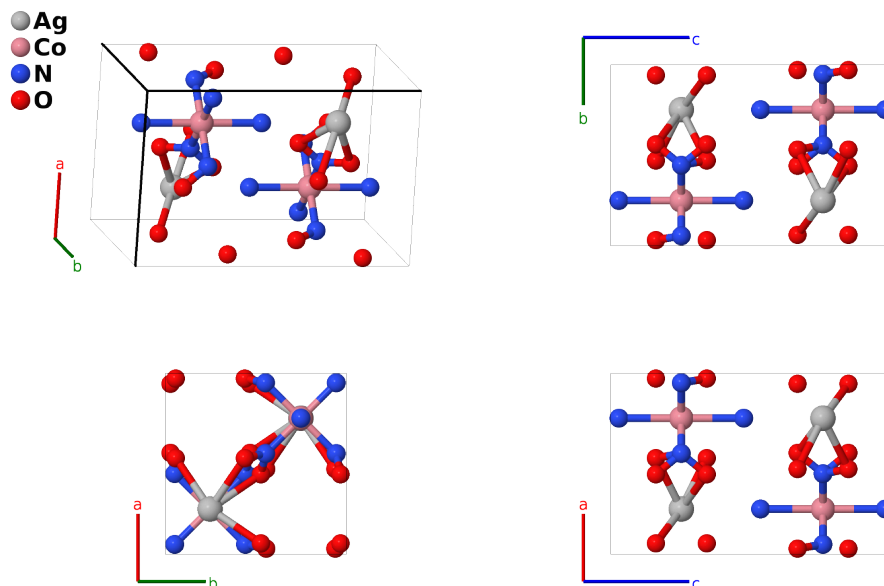
Ag[Co(NH₃)₂(NO₂)₄] (*J*₁₉) Structure: ABC4D2E8_tP32_126_a_b_h_e_k-001

This structure originally had the label ABC4D2E8_tP32_126_a_b_h_e_k. Calls to that address will be redirected here.

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<https://aflow.org/p/EW36>

https://aflow.org/p/ABC4D2E8_tP32_126_a_b_h_e_k-001

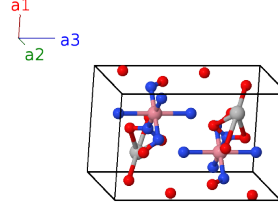


Prototype	AgCoN ₄ (NH ₃) ₂ O ₈
AFLOW prototype label	ABC4D2E8_tP32_126_a_b_h_e_k-001
<i>Strukturbericht</i> designation	<i>J</i> ₁₉
ICSD	26767
Pearson symbol	tP32
Space group number	126
Space group symbol	<i>P</i> 4/ <i>nnc</i>
AFLOW prototype command	<code>aflow --proto=ABC4D2E8_tP32_126_a_b_h_e_k-001 --params=a, c/a, z₃, x₄, x₅, y₅, z₅</code>

- The positions of the hydrogen atoms in the ammonia molecule are not determined. We only provide the positions of the nitrogen atoms (labeled as NH₃).
- (Wells, 1936) gives the lattice coordinates in setting 1 of space group *P*4/*nnc* #126. We used FINDSYM to change this to the standard setting 2.

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	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Ag I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Ag I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Co I
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Co I
\mathbf{B}_5	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	NH I
\mathbf{B}_6	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	NH I
\mathbf{B}_7	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4e)	NH I
\mathbf{B}_8	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	NH I
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{10}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{11}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{12}	$= x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{13}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{14}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{15}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{16}	$= -x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{18}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{19}	$= -(y_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{20}	$= y_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{21}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{22}	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{23}	$= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{24}	$= -(y_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{25}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{26}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	O I
\mathbf{B}_{27}	$= (y_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(16k)	O I

$$\mathbf{B}_{28} = -y_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 = -ay_5 \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (16k) \quad \text{O I}$$

$$\mathbf{B}_{29} = \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{O I}$$

$$\mathbf{B}_{30} = -x_5 \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} + a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{O I}$$

$$\mathbf{B}_{31} = -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = -ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{O I}$$

$$\mathbf{B}_{32} = \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{O I}$$

References

- [1] A. F. Wells, *The Crystal Structure of Silver Diamminotetranitro-cobaltiate* $\text{Ag}[\text{Co}(\text{NH}_3)_2(\text{NO}_2)_4]$, Z. Kristallogr. **95**, 74–82 (1936), doi:10.1524/zkri.1936.95.1.74.

Found in

- [1] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).