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Bis(2-aminopyrimidine-κN^1)dichloridozinc(II)

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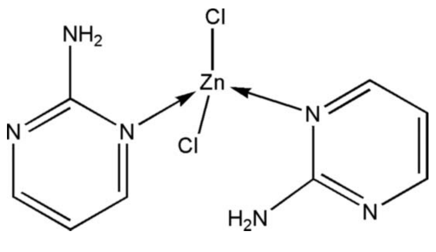
Key indicators: single-crystal X-ray study; T = 302 K; mean σ(C–C) = 0.008 Å; R factor = 0.065; wR factor = 0.174; data-to-parameter ratio = 16.4.

The title compound, $[ZnCl_2(C_4H_5N_3)_2]$, contains a four-coordinate Zn^{II} atom in an approximately tetrahedral environment. The Zn^{II} atom lies on a twofold rotation axis and is coordinated by two N atoms of two 2-aminopyrimidine ligands and by two Cl^- anions. N—H···N hydrogen bonds connect the complex molecules to form a one-dimensional supramolecular structure along the c axis. The supramolecular chains are parallel to each other and N—H···Cl hydrogen bonds link them into a two-dimensional network in the ac plane.

Related literature

For related literature, see: Arwaroli *et al.* (1997); Cookson & Tiekink (1993); Etter *et al.* (1990); Groen *et al.* (1998); Katritzky *et al.* (1984); Kennard *et al.* (1985); Lumme *et al.* (1996); Munno *et al.* (1998); Santra *et al.* (1999); Zanchini & Willett (1990).



Experimental

Crystal data

$[ZnCl_2(C_4H_5N_3)_2]$
M_r = 326.49
Monoclinic, $C2/c$
a = 10.744 (4) Å
b = 13.454 (5) Å
c = 8.806 (3) Å
β = 97.012 (6)°
V = 1263.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.35 mm^{-1}
T = 302 (2) K
0.28 × 0.18 × 0.16 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.512, T_{max} = 0.685
4933 measured reflections
1378 independent reflections
1140 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.174
S = 1.14
1378 reflections
84 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1	0.87 (2)	2.70 (5)	3.367 (5)	134 (5)
N1—H1B···N3^{i}	0.85 (2)	2.28 (4)	3.048 (6)	149 (6)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2016).

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supplementary materials

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Bis(2-aminopyrimidine-κN^1)dichloridozinc(II)

Z.-D. Lin and **W. Zeng**

Comment

Aminopyrimidine is an active component of antibiotics, antimicrobials, anticonvulsants, antispasmatics, antineoplastics and antidiabetogenics, and many derivatives have been used in seed dressings, crop-disease control and veterinary drugs *etc* (Cookson *et al.*, 1993, Katritzky *et al.*, 1984, Santra *et al.*, 1999). In coordination chemistry, the *meta*-related nitrogen in pyrimidine has played an important role in connecting different metal atoms, transmitting antiferromagnetic interactions and for obtaining magnetic systems of high nuclearity (Munno et la, 1998; Groen *et al.*, 1998). Because of the peripheral N heteroatom, the excited state of the pyrimidine moiety undergoes protonation in aqueous solution and the complexes exhibit proton-dependent photophysics and photochemistry. Recently, the design of molecular architecture with aminopyrimidine and bipyrimidine has aroused interest in the fields of coordination, bioinorganic and magnetochemistry (Arwaroli,1997). We report here a new bichlorobis(2-aminopyrimidine) zinc(II) complex(I), $(C_4H_5N_3)_2ZnCl_2$.

In the crystal structure of the title complex(I), the Zn^{II} atom lies on a twofold rotation axis, the asymmetric unit is composed of a Zn^{II} ion, two 2-aminopyrimidine ligands and two Cl anions. The molecular structure of (I) is shown in Fig. 1. The Zn^{II} ion is four-coordinated in an approximately tetrahedral environment by two N atoms[N2 and N2^{i}; symmetry code: (i) *x*- 1, *y*- 1, *z*] of two 2-aminopyrimidine ligands and two Cl anions [Cl1 and Cl1^{i}]. The bond distances and angles around the zinc atoms are quite normal. [Zn—N 2.056 (2)Å and Zn—Cl 2.249 (3) Å].

