Mercury Cyanide [$Hg(CN)_2$, $F1_1$] Structure: A2BC2_tI40_122_e_d_e-001

This structure previously used the label(s) `A2BC2_tI40_122_e_d_e`. Calls to these addresses will be redirected here.

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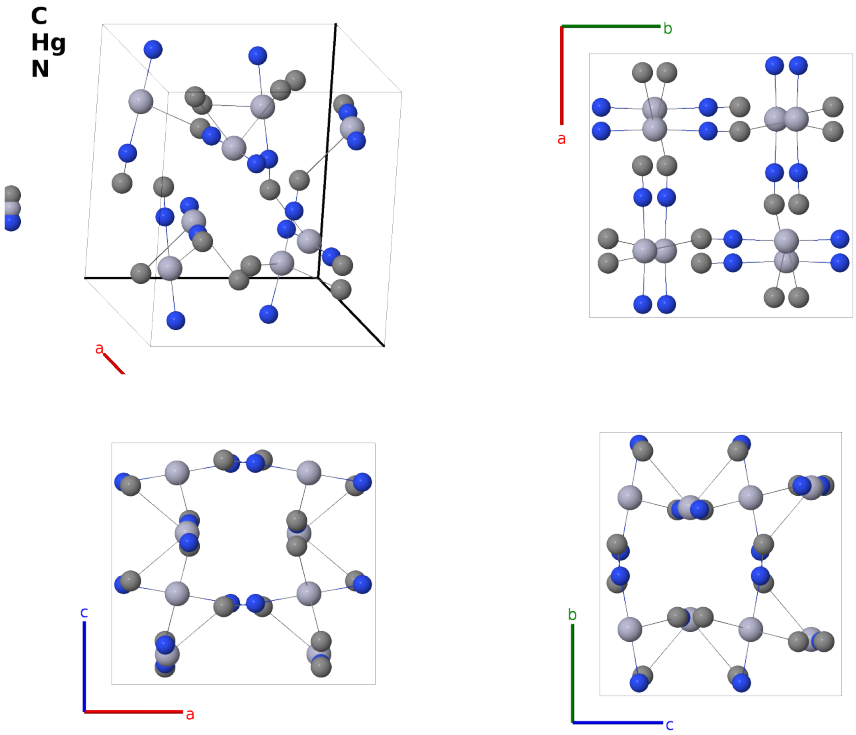
https://aflow.org/prototype-encyclopedia/05M4

https://aflow.org/prototype-encyclopedia/A2BC2_tI40_122_e_d_e-001

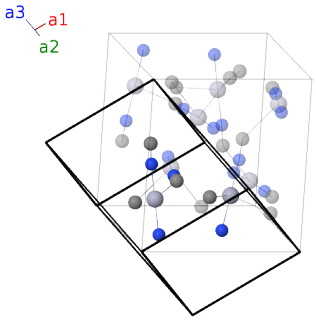


Prototype	C_2HgN_2
AFLOW prototype label	A2BC2_tI40_122_e_d_e-001
***Strukturbericht* designation**	$F1_1$
Mineral name	mercury cyanide
ICSD	412315
CCDC	1727652
Pearson symbol	tI40
Space group number	122
Space group symbol	$I\bar{4}2d$

AFLOW prototype command `aflow --proto=A2BC2_tI40_122_e_d_e-001 --params=`$a, c/a, x_1, x_2, y_2, z_2, x_3, y_3, z_3$

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_1 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8d)	Hg I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_1 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8d)	Hg I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8d)	Hg I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \left(x_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_9}$	=	$\left(y_2 - z_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_2 + z_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(-x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	C I
$\mathbf{B_{10}}$	=	$-\left(y_2 + z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_2 - z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_2 - y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	C I
$\mathbf{B_{11}}$	=	$\left(-x_2 + z_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(-y_2 + z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 + y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	C I
$\mathbf{B_{12}}$	=	$\left(x_2 + z_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_2 + z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{17}}$	=	$\left(y_3-z_3+\frac{3}{4}\right)\,\mathbf{a}_1-\left(x_3+z_3-\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	N I
$\mathbf{B_{18}}$	=	$-\left(y_3+z_3-\frac{3}{4}\right)\,\mathbf{a}_1+\left(x_3-z_3+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	N I
$\mathbf{B_{19}}$	=	$\left(-x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	N I
$\mathbf{B_{20}}$	=	$\left(x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16e)	N I

References

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First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.