

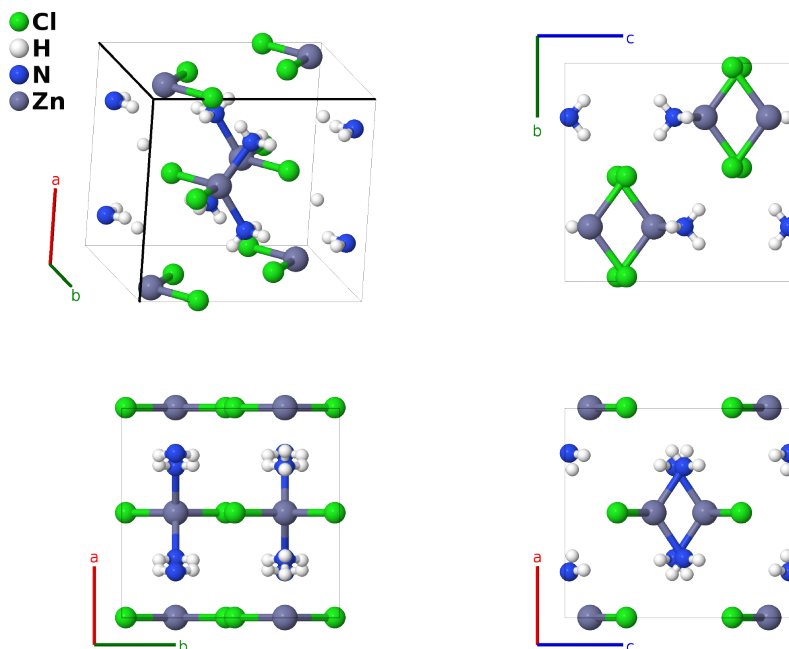
Zn(NH₃)₂Cl₂ (*E*1₂) Structure: A2B6C2D_oI44_74_i_hj_h_e-001

This structure originally had the label A2B6C2D_oI44_74_h_ij_i_e. Calls to that address will be redirected here.

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

https://aflow.org/p/A2B6C2D_oI44_74_i_hj_h_e-001



Prototype	Cl ₂ N ₂ H ₆ Zn
AFLOW prototype label	A2B6C2D_oI44_74_i_hj_h_e-001
<i>Strukturbericht</i> designation	<i>E</i> 1 ₂
ICSD	140642
Pearson symbol	oI44
Space group number	74
Space group symbol	<i>Imma</i>
AFLOW prototype command	<code>aflow --proto=A2B6C2D_oI44_74_i_hj_h_e-001 --params=a, b/a, c/a, z₁, y₂, z₂, y₃, z₃, x₄, z₄, x₅, y₅, z₅</code>

