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Dichloridobis(pyrazine-2-carboxamide-κN^4)zinc(II)

Sadif A. Shirvan* and Sara Haydari Dezfuli

Department of Chemistry, Omidieh Branch, Islamic Azad University, Omidieh, Iran
Correspondence e-mail: sadif.shirvan1@gmail.com

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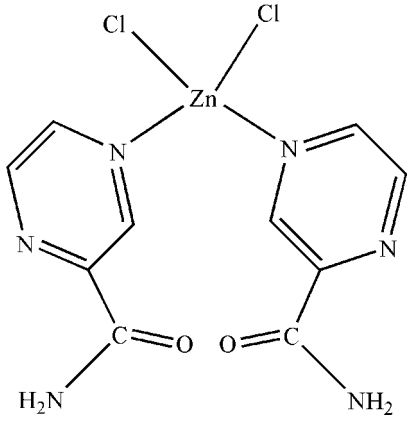
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.093; data-to-parameter ratio = 14.4.

In the crystal of the title compound, $[ZnCl_2(C_5H_5N_3O)_2]$, the molecule has m symmetry, with the Zn^{II} cation and Cl^- anions located on the mirror plane. The Zn^{II} cation is coordinated by two Cl^- anions and two pyrazine-2-carboxamide ligands in a distorted $ZnCl_2N_2$ tetrahedral geometry. The two pyrazine rings are nearly perpendicular to each other [dihedral angle = 86.61 (10)°]. Intermolecular N—H···O and N—H···N hydrogen bonds and weak C—H···O interactions stabilize the crystal packing.

Related literature

For related structures, see: Abu-Youssef *et al.* (2006); Azhdari Tehrani *et al.* (2010); Goher & Mautner (2000); Kristiansson (2002); Mir Mohammad Sadegh *et al.* (2010); Munakata *et al.* (1997); Pacigova *et al.* (2008).



Experimental

Crystal data

$[ZnCl_2(C_5H_5N_3O)_2]$
M_r = 382.53
Monoclinic, $P2_1/m$
a = 5.4296 (5) Å
b = 19.7629 (14) Å
c = 6.8396 (5) Å
β = 105.131 (7)°
V = 708.48 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.12 mm^{-1}
T = 298 K
0.40 × 0.06 × 0.05 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.881, T_{max} = 0.902
5777 measured reflections
1441 independent reflections
1064 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.093
S = 0.97
1441 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.085 (3)	Zn1—Cl2	2.1888 (16)
Zn1—Cl1	2.1945 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O1^{i}	0.86	2.02	2.875 (5)	175
N3—H3C···N2^{ii}	0.86	2.61	3.205 (5)	128
C3—H3···O1^{iii}	0.93	2.44	3.357 (5)	170

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x+1, y, z+1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the Islamic Azad University, Omidieh Branch for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5500).

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supporting information

Acta Cryst. (2012). E**68**, m546 [doi:10.1107/S1600536812013888]

Dichloridobis(pyrazine-2-carboxamide-κN^4)zinc(II)

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S1. Comment

Pyrazine-2-carboxamide (pzc), is a good ligand, and a few complexes with pzc have been prepared, such as that of mercury (Azhdari Tehrani *et al.*, 2010; Mir Mohammad Sadegh *et al.*, 2010), vanadium (Pacigova *et al.*, 2008), manganese (Abu-Youssef *et al.*, 2006) and copper (Kristiansson, 2002; Munakata *et al.*, 1997; Goher & Mautner, 2000). Here, we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound, (Fig. 1), contains one Zn^{II} atom, two Cl atoms and one pyrazine-2-carboxamide ligand. The Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from two pyrazine-2-carboxamide ligands and two terminal Cl atoms. The Zn—Cl and Zn—N bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular N—H···O, N—H···N and C—H···O hydrogen bonds (Table 2, Fig. 2) may stabilize the structure.

