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Dichloridobis(4-pyridylmethyl 1*H*-pyrrole-2-carboxylate-κ*N*)zinc

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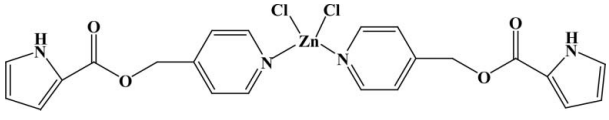
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.069; data-to-parameter ratio = 14.0.

In the title molecule, $[ZnCl_2(C_{11}H_{10}N_2O_2)_2]$, the Zn^{II} ion, situated on a twofold axis, is in a distorted tetrahedral coordination environment formed by two chloride anions and two pyridine N atoms of the two organic ligands. In the pyrrole-2-carboxylate unit, the pyrrole N—H group and the carbonyl group point approximately in the same direction. The dihedral angle between the two pyridine rings is 54.8 (3)°. The complex molecules are connected into chains extending along [101] by N—H···Cl hydrogen bonds. The chains are further assembled into ($\bar{1}$01) layers by C—H···O and C—H···Cl interactions.

Related literature

For the hydrogen-bonded assemblies of pyrrole-based structures, see: Wang & Yin (2007); Yin & Li (2006); Cui *et al.* (2009).



Experimental

Crystal data

$[ZnCl_2(C_{11}H_{10}N_2O_2)_2]$
M_r = 540.69
Monoclinic, $C2/c$
a = 27.604 (14) Å
b = 6.205 (3) Å
c = 16.087 (8) Å
β = 120.309 (6)°
V = 2379 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 296 K
0.26 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.727, T_{max} = 1.000
6100 measured reflections
2098 independent reflections
1823 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.069
S = 1.06
2098 reflections
150 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Cl1^{i}	0.86	2.57	3.306 (3)	144
C3—H3···Cl1^{ii}	0.93	2.75	3.495 (3)	138
C4—H4···O1^{iii}	0.93	2.54	3.354 (3)	146

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $x, y+1, z$; (iii) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2445).

References

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supplementary materials

Acta Cryst. (2012). E**68**, m323 [doi:10.1107/S1600536812001353]

Dichloridobis(4-pyridylmethyl 1*H*-pyrrole-2-carboxylate-κ*N*)zinc

Can Li, Guilong Zhang and Zhenming Yin

Comment

In our earlier works, we have reported the hydrogen-bonded assemblies of 4-pyridylmethyl 1*H*-pyrrole-2-carboxylate (Wang & Yin, 2007) and some other pyrrole-based compounds (Yin & Li, 2006; Cui *et al.* 2009) in the solid state. Combination of coordination bonding and hydrogen bonding is an effective strategy for the generation of supramolecular networks. Continuing our study, herein we report the crystal structure of the complex obtained with 4-pyridylmethyl-1*H*-pyrrole-2-carboxylate and $ZnCl_2$.

A perspective view of the title compound with atomic labeling is shown in Fig. 1. The complex consists of one $ZnCl_2$ and two ligand molecules, in which both the pyrrole-2-carboxylate moieties adopted *syn* conformation with the carbonyl group arranged in the same direction as the adjacent pyrrole N—H group. In the complex, the dihedral angle between the two pyridine rings is 54.8 (3)°. The complex molecules assemble into layer structrue through N—H···Cl, C—H···O and C—H···Cl hydrogen bonds (Fig. 2).

Experimental

The methanol solution of $ZnCl_2$ (0.1 M, 5 mL) was layered on $CHCl_3$ solution of 4-pyridylmethyl 1*H*-pyrrole-2-carboxylate (0.1 M, 10 mL) and then evaporated to give colorless crystals of the title compound in about 70% yield.

Refinement

All H atoms were placed in calculated positions (C—H = 0.93 -0.97 Å; N-H = 0.86 Å) and refined as riding on their carrier atoms with U_{iso}(H) = 1.2 U_{eq}(C, N).

Computing details

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

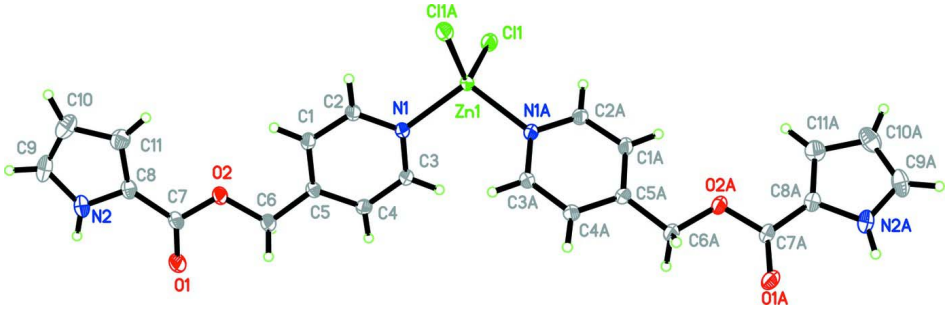

Figure 1

The molecular structure of the title compound with displacement ellipsoids shown at the 30% probability level. The atom with the ′A′ label were generated by the symmetry operation -x,y,1/2-z.

