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A monoclinic polymorph of dichlorobis(cyanoguanidine)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.004 Å
R factor = 0.035
wR factor = 0.077
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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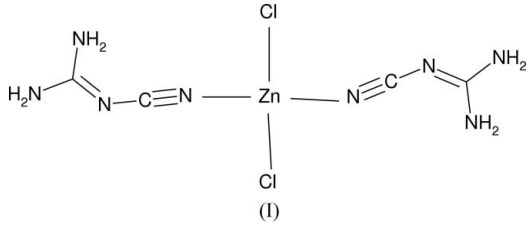
The molecular title compound, β-$[ZnCl_2(C_2H_4N_4)_2]$, crystallizes as a monoclinic polymorph of the known triclinic structure of this material. A complex network of N—H···N and N—H···Cl hydrogen bonds help to establish the crystal packing.

Comment

The title compound, (I) (Fig. 1), crystallizes as a monoclinic polymorph (space group $P2_1/c$) of the known triclinic structure (hereafter known as the α polymorph) of this material (Pickardt & Kuhn, 1995). Polymorph (I) contains isolated $[ZnCl_2(C_2H_4N_4)_2]$ molecules, with the Zn^{2+} cations coordinated by two chloride ions and two cyanide N atoms of the cyanoguanidine ligands. The geometries of the zinc ions in (I) (Table 1) and in the α polymorph [Zn—N = 1.975 (6) and 1.977 (5)Å; Zn—Cl = 2.236 (2) and 2.2565 (17)Å] are very similar. There are no significant differences in the geometries of the organic groups in the two structures. Slight differences arise in terms of the orientation of the guanidine 'arms' of the ligands. In (I), the dihedral angle between the mean planes of the C2/N2/N3/N3 and C4/N6/N7/N8 groupings is 27.7 (2)°. The equivalent value of 42.7 (5)° for the α polymorph shows that these two groupings are significantly more twisted in the triclinic polymorph (data calculated with *PLATON*; Spek, 2003).



(I)

As well as van der Waals forces, the molecules of (I) interact by way of N—H···N and N—H···Cl hydrogen bonds (Table 2) of varied lengths and strengths. The N—H···N bonds link the molecules into [100] stacks of dimers and the N—H···Cl bonds crosslink the [100] columns into a three-dimensional network (Fig. 2). Unfortunately, some of the H-atom positions in the α polymorph appear to be incorrect, so a detailed comparison of the hydrogen bonding in the two structures is not possible.

Other compounds with the stoichiometry $[M(C_2H_4N_4)_2X_2]$ (*M* = divalent metal cation and *X* = halide) include $[Cd(C_2H_4N_4)_2I_2]$ (Chiesi Villa *et al.*, 1974) and $[Cd(C_2H_4N_4)_2Br_2]$ (Pickardt & Kuhn, 1996). Neither of these shares a structure with the zinc compounds discussed here.

The iodide is molecular (space group *Pbcn*), whereas the bromide is polymeric, via Cd—(Br,Br)—Cd bridges.

Experimental

The following solutions were mixed at 293 K in a Petri dish, resulting in a colourless mixture: 10 ml of 0.1 *M* cyanoguanidine, 1 ml of 1 *M* $ZnCl_2$ and 1 ml of dilute HCl. Colourless rods and bars of (I) grew over the course of a few days as the water evaporated at 293 K.

Crystal data

$[CnCl_2(C_4H_8N_8)]$
M_r = 304.45
Monoclinic, $P2_1/c$
a = 4.9315 (3) Å
b = 14.6161 (10) Å
c = 15.5026 (11) Å
β = 93.928 (2)°
V = 1114.79 (13) Å^3
Z = 4
D_x = 1.814 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2094 reflections
θ = 2.6–26.8°
μ = 2.66 mm^{-1}
T = 293 (2) K
Bar, colourless
0.31 × 0.08 × 0.02 mm

