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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{N}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.026  
 $wR$  factor = 0.071  
Data-to-parameter ratio = 31.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*catena*-Poly[[dichlorozinc(II)]- $\mu$ -cyanoguanidine]

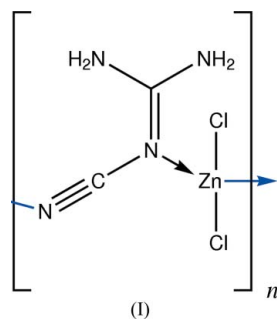
The one-dimensional title compound,  $[\text{ZnCl}_2(\text{C}_2\text{H}_4\text{N}_4)]_n$ , contains  $\text{ZnCl}_2\text{N}_2$  tetrahedra linked by *N,N*-bridging cyanoguanidine molecules. A network of  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds help to establish the crystal packing.

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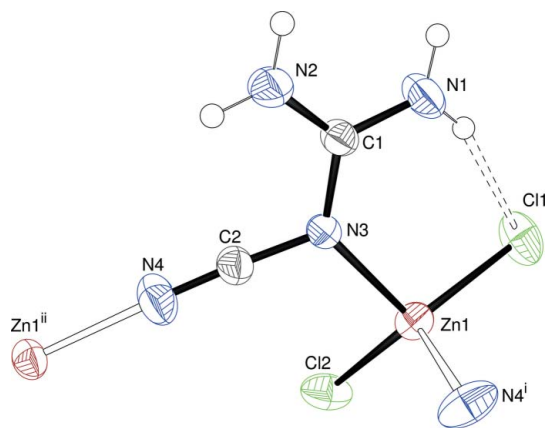
## Comment

The title compound, (I) (Fig. 1), is a one-dimensional coordination polymer containing cyanoguanidine molecules,  $\text{Zn}^{2+}$  ions and  $\text{Cl}^-$  ions. The  $\text{Zn}^{2+}$  cation is tetrahedrally coordinated by two terminal  $\text{Cl}^-$  ions and two cyanoguanidine molecules (Table 1), one bonded through the cyanide atom N4 and one from the imine atom N3. The  $\text{C1}-\text{N3}-\text{C2}$  bond angle in (I) is  $116.22(15)^\circ$ , compared with the corresponding angle of  $118.38(2)^\circ$  in the free ligand (Hirshfeld & Hope, 1980). The  $\text{C1}-\text{N3}$  [ $1.370(2)\text{ \AA}$ ] and  $\text{C2}-\text{N3}$  [ $1.308(3)\text{ \AA}$ ] bond lengths in (I) indicate that the conventional Lewis structure shown in the chemical scheme ( $\text{C1}=\text{N3}$  a formal double bond and  $\text{C2}-\text{N3}$  a formal single bond) is only a very approximate representation of the actual electron distribution in the molecule (Hughes, 1940; Hirshfeld & Hope, 1980).

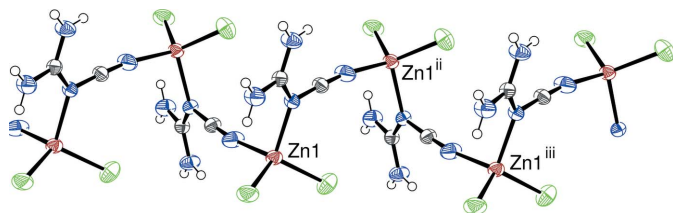


The connectivity of the building units in (I) results in a polymeric chain of stoichiometry  $\text{Zn}(\text{C}_2\text{H}_4\text{N}_4)\text{Cl}_2$  (Fig. 2), which propagates in the polar [001] direction. The chain conformation is reinforced by an intra-chain  $\text{N1}-\text{H2}\cdots\text{Cl1}$  hydrogen bond. Further  $\text{N}-\text{H}\cdots\text{Cl}$  bonds cross-link the polymeric strands (Table 2). Atom H1 has no nearby  $\text{Cl}^-$  ions but possibly forms a weak bifurcated  $\text{N}-\text{H}\cdots(\text{Cl},\text{Cl})$  interaction (bond angle sum for H1 =  $359^\circ$ ).

Two polymorphs of the molecular compound  $\text{Zn}(\text{C}_2\text{H}_4\text{N}_4)_2\text{Cl}_2$  have been reported by Pickardt & Kuhn (1995) and Fowkes & Harrison (2005). These both contain  $\text{ZnCl}_2\text{N}_2$  tetrahedra, with the two cyanoguanidine molecules both bonding through their cyanide N atoms. Other compounds with the stoichiometry of the title compound,  $M(\text{C}_2\text{H}_4\text{N}_4)_2\text{X}_2$  ( $M$  is a divalent metal cation and  $X$  is a halide) include  $\text{Hg}(\text{C}_2\text{H}_4\text{N}_4)_2\text{Cl}_2$  and  $\text{Cd}(\text{C}_2\text{H}_4\text{N}_4)_2\text{Br}_2$  (Pickardt &



**Figure 1**  
The asymmetric unit of (I), expanded to show the polymeric connectivity (open bonds) of the chain. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius. The intra-chain hydrogen bond is indicated by a double-dashed line. [Symmetry codes: (i)  $1 - x, -y, z - \frac{1}{2}$ ; (ii)  $1 - x, -y, z + \frac{1}{2}$ .]