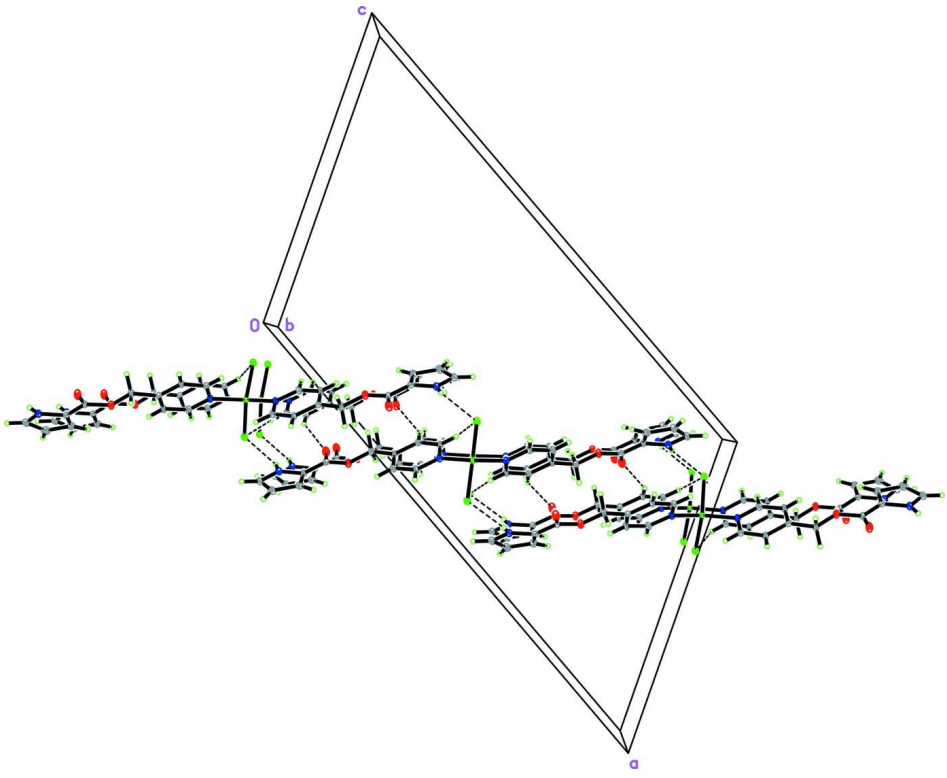

Figure 2

The layer of the title molecules assembled by intermolecular hydrogen bonds (hydrogen bonds are shown as dashed lines).

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Crystal data

$[ZnCl_2(C_{11}H_{10}N_2O_2)_2]$
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a = 27.604 (14) Å
b = 6.205 (3) Å
c = 16.087 (8) Å
β = 120.309 (6)°
V = 2379 (2) Å^3
Z = 4
F(000) = 1104
D_x = 1.510 Mg m^{-3}
Melting point: 438 K
Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 2747 reflections
θ = 2.5–26.8°
μ = 1.29 mm^{-1}
T = 296 K
Block, colourless
0.26 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.727, T_{max} = 1.000
6100 measured reflections
2098 independent reflections
1823 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −32→32
k = −7→5
l = −17→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.069
S = 1.06
2098 reflections
150 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
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.3857P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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}
Zn1	0.0000	0.41749 (4)	0.2500	0.03878 (12)
Cl1	0.01743 (2)	0.23365 (8)	0.14847 (3)	0.05019 (15)
O1	0.30330 (6)	1.1722 (3)	0.65205 (11)	0.0654 (4)
O2	0.24547 (5)	0.8880 (2)	0.60656 (9)	0.0495 (3)
N1	0.06598 (6)	0.6110 (2)	0.33725 (10)	0.0395 (3)
N2	0.37959 (7)	0.9421 (3)	0.81985 (12)	0.0555 (5)
H2	0.3931	1.0663	0.8187	0.067*
C1	0.15031 (8)	0.6615 (3)	0.48714 (13)	0.0481 (5)
H1	0.1754	0.6095	0.5483	0.058*
C2	0.10377 (8)	0.5440 (3)	0.42633 (14)	0.0470 (5)
H2A	0.0980	0.4122	0.4475	0.056*
C3	0.07520 (7)	0.8013 (3)	0.30828 (13)	0.0405 (4)
H3	0.0494	0.8502	0.2469	0.049*
C4	0.12083 (8)	0.9263 (3)	0.36502 (14)	0.0427 (4)

