

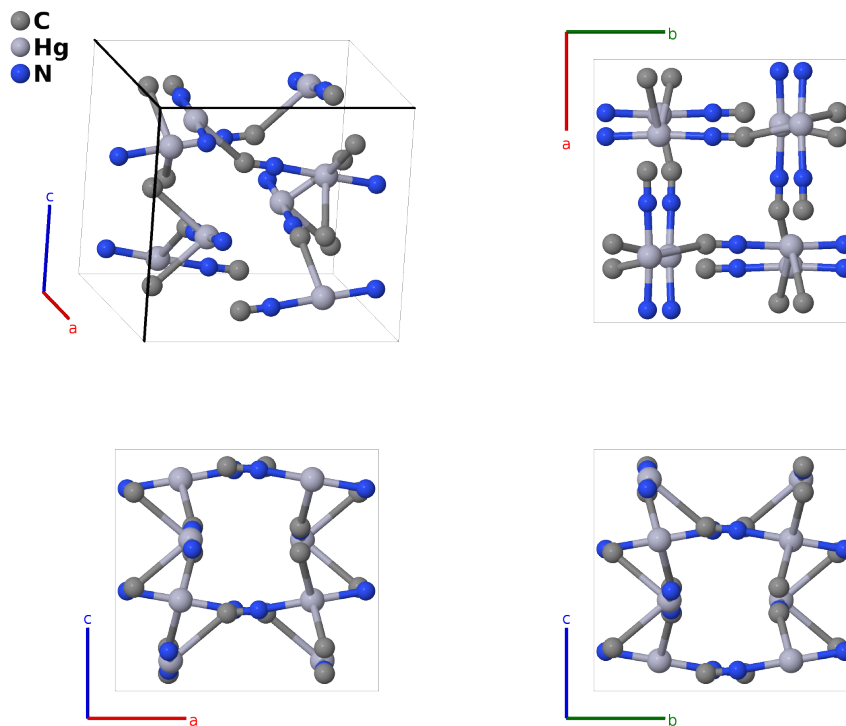
Mercury Cyanide [Hg(CN)₂, *F*1₁] Structure: A2BC2_tI40_122_e_d_e-001

This structure originally had the label A2BC2_tI40_122_e_d_e. Calls to that address will be redirected here.

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<https://aflow.org/p/05M4>

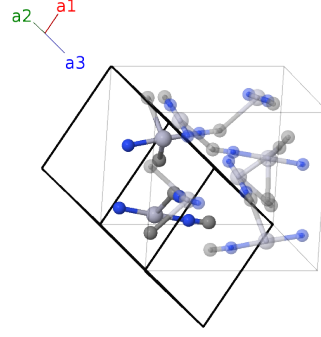
https://aflow.org/p/A2BC2_tI40_122_e_d_e-001



Prototype	C ₂ HgN ₂
AFLOW prototype label	A2BC2_tI40_122_e_d_e-001
<i>Strukturbericht</i> designation	<i>F</i> 1 ₁
Mineral name	mercury cyanide
ICSD	412315
Pearson symbol	tI40
Space group number	122
Space group symbol	<i>I</i> $\bar{4}2d$
AFLOW prototype command	<code>aflow --proto=A2BC2_tI40_122_e_d_e-001 --params=a, c/a, x₁, x₂, y₂, z₂, x₃, y₃, z₃</code>

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{3}{8} \mathbf{a}_1 + (x_1 + \frac{1}{8}) \mathbf{a}_2 + (x_1 + \frac{1}{4}) \mathbf{a}_3 =$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Hg I
\mathbf{B}_2	$= \frac{7}{8} \mathbf{a}_1 - (x_1 - \frac{1}{8}) \mathbf{a}_2 - (x_1 - \frac{3}{4}) \mathbf{a}_3 =$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Hg I
\mathbf{B}_3	$= -(x_1 - \frac{7}{8}) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 - (x_1 - \frac{1}{4}) \mathbf{a}_3 =$	$-\frac{1}{4}a \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Hg I
\mathbf{B}_4	$= (x_1 + \frac{7}{8}) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + (x_1 + \frac{3}{4}) \mathbf{a}_3 =$	$\frac{1}{4}a \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Hg I
\mathbf{B}_5	$= (y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3 =$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_6	$= -(y_2 - z_2) \mathbf{a}_1 - (x_2 - z_2) \mathbf{a}_2 - (x_2 + y_2) \mathbf{a}_3 =$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_7	$= -(x_2 + z_2) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3 =$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_8	$= (x_2 - z_2) \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3 =$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_9	$= (y_2 - z_2 + \frac{3}{4}) \mathbf{a}_1 - (x_2 + z_2 - \frac{1}{4}) \mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3 =$	$-ax_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_{10}	$= -(y_2 + z_2 - \frac{3}{4}) \mathbf{a}_1 + (x_2 - z_2 + \frac{1}{4}) \mathbf{a}_2 + (x_2 - y_2 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_{11}	$= (-x_2 + z_2 + \frac{3}{4}) \mathbf{a}_1 + (-y_2 + z_2 + \frac{1}{4}) \mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_3 =$	$-ay_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_{12}	$= (x_2 + z_2 + \frac{3}{4}) \mathbf{a}_1 + (y_2 + z_2 + \frac{1}{4}) \mathbf{a}_2 + (x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3 =$	$ay_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(16e)	C I
\mathbf{B}_{13}	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3 =$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16e)	N I
\mathbf{B}_{14}	$= -(y_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3 =$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16e)	N I
\mathbf{B}_{15}	$= -(x_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 =$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16e)	N I
\mathbf{B}_{16}	$= (x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 =$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16e)	N I

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{pmatrix} (y_3 - z_3 + \frac{3}{4}) \mathbf{a}_1 - \\ (x_3 + z_3 - \frac{1}{4}) \mathbf{a}_2 + \\ (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{N I} \\
\mathbf{B}_{18} &= \begin{pmatrix} -(y_3 + z_3 - \frac{3}{4}) \mathbf{a}_1 + \\ (x_3 - z_3 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{N I} \\
\mathbf{B}_{19} &= \begin{pmatrix} (-x_3 + z_3 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 - \\ (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{N I} \\
\mathbf{B}_{20} &= \begin{pmatrix} (x_3 + z_3 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{N I}
\end{aligned}$$

References

- [1] O. Reckeweg and A. Simon, *X-Ray and Raman Investigations on Cyanides of Mono- and Divalent Metals and Synthesis, Crystal Structure and Raman Spectrum of $Tl_5(CO_3)_2(CN)$* , Z. f. Naturf. B **57**, 895–900 (2002), doi:10.1515/znb-2002-0809.

Found in

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