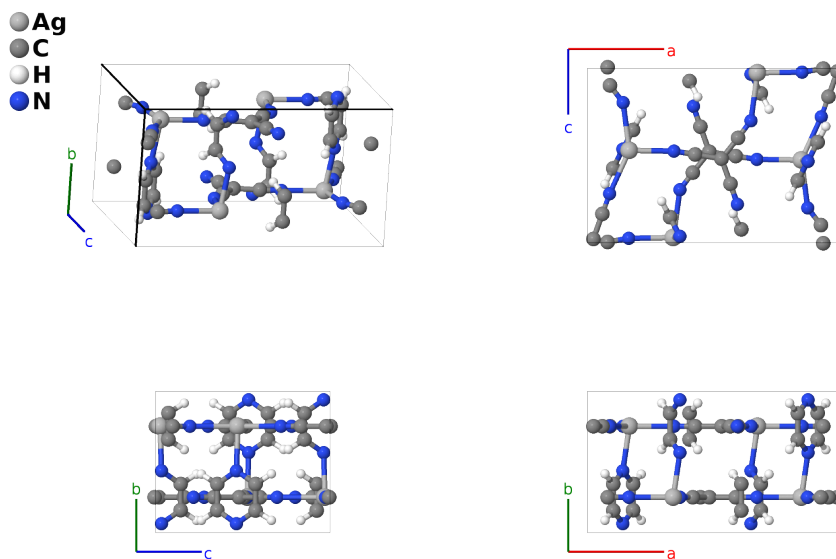


# Ag(tcm)(pyz) [AgC<sub>8</sub>N<sub>5</sub>H<sub>4</sub>] Structure: AB8C4D5\_oP72\_62\_c\_4c2d\_2d\_3cd-001

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<https://aflow.org/p/L9Y6>

[https://aflow.org/p/AB8C4D5\\_oP72\\_62\\_c\\_4c2d\\_2d\\_3cd-001](https://aflow.org/p/AB8C4D5_oP72_62_c_4c2d_2d_3cd-001)

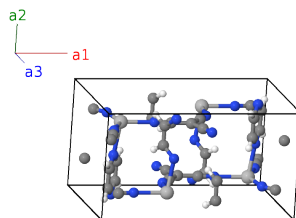


Prototype	AgC <sub>8</sub> H <sub>4</sub> N <sub>5</sub>
AFLOW prototype label	AB8C4D5_oP72_62_c_4c2d_2d_3cd-001
CCDC	671414
Pearson symbol	oP72
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=AB8C4D5_oP72_62_c_4c2d_2d_3cd-001</code> <code>--params=a,b/a,c/a,x<sub>1</sub>,z<sub>1</sub>,x<sub>2</sub>,z<sub>2</sub>,x<sub>3</sub>,z<sub>3</sub>,x<sub>4</sub>,z<sub>4</sub>,x<sub>5</sub>,z<sub>5</sub>,x<sub>6</sub>,z<sub>6</sub>,x<sub>7</sub>,z<sub>7</sub>,x<sub>8</sub>,z<sub>8</sub>,x<sub>9</sub>,y<sub>9</sub>,z<sub>9</sub>,x<sub>10</sub>,y<sub>10</sub>,z<sub>10</sub>,x<sub>11</sub>,y<sub>11</sub>,z<sub>11</sub>,x<sub>12</sub>,y<sub>12</sub>,z<sub>12</sub>,x<sub>13</sub>,y<sub>13</sub>,z<sub>13</sub></code>

- In the chemical literature tcm=tricyanomethanide (C(CN)<sub>3</sub><sup>-</sup>), and phz=pyrazine.

## Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{x} \\ \mathbf{a}_2 &= b \hat{y} \\ \mathbf{a}_3 &= c \hat{z} \end{aligned}$$







$$\begin{aligned}
\mathbf{B}_{63} &= x_{12} \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = ax_{12} \hat{\mathbf{x}} - b \left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8d) & \text{H II} \\
\mathbf{B}_{64} &= -\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{H II} \\
\mathbf{B}_{65} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 = ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{66} &= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 - y_{13} \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c \left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{67} &= -x_{13} \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 - z_{13} \mathbf{a}_3 = -ax_{13} \hat{\mathbf{x}} + b \left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{68} &= \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{69} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 = -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{70} &= \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 + y_{13} \mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - c \left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{71} &= x_{13} \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + z_{13} \mathbf{a}_3 = ax_{13} \hat{\mathbf{x}} - b \left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8d) & \text{N IV} \\
\mathbf{B}_{72} &= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{N IV}
\end{aligned}$$

## References

- [1] S. R. Batten, B. F. Hoskins, and R. Robson, *Structures of [Ag(tcm)], [Ag(tcm)(phz)<sub>1/2</sub>] and [Ag(tcm)(pyz)] (tcm-tricyanomethanide, C(CN)<sub>3</sub><sup>-</sup>, phz-phenazine, pyz-pyrazine)*, New J. Chem. **22**, 173–175 (1998), doi:10.1039/A707639H.

## Found in

- [1] S. A. Hodgson, J. Adamson, S. J. Hunt, M. J. Cliffe, A. B. Cairns, A. L. Thompson, M. G. Tucker, N. P. Funnell, and A. L. Goodwin, *Negative area compressibility in silver(I) tricyanomethanide*, Chem. Commun. **50**, 5264–5266 (2014), doi:10.1039/C3CC47032F.
- [2] J. Konnert and D. Britton, *The Crystal Structure of AgC(CN)<sub>3</sub>*, Inorg. Chem. **5**, 1191–1196 (1966), doi:10.1021/ic50041a026.