**Figure 2**  
Part of an [001] polymeric chain in (I). [Symmetry codes: (ii)  $1 - x, -y, z + \frac{1}{2}$ , (iii)  $x, y, z + 1$ .]

Kuhn, 1996). The mercury compound contains *N,N*-bonded cyanoguanidine molecules, as seen here in (I), but the  $\text{Cl}^-$  ions also act as  $\mu_2$  bridges between the irregularly-coordinated  $\text{Hg}^{2+}$  ions, leading to a layered polymeric network. The cadmium compound features cyanide-*N*-bonded cyanoguanidine molecules and bridging  $\text{Br}^-$  ions, leading to one-dimensional chains of distorted tetrahedral  $\text{CdN}_2\text{Br}_2$  units.

### Experimental

An aqueous solution (10 ml) of cyanoguanidine (0.73 M) and a methanolic solution (10 ml) of  $\text{ZnCl}_2$  (0.73 M) were mixed at 293 K in a Petri dish, resulting in a colourless mixture. Colourless blocks and slabs of (I) grew over the course of a few days as the water/methanol evaporated at 293 K.

#### Crystal data

|   |   |
|---|---|
| $[\text{ZnCl}_2(\text{C}_2\text{H}_4\text{N}_4)]$ | $Z = 4$                                   |
| $M_r = 220.36$                                    | $D_x = 1.957 \text{ Mg m}^{-3}$           |
| Orthorhombic, $Pca2_1$                            | Mo $K\alpha$ radiation                    |
| $a = 13.6756(8) \text{ \AA}$                      | $\mu = 3.92 \text{ mm}^{-1}$              |
| $b = 7.3710(5) \text{ \AA}$                       | $T = 293(2) \text{ K}$                    |
| $c = 7.4200(5) \text{ \AA}$                       | Slab, colourless                          |
| $V = 747.96(8) \text{ \AA}^3$                     | $0.51 \times 0.49 \times 0.09 \text{ mm}$ |

#### Data collection

|  |  |
|--|--|
| Bruker SMART1000 CCD area-detector diffractometer        | 9597 measured reflections              |
| $\omega$ scans   | 2612 independent reflections           |
| Absorption correction: multi-scan (SADABS; Bruker, 1999) | 2481 reflections with $I > 2\sigma(I)$ |
| $T_{\min} = 0.240, T_{\max} = 0.720$                     | $R_{\text{int}} = 0.039$               |
|  | $\theta_{\max} = 32.5^\circ$           |

#### Refinement

|  |   |
|--|---|
| Refinement on $F^2$                    | $(\Delta/\sigma)_{\max} < 0.001$                          |
| $R[F^2 > 2\sigma(F^2)] = 0.026$        | $\Delta\rho_{\max} = 0.49 \text{ e \AA}^{-3}$             |
| $wR(F^2) = 0.071$                      | $\Delta\rho_{\min} = -0.57 \text{ e \AA}^{-3}$            |
| $S = 1.05$                             | Extinction correction: SHELXL97 (Sheldrick, 1997)         |
| 2612 reflections                       | Extinction coefficient: 0.0218 (16)                       |
| 83 parameters                          | Absolute structure: Flack (1983), with 1163 Friedel pairs |
| H-atom parameters constrained          | Flack parameter: 0.027 (11)                               |
| $w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$ |   |
| where $P = (F_o^2 + 2F_c^2)/3$         |   |

**Table 1**

Selected bond lengths ( $\text{\AA}$ ).

|                      |             |         |            |
|----------------------|-------------|---------|------------|
| Zn1—N4 <sup>iv</sup> | 1.985 (2)   | Zn1—Cl2 | 2.2238 (7) |
| Zn1—N3               | 2.0887 (14) | Zn1—Cl1 | 2.2252 (7) |

Symmetry code: (iv)  $-x + 1, -y, z - \frac{1}{2}$ .

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

| $D-H\cdots A$                     | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| N1—H1 $\cdots$ Cl1 <sup>v</sup>   | 0.86  | 2.92        | 3.6437 (18) | 144           |
| N1—H1 $\cdots$ Cl2 <sup>vi</sup>  | 0.86  | 2.92        | 3.389 (2)   | 116           |
| N1—H2 $\cdots$ Cl1                | 0.86  | 2.48        | 3.3050 (18) | 161           |
| N2—H3 $\cdots$ Cl1 <sup>v</sup>   | 0.86  | 2.42        | 3.262 (2)   | 166           |
| N2—H4 $\cdots$ Cl2 <sup>vii</sup> | 0.86  | 2.50        | 3.289 (2)   | 153           |

Symmetry codes: (v)  $x + \frac{1}{2}, -y + 1, z$ ; (vi)  $-x + 1, -y + 1, z - \frac{1}{2}$ ; (vii)  $x + \frac{1}{2}, -y, z$ .

H atoms were placed in idealized locations, with  $\text{N—H} = 0.86 \text{ \AA}$ , and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ .

Data collection: SMART (Bruker, 1999); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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