

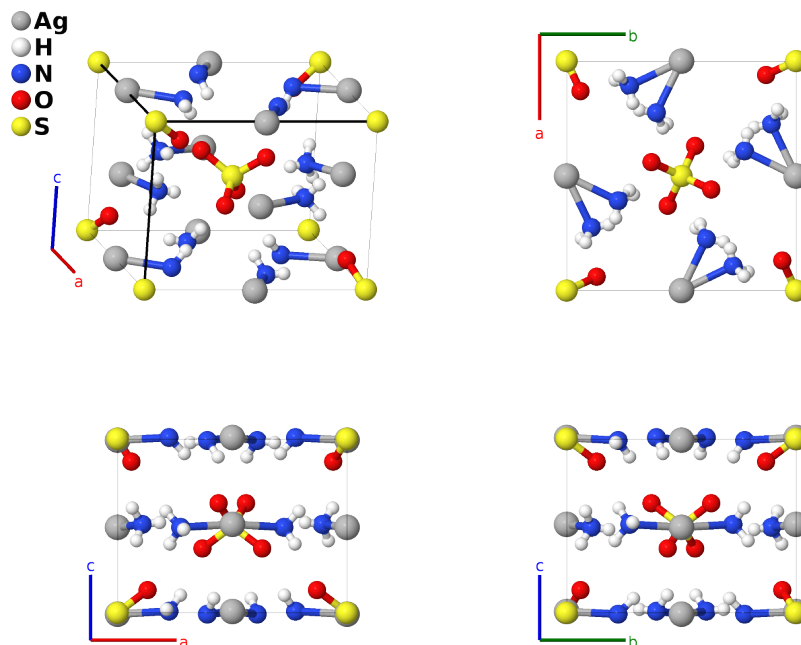
Ag₂SO₄·4NH₃ (*H*₄₁₇) Structure: A2B12C4D4E_tP46_114_d_3e_e_e_a-001

This structure originally had the label A2B12C4D4E_tP46_114_d_3e_e_e_a. Calls to that address will be redirected here.

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

https://aflow.org/p/A2B12C4D4E_tP46_114_d_3e_e_e_a-001

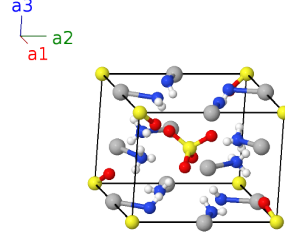


Prototype	Ag ₂ H ₁₂ N ₄ O ₄ S
AFLOW prototype label	A2B12C4D4E_tP46_114_d_3e_e_e_a-001
<i>Strukturbericht</i> designation	<i>H</i> ₄₁₇
ICSD	36585
Pearson symbol	tP46
Space group number	114
Space group symbol	<i>P</i> $\bar{4}$ ₂ <i>c</i>
AFLOW prototype command	<code>aflow --proto=A2B12C4D4E_tP46_114_d_3e_e_e_a-001 --params=a, c/a, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</code>

- We use the data from (Zachwieja, 1992), which refines the data of the original *H*₄₁₇ structure of (Corey, 1934) and locates the hydrogen atoms.

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	0	$=$	0	(2a)	S I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	S I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4d)	Ag I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(4d)	Ag I
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ag I
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Ag I
\mathbf{B}_7	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_8	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_9	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_{10}	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_{11}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_{12}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_{13}	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_{14}	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H I
\mathbf{B}_{15}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{16}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{17}	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{18}	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{19}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{20}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{21}	$-(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H II
\mathbf{B}_{22}	$(y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	H II

$$\begin{aligned}
\mathbf{B}_{23} &= 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}} & (8e) & \text{H III} \\
\mathbf{B}_{24} &= -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}} & (8e) & \text{H III} \\
\mathbf{B}_{25} &= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8e) & \text{H III} \\
\mathbf{B}_{26} &= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8e) & \text{H III} \\
\mathbf{B}_{27} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_5 - \frac{1}{2}\right) \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}} & (8e) & \text{H III} \\
\mathbf{B}_{28} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_5 + \frac{1}{2}\right) \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}} & (8e) & \text{H III} \\
\mathbf{B}_{29} &= -\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}} & (8e) & \text{H III} \\
\mathbf{B}_{30} &= \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}} & (8e) & \text{H III} \\
\mathbf{B}_{31} &= 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}} & (8e) & \text{N I} \\
\mathbf{B}_{32} &= -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}} & (8e) & \text{N I} \\
\mathbf{B}_{33} &= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8e) & \text{N I} \\
\mathbf{B}_{34} &= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8e) & \text{N I} \\
\mathbf{B}_{35} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{N I} \\
\mathbf{B}_{36} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{N I} \\
\mathbf{B}_{37} &= -\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}} & (8e) & \text{N I} \\
\mathbf{B}_{38} &= \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}} & (8e) & \text{N I} \\
\mathbf{B}_{39} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{40} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{41} &= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{42} &= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{43} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{44} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{45} &= -\left(y_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{O I} \\
\mathbf{B}_{46} &= \left(y_7 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{O I}
\end{aligned}$$

References

- [1] U. Zachwieja and H. Jacobs, *Redetermination of the crystal structure of diammine silver(I)-sulfate, $[\text{Ag}(\text{NH}_3)_2]_2\text{SO}_4$* , Z. Kristallogr. **201**, 207–212 (1992), doi:10.1524/zkri.1992.201.14.207.
- [2] R. B. Corey and R. W. G. Wyckoff, *The Crystal Structure of Silver Sulfate Tetrammoniate*, Z. Kristallogr. **87**, 264–274 (1934), doi:10.1524/zkri.1934.87.1.264.