

Diamminetriamidodizinc Chloride ($[\text{Zn}_2(\text{NH}_3)_2(\text{NH}_2)_3]\text{Cl}$) Structure:

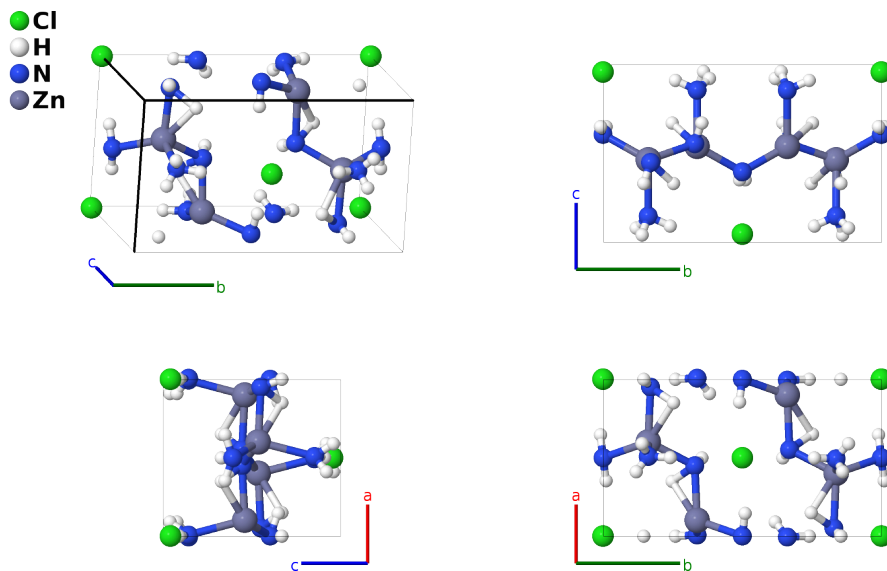
AB12C5D2_oP40_18_a_6c_b2c_c-001

This structure originally had the label AB12C5D2_oP40_18_a_6c_b2c_c. Calls to that address will be redirected here.

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<https://afLOW.org/p/5HSN>

https://afLOW.org/p/AB12C5D2_oP40_18_a_6c_b2c_c-001

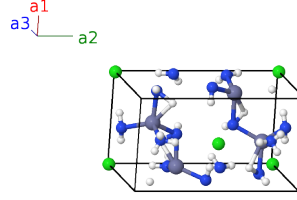


Prototype	$\text{ClH}_{12}\text{N}_5\text{Zn}$
AFLOW prototype label	AB12C5D2_oP40_18_a_6c_b2c_c-001
Mineral name	diamminetriamidodizinc chloride
ICSD	31831
Pearson symbol	oP40
Space group number	18
Space group symbol	$P2_12_12$
AFLOW prototype command	<pre>afLOW --proto=AB12C5D2_oP40_18_a_6c_b2c_c-001 --params=a,b/a,c/a,z1,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8, x9,y9,z9,x10,y10,z10,x11,y11,z11</pre>

- The ICSD entry has Wyckoff coordinates that significantly disagree with the those in (Richter, 2016). We use the values from Table 2 of that paper.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	Cl I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(2a)	Cl I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	N I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(2b)	N I
\mathbf{B}_5	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_6	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_7	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_8	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_9	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{10}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{11}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{12}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{13}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	H III
\mathbf{B}_{14}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	H III
\mathbf{B}_{15}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	H III
\mathbf{B}_{16}	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	H III
\mathbf{B}_{17}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	H IV
\mathbf{B}_{18}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	H IV
\mathbf{B}_{19}	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	H IV
\mathbf{B}_{20}	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	H IV
\mathbf{B}_{21}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	H V
\mathbf{B}_{22}	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	H V
\mathbf{B}_{23}	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4c)	H V
\mathbf{B}_{24}	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4c)	H V
\mathbf{B}_{25}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4c)	H VI
\mathbf{B}_{26}	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4c)	H VI

$$\begin{aligned}
\mathbf{B}_{27} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 = -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (4c) & \text{H VI} \\
\mathbf{B}_{28} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 = a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (4c) & \text{H VI} \\
\mathbf{B}_{29} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4c) & \text{N II} \\
\mathbf{B}_{30} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4c) & \text{N II} \\
\mathbf{B}_{31} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 = -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (4c) & \text{N II} \\
\mathbf{B}_{32} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 = a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (4c) & \text{N II} \\
\mathbf{B}_{33} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (4c) & \text{N III} \\
\mathbf{B}_{34} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (4c) & \text{N III} \\
\mathbf{B}_{35} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (4c) & \text{N III} \\
\mathbf{B}_{36} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (4c) & \text{N III} \\
\mathbf{B}_{37} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (4c) & \text{Zn I} \\
\mathbf{B}_{38} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (4c) & \text{Zn I} \\
\mathbf{B}_{39} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (4c) & \text{Zn I} \\
\mathbf{B}_{40} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (4c) & \text{Zn I}
\end{aligned}$$

References

- [1] T. M. M. Richter, S. Strobel, N. S. A. Alt, E. Schlücker, and R. Niewa, *Ammonothermal Synthesis and Crystal Structures of Diamminetriamidodizinc Chloride $[\text{Zn}_2(\text{NH}_3)_2(\text{NH}_2)_3]\text{Cl}$ and Diamminemonoamidozinc Bromide $[\text{Zn}(\text{NH}_3)_2(\text{NH}_2)]\text{Br}$* , *Inorganics* **4**, 41 (2016).