The 2-aminopyrimidine molecules are planar within experimental error (pyrimidine ring the greatest deviation C3 within 0.0119 (3) Å)) and the amino N atoms lie approximately in the corresponding molecular planes (N1 off of the pyrimidine ring plane within 0.0183 (3) Å). The bond distances and angles of the 2-aminopyrimidine ligand are similar to those found in other complexes (Kennard *et al.*, 1985; Etter *et al.*, 1990; Zanchini *et al.*, 1990;Lumme *et al.*, 1996).

A large number of N—H···N hydrogen bonds and N—H···Cl hydrogen bonds (Table 2) help to establish the crystal packing. The N—H···N hydrogen bonds bind the complex molecules to form a one-dimensional supramolecular structure along the *c* axis. The supramolecular chains are parallel to each other and the N—H···Cl hydrogen bonds link them into a two-dimensional network into the *ac* plane. There are only weaker van der Waals interactions in the *b* axis (Fig.2).

Experimental

A solution of $ZnCl_2$ (0.5 mmol) in ethanol (10 ml) and 2-aminopyrimidine (1.0 mmol) was stirred at room temperature for 12 h and then filtered. The filtrate was kept at room temperature in the dark for two weeks, affording white crystals of (I). The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous $CaCl_2$. Analysis calculated for $C_8N_6H_{10}$ Zn Cl_2: C 29.43, N 25.74, H 3.09%; found: C 29.11, N 25.34,H 3.22%.

Refinement

The H atoms bonded to the C atoms were placed in calculated positions, and were allowed to ride on their parent atoms, with a C—H distance of 0.93 Å for aromatic H atoms and U_{iso}(H) = 1.2 times of its parent atom. The H atom positions of the NH_2 group were obtained from a Fourier difference map and were refined with a restrained N—H distance of 0.86 (0.02) Å. The isotropic displacement parameters were set equal to $1.2U_{eq}$(parent atom). The highest and lowest residual density peaks are 0.94 Å and 0.77 Å respectively from the Zn atom.

Figures

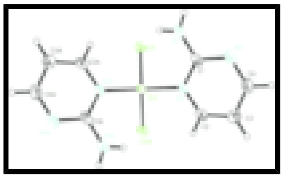

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes:(i) $-x$, y, $-z + 1/2$]

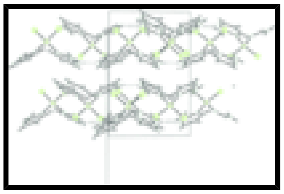

Fig. 2. Crystal packing of (I) viewing along the *a* axis. The N–H···N and N—H···Cl hydrogen bonding interactions are shown as dashed lines.

Bis(2-aminopyrimidine-κN^1)dichloridozinc(II)