S2. Experimental

A solution of pyrazine-2-carboxamide (0.25 g, 2.0 mmol) in methanol (10 ml) was added to a solution of $ZnCl_2$ (0.13 g, 1.0 mmol) in methanol (10 ml) and the resulting colorless solution was stirred for 15 min at room temperature. This solution was left to evaporate slowly at room temperature. After one week, colorless plate crystals of the title compound were isolated (yield 0.30 g, 78.4%).

S3. Refinement

All H atoms were positioned geometrically, with C—H = 0.93 and N—H = 0.86 Å, and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

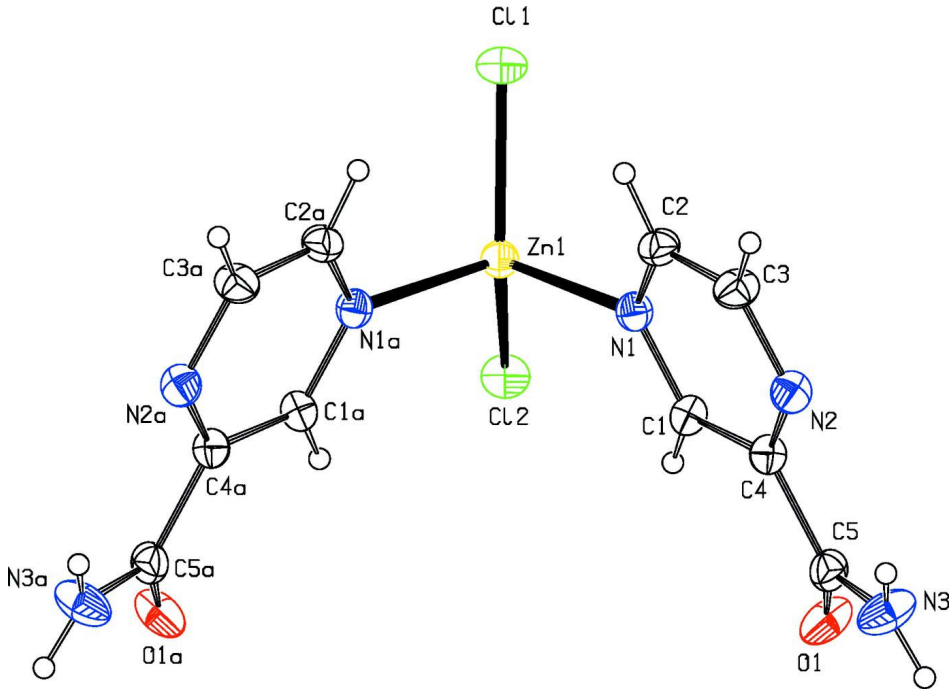

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (*a*) *x*,1/2 - *y*,*z*].

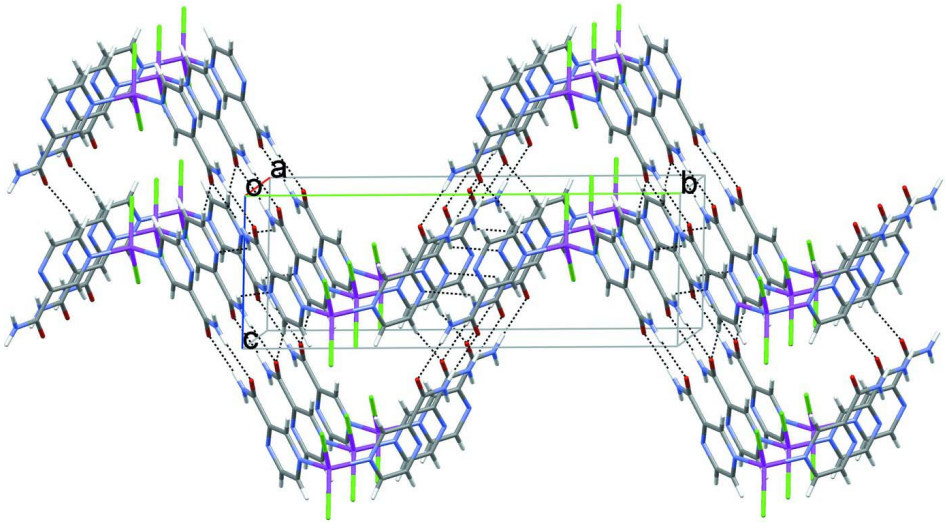

Figure 2

Unit-cell packing diagram for title molecule. Hydrogen bonds are shown as dashed lines