H4	0.1258	1.0569	0.3420	0.051*
C5	0.15987 (7)	0.8576 (3)	0.45746 (13)	0.0394 (4)
C6	0.20924 (8)	0.9974 (3)	0.51816 (14)	0.0501 (5)
H6A	0.2293	1.0285	0.4844	0.060*
H6B	0.1968	1.1328	0.5313	0.060*
C7	0.29241 (8)	0.9944 (4)	0.66858 (13)	0.0444 (4)
C8	0.32739 (8)	0.8683 (3)	0.75342 (13)	0.0460 (4)
C9	0.40637 (10)	0.7894 (5)	0.88712 (16)	0.0712 (7)
H9	0.4427	0.7994	0.9392	0.085*
C10	0.37168 (12)	0.6193 (5)	0.86637 (18)	0.0767 (8)
H10	0.3796	0.4930	0.9020	0.092*
C11	0.32176 (10)	0.6672 (4)	0.78171 (16)	0.0607 (5)
H11	0.2904	0.5784	0.7504	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03178 (17)	0.03411 (18)	0.03693 (18)	0.000	0.00734 (13)	0.000
Cl1	0.0473 (3)	0.0494 (3)	0.0450 (3)	0.0092 (2)	0.0167 (2)	−0.0014 (2)
O1	0.0573 (9)	0.0543 (9)	0.0588 (9)	−0.0232 (8)	0.0102 (8)	0.0022 (8)
O2	0.0393 (7)	0.0473 (8)	0.0451 (7)	−0.0124 (6)	0.0089 (6)	0.0012 (6)
N1	0.0343 (8)	0.0366 (8)	0.0373 (8)	−0.0042 (6)	0.0104 (7)	0.0007 (6)
N2	0.0416 (9)	0.0756 (13)	0.0404 (9)	−0.0067 (9)	0.0142 (8)	−0.0053 (8)
C1	0.0428 (10)	0.0460 (11)	0.0378 (10)	−0.0054 (9)	0.0071 (9)	0.0065 (9)
C2	0.0450 (11)	0.0395 (11)	0.0426 (10)	−0.0090 (8)	0.0118 (9)	0.0066 (8)
C3	0.0382 (10)	0.0378 (10)	0.0368 (9)	0.0010 (8)	0.0124 (8)	0.0037 (8)
C4	0.0404 (10)	0.0370 (10)	0.0457 (10)	−0.0039 (8)	0.0181 (9)	0.0047 (8)
C5	0.0341 (9)	0.0381 (9)	0.0416 (10)	−0.0050 (8)	0.0159 (8)	−0.0028 (8)
C6	0.0425 (11)	0.0455 (11)	0.0460 (11)	−0.0106 (9)	0.0103 (9)	0.0023 (9)
C7	0.0357 (10)	0.0500 (11)	0.0417 (10)	−0.0097 (9)	0.0152 (9)	−0.0063 (9)
C8	0.0386 (10)	0.0565 (12)	0.0412 (10)	−0.0040 (9)	0.0190 (9)	−0.0036 (9)
C9	0.0527 (13)	0.112 (2)	0.0409 (12)	0.0165 (15)	0.0176 (11)	0.0113 (13)
C10	0.0786 (18)	0.092 (2)	0.0623 (15)	0.0227 (16)	0.0379 (14)	0.0292 (14)
C11	0.0610 (13)	0.0659 (14)	0.0588 (13)	−0.0012 (12)	0.0328 (12)	0.0075 (11)

Geometric parameters (Å, º)

Zn1—N1	2.0367 (15)	C2—H2A	0.9300
Zn1—N1^{i}	2.0367 (15)	C3—C4	1.364 (3)
Zn1—Cl1^{i}	2.2347 (9)	C3—H3	0.9300
Zn1—Cl1	2.2347 (9)	C4—C5	1.392 (3)
O1—C7	1.208 (3)	C4—H4	0.9300
O2—C7	1.344 (2)	C5—C6	1.490 (3)
O2—C6	1.431 (2)	C6—H6A	0.9700
N1—C3	1.340 (2)	C6—H6B	0.9700
N1—C2	1.344 (2)	C7—C8	1.441 (3)
N2—C9	1.345 (3)	C8—C11	1.364 (3)
N2—C8	1.369 (3)	C9—C10	1.349 (4)
N2—H2	0.8600	C9—H9	0.9300
C1—C2	1.368 (3)	C10—C11	1.396 (3)