Crystal data

$[ZnCl_2(C_4H_5N_3)_2]$

$M_r = 326.49$

Monoclinic, *C*2/*c*

Hall symbol: -C 2yc

$a = 10.744$ (4) Å

$b = 13.454$ (5) Å

$c = 8.806$ (3) Å

$\beta = 97.012$ (6)°

$V = 1263.4$ (8) $Å^3$

$Z = 4$

$F_{000} = 656$

$D_x = 1.716$ Mg m^{-3}

Mo *K*α radiation
$\lambda = 0.71073$ Å

Cell parameters from 2860 reflections

$\theta = 2.0–28.3°$

$\mu = 2.35$ mm^{-1}

$T = 302$ (2) K

Block, white

0.28 × 0.18 × 0.16 mm

Data collection

Siemens SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 302(2)$ K

1378 independent reflections

1140 reflections with $I > 2\sigma(I)$

$R_{int} = 0.045$

$\theta_{max} = 27.0°$

φ and ω scans	$\theta_{min} = 2.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -13 \rightarrow 12$
$T_{min} = 0.512$, $T_{max} = 0.685$	$k = -17 \rightarrow 17$
4933 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.065$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.174$	$w = 1/[\sigma^2(F_o^2) + (0.0993P)^2 + 1.9733P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} = 0.002$
1378 reflections	$\Delta\rho_{max} = 1.35$ e Å^{-3}
84 parameters	$\Delta\rho_{min} = -0.66$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.0000	0.24505 (6)	0.2500	0.0411 (3)
C1	0.0696 (5)	0.3725 (4)	−0.0120 (5)	0.0419 (11)
C2	0.2323 (5)	0.3378 (4)	0.1742 (6)	0.0494 (13)
H2	0.2627	0.3089	0.2673	0.059*
C3	0.3158 (6)	0.3857 (5)	0.0918 (7)	0.0586 (15)
H3	0.4001	0.3929	0.1291	0.070*
C4	0.2666 (5)	0.4222 (4)	−0.0492 (6)	0.0521 (13)
H4	0.3210	0.4522	−0.1099	0.063*
Cl1	−0.12680 (12)	0.15173 (10)	0.08506 (13)	0.0479 (4)
N1	−0.0526 (4)	0.3712 (4)	−0.0641 (5)	0.0553 (12)
H1A	−0.108 (5)	0.340 (4)	−0.018 (7)	0.066*

H1B	−0.088 (5)	0.404 (4)	−0.140 (5)	0.066*
N2	0.1090 (4)	0.3313 (3)	0.1258 (4)	0.0403 (9)
N3	0.1469 (4)	0.4169 (3)	−0.1027 (5)	0.0491 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0449 (5)	0.0541 (6)	0.0248 (4)	0.000	0.0067 (3)	0.000
C1	0.056 (3)	0.047 (3)	0.025 (2)	0.001 (2)	0.0112 (19)	−0.0044 (17)
C2	0.052 (3)	0.065 (3)	0.030 (2)	−0.005 (2)	0.002 (2)	−0.003 (2)
C3	0.052 (3)	0.077 (4)	0.047 (3)	−0.020 (3)	0.003 (2)	−0.003 (3)
C4	0.058 (3)	0.057 (3)	0.044 (3)	−0.013 (2)	0.020 (2)	−0.006 (2)
Cl1	0.0497 (8)	0.0568 (8)	0.0362 (6)	−0.0088 (5)	0.0012 (5)	−0.0068 (5)
N1	0.047 (3)	0.083 (4)	0.037 (2)	0.005 (2)	0.0075 (19)	0.013 (2)
N2	0.046 (2)	0.052 (2)	0.0238 (18)	−0.0043 (18)	0.0078 (15)	−0.0017 (15)
N3	0.062 (3)	0.057 (3)	0.030 (2)	−0.007 (2)	0.0117 (19)	−0.0010 (17)

Geometric parameters (Å, °)