Dichloridobis(pyrazine-2-carboxamide-κN^4)zinc(II)

Crystal data

$[ZnCl_2(C_5H_5N_3O)_2]$
M_r = 382.53
Monoclinic, $P2_1/m$

Hall symbol: -P 2yb
a = 5.4296 (5) Å
b = 19.7629 (14) Å

c = 6.8396 (5) Å
β = 105.131 (7)°
V = 708.48 (10) Å^3
Z = 2
F(000) = 384
D_x = 1.793 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 5777 reflections
θ = 2.1–26.0°
μ = 2.12 mm^{-1}
T = 298 K
Plate, colorless
0.40 × 0.06 × 0.05 mm

Data collection

Bruker APEXII CCD area-detector′ diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.881, T_{max} = 0.902

5777 measured reflections
1441 independent reflections
1064 reflections with $I > 2\sigma(I)$
R_{int} = 0.085
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −6→6
k = −21→24
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.093
S = 0.97
1441 reflections
100 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
C1	0.3963 (7)	0.3616 (2)	0.4810 (6)	0.0307 (9)
H1	0.2583	0.3512	0.3724	0.037*
C2	0.6226 (8)	0.3464 (2)	0.8085 (6)	0.0364 (10)
H2	0.6435	0.3262	0.9347	0.044*
C3	0.8016 (8)	0.3930 (2)	0.7802 (6)	0.0391 (10)
H3	0.9428	0.4022	0.8873	0.047*
C4	0.5722 (7)	0.4094 (2)	0.4563 (6)	0.0310 (8)
C5	0.5370 (8)	0.4445 (2)	0.2579 (6)	0.0366 (9)
N1	0.4213 (6)	0.33021 (16)	0.6574 (5)	0.0312 (7)
N2	0.7776 (6)	0.42473 (18)	0.6048 (5)	0.0366 (8)

N3	0.7336 (7)	0.4801 (2)	0.2331 (6)	0.0535 (11)
H3B	0.7210	0.5022	0.1226	0.064*
H3C	0.8736	0.4812	0.3276	0.064*
O1	0.3309 (6)	0.44069 (17)	0.1293 (4)	0.0506 (8)
Zn1	0.18582 (12)	0.2500	0.69002 (10)	0.0304 (2)
Cl1	0.1855 (3)	0.2500	1.0108 (2)	0.0480 (4)
Cl2	−0.1427 (3)	0.2500	0.4244 (2)	0.0416 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0264 (19)	0.030 (2)	0.034 (2)	−0.0008 (16)	0.0050 (17)	0.0030 (17)
C2	0.040 (2)	0.038 (2)	0.028 (2)	−0.0004 (18)	0.0041 (18)	0.0030 (18)
C3	0.036 (2)	0.046 (3)	0.030 (2)	−0.0092 (19)	−0.0004 (18)	0.0013 (19)
C4	0.0278 (19)	0.030 (2)	0.034 (2)	−0.0010 (16)	0.0063 (16)	−0.0002 (17)
C5	0.041 (2)	0.031 (2)	0.036 (2)	−0.0065 (18)	0.0050 (19)	0.0002 (18)
N1	0.0300 (16)	0.0295 (18)	0.0341 (19)	−0.0027 (14)	0.0081 (14)	−0.0011 (14)
N2	0.0325 (18)	0.037 (2)	0.037 (2)	−0.0053 (14)	0.0032 (15)	−0.0011 (15)
N3	0.041 (2)	0.073 (3)	0.042 (2)	−0.0229 (19)	0.0026 (17)	0.017 (2)
O1	0.0432 (17)	0.058 (2)	0.0413 (18)	−0.0198 (15)	−0.0053 (15)	0.0173 (16)
Zn1	0.0290 (3)	0.0313 (4)	0.0329 (4)	0.000	0.0114 (3)	0.000
Cl1	0.0570 (10)	0.0575 (11)	0.0328 (8)	0.000	0.0174 (7)	0.000
Cl2	0.0303 (7)	0.0525 (10)	0.0408 (8)	0.000	0.0069 (6)	0.000

