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Bis(2-aminopyrazine-κN^4)dichloridozinc

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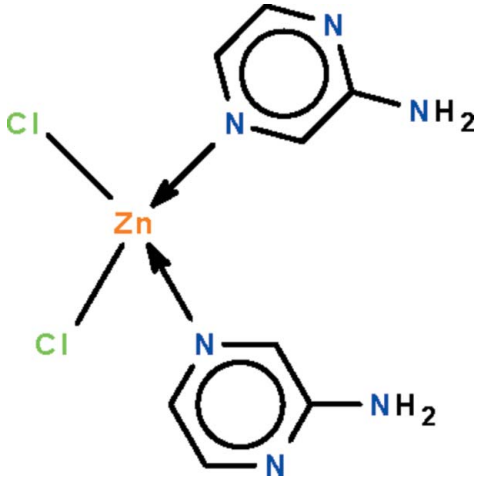
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.066; data-to-parameter ratio = 17.0.

In the title adduct, $[ZnCl_2(C_4H_5N_3)_2]$, the Zn^{II} atom lies on a twofold rotation axis that relates one Cl atom to the other as well as one 2-aminopyrazine ligand to the other; the coordination geometry is a distorted tetrahedron. In the crystal, adjacent molecules are linked by N—H···N hydrogen bonds across the center of inversion, generating a chain; neighboring chains are linked by N—H···Cl hydrogen bonds, forming a three-dimensional network.

Related literature

For a related compound, $CoCl_2(C_4H_5N_3)_4$, see: Kang *et al.* (2009).



Experimental

Crystal data

$[ZnCl_2(C_4H_5N_3)_2]$
M_r = 326.49
Monoclinic, $C2/c$
a = 17.1445 (12) Å
b = 6.1660 (4) Å
c = 12.0198 (8) Å
β = 98.608 (2)°
V = 1256.34 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.37 mm^{-1}
T = 293 K
0.35 × 0.30 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.491, T_{max} = 0.718
5769 measured reflections
1432 independent reflections
1350 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.066
S = 1.06
1432 reflections
84 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N3	2.0576 (12)	Zn1—Cl1	2.2403 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.87 (1)	2.27 (1)	3.141 (2)	176 (3)
N1—H2···Cl1^{ii}	0.87 (1)	2.63 (2)	3.392 (2)	147 (2)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5256).

References

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supplementary materials

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Bis(2-aminopyrazine-κN^4)dichloridozinc

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Comment

We have reported the metal(II) dichloride adducts of 2-aminopyrazine. For example, cobalt(II) dichloride forms a tetrakis adduct (Kang *et al.*, 2009). The corresponding zinc(II) dichloride is a bis adduct; in the adduct, $ZnCl_2(C_4H_5N_3)_2$ (Scheme I, Fig. 1), the Zn^{II} atom lies on a twofold axis and the geometry is a tetrahedron. Adjacent adduct molecules are linked by an N–H···N hydrogen across a center-of-inversion to generate a chain; neighboring chains are linked by an N–H···Cl hydrogen bond to form a layer (Table 1).

Experimental

Zinc dichloride hexahydrate (2 mmol) and 2-aminopyrazine (2 mmol) were dissolved in water (20 ml); the solution was filtered. Colorless crystals separated from solution after several days.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The amino H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N–H 0.88±0.01 Å; their temperature factors were refined.

Figures

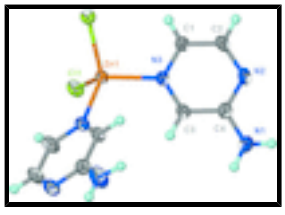

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $ZnCl_2(C_4H_5N_3)_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The Zn atom lies on a twofold axis and the unlabeled atoms are related to the labeled ones by 1 - *x*, *y*, 1/2 - *z*.

Bis(2-aminopyrazine-κN^4)dichloridozinc

Crystal data

$[ZnCl_2(C_4H_5N_3)_2]$	$F(000) = 656$
$M_r = 326.49$	$D_x = 1.726$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 5413 reflections
a = 17.1445 (12) Å	θ = 3.4–27.5°
b = 6.1660 (4) Å	μ = 2.37 mm^{-1}

c = 12.0198 (8) Å	T = 293 K
β = 98.608 (2)°	Prism, colorless
V = 1256.34 (15) Å^3	0.35 × 0.30 × 0.15 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	1432 independent reflections
Radiation source: fine-focus sealed tube	1350 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.029
ω scans	θ_{max} = 27.5°, θ_{min} = 3.4°
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	h = −22→22
T_{min} = 0.491, T_{max} = 0.718	k = −7→7
5769 measured reflections	l = −15→15