C1—C5	1.380 (3)	C10—H10	0.9300
C1—H1	0.9300	C11—H11	0.9300
N1—Zn1—N1^{i}	107.76 (9)	C1—C5—C4	117.34 (17)
N1—Zn1—Cl1^{i}	104.16 (6)	C1—C5—C6	123.90 (17)
N1^{i}—Zn1—Cl1^{i}	110.92 (6)	C4—C5—C6	118.76 (17)
N1—Zn1—Cl1	110.92 (6)	O2—C6—C5	108.94 (16)
N1^{i}—Zn1—Cl1	104.16 (6)	O2—C6—H6A	109.9
Cl1^{i}—Zn1—Cl1	118.61 (4)	C5—C6—H6A	109.9
C7—O2—C6	115.69 (15)	O2—C6—H6B	109.9
C3—N1—C2	117.51 (15)	C5—C6—H6B	109.9
C3—N1—Zn1	122.71 (12)	H6A—C6—H6B	108.3
C2—N1—Zn1	119.71 (12)	O1—C7—O2	122.62 (18)
C9—N2—C8	109.1 (2)	O1—C7—C8	125.59 (17)
C9—N2—H2	125.4	O2—C7—C8	111.77 (17)
C8—N2—H2	125.4	C11—C8—N2	107.33 (19)
C2—C1—C5	119.81 (18)	C11—C8—C7	132.68 (19)
C2—C1—H1	120.1	N2—C8—C7	119.74 (18)
C5—C1—H1	120.1	N2—C9—C10	108.6 (2)
N1—C2—C1	122.78 (17)	N2—C9—H9	125.7
N1—C2—H2A	118.6	C10—C9—H9	125.7
C1—C2—H2A	118.6	C9—C10—C11	107.6 (2)
N1—C3—C4	122.79 (17)	C9—C10—H10	126.2
N1—C3—H3	118.6	C11—C10—H10	126.2
C4—C3—H3	118.6	C8—C11—C10	107.3 (2)
C3—C4—C5	119.77 (17)	C8—C11—H11	126.3
C3—C4—H4	120.1	C10—C11—H11	126.3
C5—C4—H4	120.1		
N1^{i}—Zn1—N1—C3	−34.15 (12)	C7—O2—C6—C5	179.31 (16)
Cl1^{i}—Zn1—N1—C3	−152.03 (13)	C1—C5—C6—O2	4.0 (3)
Cl1—Zn1—N1—C3	79.27 (15)	C4—C5—C6—O2	−175.71 (16)
N1^{i}—Zn1—N1—C2	149.00 (17)	C6—O2—C7—O1	1.0 (3)
Cl1^{i}—Zn1—N1—C2	31.12 (15)	C6—O2—C7—C8	−177.45 (16)
Cl1—Zn1—N1—C2	−97.58 (15)	C9—N2—C8—C11	1.1 (2)
C3—N1—C2—C1	0.1 (3)	C9—N2—C8—C7	−173.90 (18)
Zn1—N1—C2—C1	177.12 (16)	O1—C7—C8—C11	−178.6 (2)
C5—C1—C2—N1	−0.1 (3)	O2—C7—C8—C11	−0.2 (3)
C2—N1—C3—C4	0.2 (3)	O1—C7—C8—N2	−5.1 (3)
Zn1—N1—C3—C4	−176.75 (14)	O2—C7—C8—N2	173.28 (17)
N1—C3—C4—C5	−0.5 (3)	C8—N2—C9—C10	−1.4 (3)
C2—C1—C5—C4	−0.2 (3)	N2—C9—C10—C11	1.2 (3)
C2—C1—C5—C6	−179.95 (19)	N2—C8—C11—C10	−0.4 (2)
C3—C4—C5—C1	0.5 (3)	C7—C8—C11—C10	173.7 (2)
C3—C4—C5—C6	−179.77 (18)	C9—C10—C11—C8	−0.5 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cl1^{ii}	0.86	2.57	3.306 (3)	144
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C4—H4···O1^{iv}	0.93	2.54	3.354 (3)	146

Symmetry codes: (ii) −*x*+1/2, −*y*+3/2, −*z*+1; (iii) *x*, *y*+1, *z*; (iv) −*x*+1/2, −*y*+5/2, −*z*+1.