Data collection

Bruker SMART1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.495, T_{max} = 0.950
7331 measured reflections
2444 independent reflections
1610 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 27.0°
$h = -6 \rightarrow 6$
$k = -18 \rightarrow 13$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.077
S = 0.91
2444 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	1.974 (3)	Zn1—Cl2	2.2302 (10)
Zn1—N5	1.984 (3)	Zn1—Cl1	2.2664 (10)
C1—N1—Zn1	166.5 (3)	C3—N5—Zn1	174.2 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H3···N6^{i}	0.86	2.46	3.082 (4)	130
N4—H4···N2^{ii}	0.86	2.31	3.156 (4)	168
N3—H1···Cl1^{iii}	0.86	2.57	3.365 (3)	155
N4—H3···Cl1^{iii}	0.86	2.77	3.520 (3)	147
N7—H5···Cl2^{iv}	0.86	2.47	3.282 (3)	158
N7—H6···Cl1^{v}	0.86	2.56	3.368 (3)	156
N8—H7···Cl2^{iv}	0.86	2.63	3.402 (3)	151
N8—H8···Cl1^{vi}	0.86	2.50	3.322 (3)	160

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $-x+3, -y, -z+1$; (iii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $x-1, y, z$; (vi) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

The H atoms were placed in idealized positions (N—H = 0.86Å) and refined as riding with the constraint $U_{iso}(H) = 1.2U_{eq}(N)$ applied.

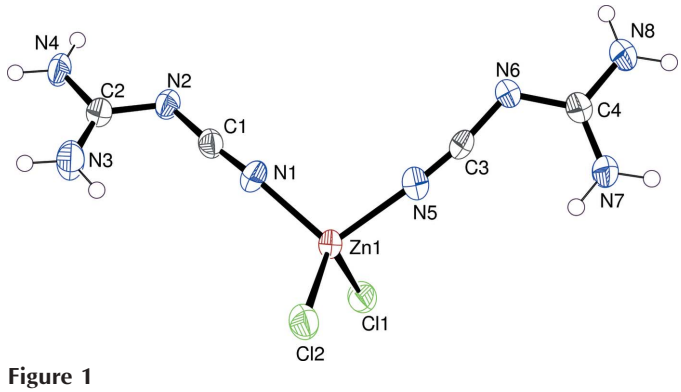


Figure 1
The molecular structure of (I), showing 50% displacement ellipsoids (H atoms are drawn as spheres of arbitrary radius).

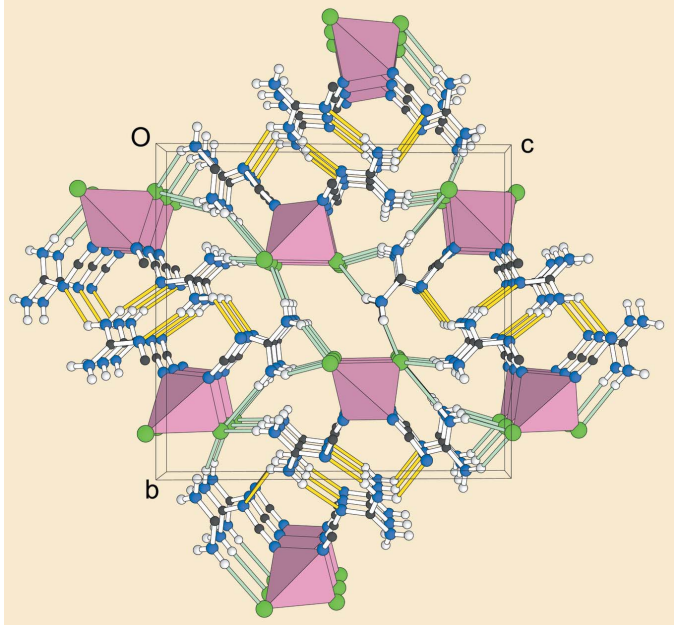


Figure 2
[100] projection of the packing in (I), with the ZnN_2Cl_2 groupings represented by polyhedra. Colour key: C black, H white, N blue, and Cl green. The H···N and H···Cl portions of the hydrogen bonds are highlighted in yellow and green, respectively.

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: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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