Geometric parameters (Å, º)

C1—N1	1.332 (5)	C5—O1	1.232 (5)
C1—C4	1.384 (5)	C5—N3	1.326 (5)
C1—H1	0.9300	N1—Zn1	2.085 (3)
C2—N1	1.333 (5)	N3—H3B	0.8600
C2—C3	1.388 (6)	N3—H3C	0.8600
C2—H2	0.9300	Zn1—N1	2.085 (3)
C3—N2	1.330 (5)	Zn1—N1^{i}	2.085 (3)
C3—H3	0.9300	Zn1—Cl1	2.1945 (16)
C4—N2	1.333 (5)	Zn1—Cl2	2.1888 (16)
C4—C5	1.491 (6)		
N1—C1—C4	121.2 (4)	N3—C5—C4	116.6 (4)
N1—C1—H1	119.4	C1—N1—C2	117.4 (3)
C4—C1—H1	119.4	C1—N1—Zn1	122.1 (3)
N1—C2—C3	120.9 (4)	C2—N1—Zn1	120.1 (3)
N1—C2—H2	119.6	C3—N2—C4	116.4 (3)
C3—C2—H2	119.6	C5—N3—H3B	120.0
N2—C3—C2	122.1 (4)	C5—N3—H3C	120.0
N2—C3—H3	118.9	H3B—N3—H3C	120.0
C2—C3—H3	118.9	N1—Zn1—N1^{i}	99.00 (18)
N2—C4—C1	121.9 (4)	N1—Zn1—Cl2	107.51 (10)
N2—C4—C5	118.1 (3)	N1^{i}—Zn1—Cl2	107.51 (10)

C1—C4—C5	120.0 (3)	N1—Zn1—Cl1	105.53 (9)
O1—C5—N3	123.5 (4)	N1^{i}—Zn1—Cl1	105.53 (9)
O1—C5—C4	119.9 (4)	Cl2—Zn1—Cl1	128.07 (6)
N1—C2—C3—N2	1.9 (7)	C3—C2—N1—Zn1	170.7 (3)
N1—C1—C4—N2	2.1 (6)	C2—C3—N2—C4	−0.2 (6)
N1—C1—C4—C5	−179.0 (4)	C1—C4—N2—C3	−1.7 (6)
N2—C4—C5—O1	−167.5 (4)	C5—C4—N2—C3	179.4 (4)
C1—C4—C5—O1	13.5 (6)	C1—N1—Zn1—N1^{i}	96.5 (3)
N2—C4—C5—N3	10.8 (6)	C2—N1—Zn1—N1^{i}	−75.5 (3)
C1—C4—C5—N3	−168.2 (4)	C1—N1—Zn1—Cl2	−15.2 (3)
C4—C1—N1—C2	−0.3 (6)	C2—N1—Zn1—Cl2	172.9 (3)
C4—C1—N1—Zn1	−172.5 (3)	C1—N1—Zn1—Cl1	−154.6 (3)
C3—C2—N1—C1	−1.5 (6)	C2—N1—Zn1—Cl1	33.5 (3)

Symmetry code: (i) x, $-y+1/2$, z.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*B*···O1^{ii}	0.86	2.02	2.875 (5)	175
N3—H3*C*···N2^{iii}	0.86	2.61	3.205 (5)	128
C3—H3···O1^{iv}	0.93	2.44	3.357 (5)	170

Symmetry codes: (ii) $-x+1$, $-y+1$, $-z$; (iii) $-x+2$, $-y+1$, $-z+1$; (iv) $x+1$, y, $z+1$.