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.024	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.066	H atoms treated by a mixture of independent and constrained refinement
S = 1.06	$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.3611P]$ where $P = (F_o^2 + 2F_c^2)/3$
1432 reflections	$(\Delta/\sigma)_{max}$ = 0.001
84 parameters	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
2 restraints	$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.5000	0.04567 (4)	0.2500	0.03073 (11)
Cl1	0.44416 (2)	−0.15067 (7)	0.37370 (3)	0.04100 (13)
N1	0.63303 (10)	0.7312 (3)	0.48482 (17)	0.0590 (5)
H1	0.6731 (12)	0.808 (4)	0.516 (2)	0.088*
H2	0.5858 (9)	0.779 (5)	0.486 (2)	0.088*
N2	0.71831 (9)	0.4959 (3)	0.41464 (14)	0.0431 (3)
N3	0.59049 (7)	0.2453 (2)	0.31966 (11)	0.0330 (3)
C1	0.66520 (10)	0.1889 (3)	0.30962 (16)	0.0439 (4)
H1A	0.6746	0.0646	0.2698	0.053*
C2	0.72731 (10)	0.3139 (3)	0.35775 (17)	0.0456 (4)
H2A	0.7782	0.2698	0.3504	0.055*
C3	0.57962 (10)	0.4231 (3)	0.37660 (14)	0.0352 (3)
H3	0.5287	0.4646	0.3850	0.042*

C4	0.64450 (10)	0.5519 (2)	0.42521 (15)	0.0380 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02308 (15)	0.02663 (16)	0.04198 (17)	0.000	0.00323 (10)	0.000
Cl1	0.0322 (2)	0.0426 (2)	0.0489 (2)	0.00146 (16)	0.00822 (16)	0.01054 (17)
N1	0.0411 (9)	0.0467 (9)	0.0853 (12)	−0.0010 (8)	−0.0031 (8)	−0.0283 (9)
N2	0.0292 (7)	0.0403 (7)	0.0577 (9)	−0.0066 (6)	−0.0007 (6)	−0.0060 (7)
N3	0.0265 (6)	0.0298 (6)	0.0422 (6)	−0.0028 (5)	0.0035 (5)	−0.0027 (5)
C1	0.0301 (8)	0.0404 (9)	0.0617 (10)	−0.0027 (7)	0.0086 (7)	−0.0139 (8)
C2	0.0257 (8)	0.0477 (9)	0.0636 (11)	−0.0030 (7)	0.0070 (7)	−0.0081 (8)
C3	0.0261 (8)	0.0330 (7)	0.0460 (8)	0.0003 (6)	0.0034 (6)	−0.0016 (6)
C4	0.0350 (9)	0.0320 (8)	0.0450 (9)	−0.0022 (6)	−0.0008 (7)	−0.0023 (6)

Geometric parameters (Å, °)

Zn1—N3	2.0576 (12)	N2—C4	1.336 (2)
Zn1—N3^{i}	2.0576 (12)	N3—C3	1.320 (2)
Zn1—Cl1	2.2403 (4)	N3—C1	1.350 (2)
Zn1—Cl1^{i}	2.2403 (4)	C1—C2	1.371 (2)
N1—C4	1.348 (2)	C1—H1A	0.9300
N1—H1	0.87 (1)	C2—H2A	0.9300
N1—H2	0.87 (1)	C3—C4	1.419 (2)
N2—C2	1.335 (2)	C3—H3	0.9300
N3—Zn1—N3^{i}	106.52 (7)	N3—C1—C2	120.33 (16)
N3—Zn1—Cl1	115.10 (4)	N3—C1—H1A	119.8
N3^{i}—Zn1—Cl1	102.85 (4)	C2—C1—H1A	119.8
N3—Zn1—Cl1^{i}	102.85 (4)	N2—C2—C1	123.16 (17)
N3^{i}—Zn1—Cl1^{i}	115.10 (4)	N2—C2—H2A	118.4
Cl1—Zn1—Cl1^{i}	114.58 (2)	C1—C2—H2A	118.4
C4—N1—H1	120.5 (19)	N3—C3—C4	121.01 (15)
C4—N1—H2	120 (2)	N3—C3—H3	119.5
H1—N1—H2	119 (3)	C4—C3—H3	119.5
C2—N2—C4	116.72 (15)	N2—C4—N1	118.57 (16)
C3—N3—C1	118.01 (14)	N2—C4—C3	120.76 (15)
C3—N3—Zn1	123.46 (11)	N1—C4—C3	120.67 (17)
C1—N3—Zn1	118.50 (10)		
N3^{i}—Zn1—N3—C3	41.52 (11)	C4—N2—C2—C1	1.2 (3)
Cl1—Zn1—N3—C3	−71.75 (13)	N3—C1—C2—N2	−1.0 (3)
Cl1^{i}—Zn1—N3—C3	162.95 (12)	C1—N3—C3—C4	0.4 (2)
N3^{i}—Zn1—N3—C1	−140.45 (14)	Zn1—N3—C3—C4	178.43 (12)
Cl1—Zn1—N3—C1	106.28 (13)	C2—N2—C4—N1	178.12 (19)
Cl1^{i}—Zn1—N3—C1	−19.02 (13)	C2—N2—C4—C3	−0.7 (3)
C3—N3—C1—C2	0.1 (3)	N3—C3—C4—N2	−0.1 (3)
Zn1—N3—C1—C2	−178.02 (15)	N3—C3—C4—N1	−178.88 (17)

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{ii}	0.87 (1)	2.27 (1)	3.141 (2)	176 (3)
N1—H2···Cl1^{iii}	0.87 (1)	2.63 (2)	3.392 (2)	147 (2)

Symmetry codes: (ii) −*x*+3/2, −*y*+3/2, −*z*+1; (iii) *x*, *y*+1, *z*.

Fig. 1