Zn1—N2	2.056 (4)	C2—C3	1.380 (8)
Zn1—N2^{i}	2.056 (4)	C2—H2	0.9300
Zn1—Cl1	2.2492 (13)	C3—C4	1.380 (8)
Zn1—Cl1^{i}	2.2492 (13)	C3—H3	0.9300
C1—N1	1.337 (7)	C4—N3	1.316 (7)
C1—N2	1.355 (6)	C4—H4	0.9300
C1—N3	1.358 (6)	N1—H1A	0.87 (2)
C2—N2	1.344 (6)	N1—H1B	0.85 (2)
N2—Zn1—N2^{i}	111.3 (2)	C4—C3—H3	122.0
N2—Zn1—Cl1	108.13 (11)	C2—C3—H3	122.0
N2^{i}—Zn1—Cl1	108.59 (12)	N3—C4—C3	123.5 (5)
N2—Zn1—Cl1^{i}	108.59 (12)	N3—C4—H4	118.2
N2^{i}—Zn1—Cl1^{i}	108.13 (11)	C3—C4—H4	118.2
Cl1—Zn1—Cl1^{i}	112.13 (8)	C1—N1—H1A	123 (4)
N1—C1—N2	119.2 (4)	C1—N1—H1B	126 (4)
N1—C1—N3	116.7 (4)	H1A—N1—H1B	111 (6)
N2—C1—N3	124.0 (5)	C2—N2—C1	116.5 (4)
N2—C2—C3	122.9 (5)	C2—N2—Zn1	118.2 (3)
N2—C2—H2	118.6	C1—N2—Zn1	124.8 (3)
C3—C2—H2	118.6	C4—N3—C1	117.1 (4)
C4—C3—C2	115.9 (5)		
N2—C2—C3—C4	−3.6 (8)	Cl1—Zn1—N2—C2	−134.8 (3)
C2—C3—C4—N3	2.9 (9)	Cl1^{i}—Zn1—N2—C2	−12.9 (4)
C3—C2—N2—C1	1.5 (8)	N2^{i}—Zn1—N2—C1	−82.6 (4)
C3—C2—N2—Zn1	173.6 (4)	Cl1—Zn1—N2—C1	36.6 (4)
N1—C1—N2—C2	−177.9 (5)	Cl1^{i}—Zn1—N2—C1	158.5 (4)
N3—C1—N2—C2	1.6 (7)	C3—C4—N3—C1	−0.1 (8)

N1—C1—N2—Zn1	10.6 (7)	N1—C1—N3—C4	177.2 (5)
N3—C1—N2—Zn1	−169.9 (4)	N2—C1—N3—C4	−2.3 (7)
N2^{i}—Zn1—N2—C2	106.0 (4)		

Symmetry codes: (i) −x, y, −z+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···Cl1	0.87 (2)	2.70 (5)	3.367 (5)	134 (5)
N1—H1B···N3^{ii}	0.85 (2)	2.28 (4)	3.048 (6)	149 (6)

Symmetry codes: (ii) −x, y, −z−1/2.

Fig. 1

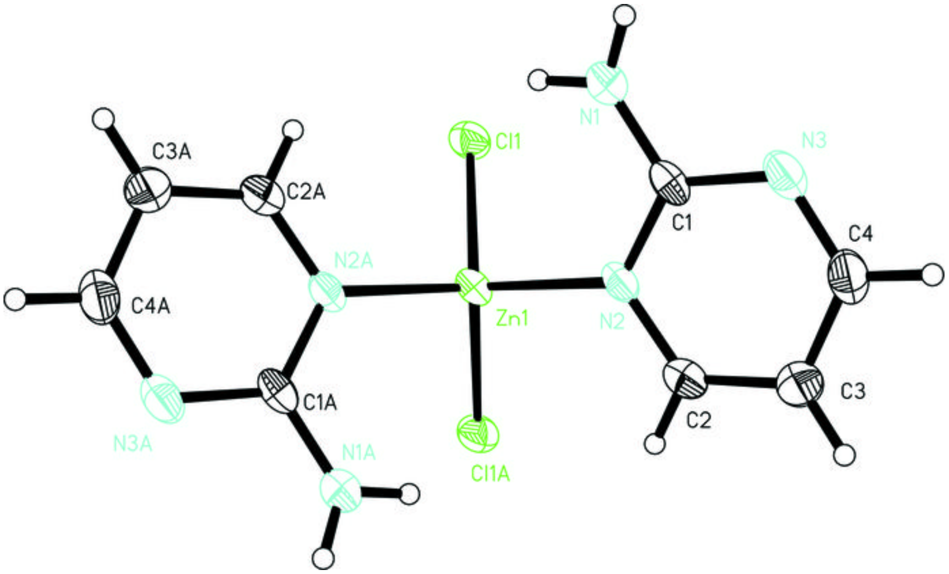

Fig. 2