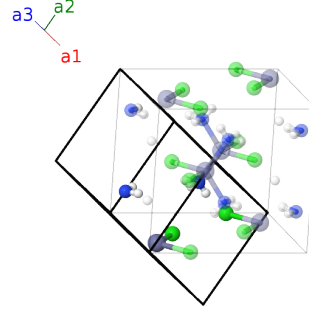
Other compounds with this structure

Zn(NH₃)₂Br₂

- (Ivšić, 2019) studied this system at 100K and were able to locate the hydrogen atoms. The positions of the other atoms are similar to those in earlier works such as (Yamaguchi, 1981) and the space group is unchanged, so we use this as the prototype for the *E*1₂ label.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$(z_1 + \frac{1}{4})\mathbf{a}_1 + z_1\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}b\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(4e)	Zn I
\mathbf{B}_2	$-(z_1 - \frac{3}{4})\mathbf{a}_1 - z_1\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}b\hat{\mathbf{y}} - cz_1\hat{\mathbf{z}}$	(4e)	Zn I
\mathbf{B}_3	$(y_2 + z_2)\mathbf{a}_1 + z_2\mathbf{a}_2 + y_2\mathbf{a}_3$	=	$by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(8h)	H I
\mathbf{B}_4	$(-y_2 + z_2 + \frac{1}{2})\mathbf{a}_1 + z_2\mathbf{a}_2 - (y_2 - \frac{1}{2})\mathbf{a}_3$	=	$-b(y_2 - \frac{1}{2})\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(8h)	H I
\mathbf{B}_5	$(y_2 - z_2 + \frac{1}{2})\mathbf{a}_1 - z_2\mathbf{a}_2 + (y_2 + \frac{1}{2})\mathbf{a}_3$	=	$b(y_2 + \frac{1}{2})\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(8h)	H I
\mathbf{B}_6	$-(y_2 + z_2)\mathbf{a}_1 - z_2\mathbf{a}_2 - y_2\mathbf{a}_3$	=	$-by_2\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(8h)	H I
\mathbf{B}_7	$(y_3 + z_3)\mathbf{a}_1 + z_3\mathbf{a}_2 + y_3\mathbf{a}_3$	=	$by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_8	$(-y_3 + z_3 + \frac{1}{2})\mathbf{a}_1 + z_3\mathbf{a}_2 - (y_3 - \frac{1}{2})\mathbf{a}_3$	=	$-b(y_3 - \frac{1}{2})\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_9	$(y_3 - z_3 + \frac{1}{2})\mathbf{a}_1 - z_3\mathbf{a}_2 + (y_3 + \frac{1}{2})\mathbf{a}_3$	=	$b(y_3 + \frac{1}{2})\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{10}	$-(y_3 + z_3)\mathbf{a}_1 - z_3\mathbf{a}_2 - y_3\mathbf{a}_3$	=	$-by_3\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(8h)	N I
\mathbf{B}_{11}	$(z_4 + \frac{1}{4})\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + (x_4 + \frac{1}{4})\mathbf{a}_3$	=	$ax_4\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(8i)	Cl I
\mathbf{B}_{12}	$(z_4 + \frac{1}{4})\mathbf{a}_1 - (x_4 - z_4)\mathbf{a}_2 - (x_4 - \frac{1}{4})\mathbf{a}_3$	=	$-ax_4\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(8i)	Cl I
\mathbf{B}_{13}	$-(z_4 - \frac{3}{4})\mathbf{a}_1 - (x_4 + z_4)\mathbf{a}_2 - (x_4 - \frac{3}{4})\mathbf{a}_3$	=	$-ax_4\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(8i)	Cl I
\mathbf{B}_{14}	$-(z_4 - \frac{3}{4})\mathbf{a}_1 + (x_4 - z_4)\mathbf{a}_2 + (x_4 + \frac{3}{4})\mathbf{a}_3$	=	$ax_4\hat{\mathbf{x}} + \frac{3}{4}b\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(8i)	Cl I
\mathbf{B}_{15}	$(y_5 + z_5)\mathbf{a}_1 + (x_5 + z_5)\mathbf{a}_2 + (x_5 + y_5)\mathbf{a}_3$	=	$ax_5\hat{\mathbf{x}} + by_5\hat{\mathbf{y}} + cz_5\hat{\mathbf{z}}$	(16j)	H II
\mathbf{B}_{16}	$(-y_5 + z_5 + \frac{1}{2})\mathbf{a}_1 - (x_5 - z_5)\mathbf{a}_2 - (x_5 + y_5 - \frac{1}{2})\mathbf{a}_3$	=	$-ax_5\hat{\mathbf{x}} - b(y_5 - \frac{1}{2})\hat{\mathbf{y}} + cz_5\hat{\mathbf{z}}$	(16j)	H II
\mathbf{B}_{17}	$(y_5 - z_5 + \frac{1}{2})\mathbf{a}_1 - (x_5 + z_5)\mathbf{a}_2 + (-x_5 + y_5 + \frac{1}{2})\mathbf{a}_3$	=	$-ax_5\hat{\mathbf{x}} + b(y_5 + \frac{1}{2})\hat{\mathbf{y}} - cz_5\hat{\mathbf{z}}$	(16j)	H II
\mathbf{B}_{18}	$-(y_5 + z_5)\mathbf{a}_1 + (x_5 - z_5)\mathbf{a}_2 + (x_5 - y_5)\mathbf{a}_3$	=	$ax_5\hat{\mathbf{x}} - by_5\hat{\mathbf{y}} - cz_5\hat{\mathbf{z}}$	(16j)	H II
\mathbf{B}_{19}	$-(y_5 + z_5)\mathbf{a}_1 - (x_5 + z_5)\mathbf{a}_2 - (x_5 + y_5)\mathbf{a}_3$	=	$-ax_5\hat{\mathbf{x}} - by_5\hat{\mathbf{y}} - cz_5\hat{\mathbf{z}}$	(16j)	H II

$$\mathbf{B}_{20} = \begin{pmatrix} (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 - z_5) \mathbf{a}_2 + (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (16j) \quad \text{H II}$$

$$\mathbf{B}_{21} = \begin{pmatrix} (-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 + z_5) \mathbf{a}_2 + (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} \quad (16j) \quad \text{H II}$$

$$\mathbf{B}_{22} = \begin{pmatrix} (y_5 + z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - \\ (x_5 - y_5) \mathbf{a}_3 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} \quad (16j) \quad \text{H II}$$

References

- [1] T. Ivšić, D. W. Bi, and A. Magrez, *New refinement of the crystal structure of $\text{Zn}(\text{NH}_3)\text{Cl}_2$ at 100K*, Acta Crystallogr. Sect. E **75**, 1386–1388 (2019), doi:10.1107/S2056989019011757.
- [2] T. Yamaguchi and O. Lindqvist, *The Crystal Structure of Diamminedichlorozinc(II), $\text{ZnCl}_2(\text{NH}_3)_2$. A New Refinement.*, Acta Chem. Scand. **37a**, 727–728 (1981), doi:10.3891/acta.chem.scand.35a-0727.