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Dichlorido(2,6-dipyrazol-1-ylpyridine)-zinc(II)

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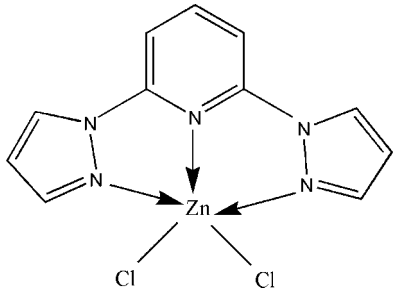
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.078; data-to-parameter ratio = 16.5.

In the title complex, $[ZnCl_2(C_{11}H_9N_5)]$, the Zn^{II} ion assumes a distorted trigonal–bipyramidal ZnN_3Cl_2 coordination geometry [Zn—N = 2.1397 (16)–2.2117 (17) Å, Zn—Cl = 2.2470 (6) and 2.2564 (6) Å]. The crystal packing exhibits π–π stacking interactions between the 2,6-dipyrazol-1-ylpyridine ligands of neighbouring molecules.

Related literature

For the related crystal structure of dichlorido[2,6-bis-(pyrazolylmethyl)pyridine]zinc(II), see Balamurugan *et al.* (2004).



Experimental

Crystal data

$[ZnCl_2(C_{11}H_9N_5)]$
M_r = 347.50
Monoclinic, $P2_1/c$
a = 10.9630 (17) Å
b = 8.0263 (13) Å
c = 14.943 (2) Å
β = 93.079 (2)°
V = 1313.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.27 mm^{-1}
T = 298 (2) K
0.48 × 0.42 × 0.29 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.409, T_{max} = 0.559
(expected range = 0.379–0.518)
7375 measured reflections
2848 independent reflections
2431 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.05
2848 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected interatomic distances (Å).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C4/N1/N4/N5/Zn1, C1–C3/N4/N5 and C4–C8/N1 rings, respectively.

$Cg1\cdots Cg2^{i}$	3.4087 (12)	$Cg2\cdots Cg3^{i}$	3.6253 (13)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2454).

References

Balamurugan, V., Hundal, M. S. & Mukherjee, R. (2004). *Chem. Eur. J.* **10**, 1683–1690.
Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m1374 [doi:10.1107/S1600536808031152]

Dichlorido(2,6-dipyrazol-1-ylpyridine)zinc(II)

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S1. Comment

2,6-Dipyrazol-1-ylpyridine and the relevant homologues as a tridentate ligand play an important role in modern coordination chemistry (Balamurugan *et al.*, 2004), and the interest in complexes with 2,6-dipyrazol-1-ylpyridine ligand stimulted us to prepare the title complex, (I). Herein we report its crystal structure.

In (I) (Fig. 1), each Zn^{II} ion has a distorted trigonal-bipyramidal coordination environment. In the crystal, there exist π-π stacking interactions involving symmetry related 2,6-dipyrazol-1-ylpyridine ligands (Talbe 1).

S2. Experimental

15 ml me thanol solution containing 2,6-dipyrazol-1-ylpyridine (0.0522 g, 0.247 mmol) and pyrazine-1,4-dioxide (0.0414 g, 0.369 mmol) was added into 5 ml H_2O solution of $ZnCl_2$ (0.0783 g, 0.575 mmol), and the mixed solution was stirred for a few minutes. Colorless single crystals were obtained after the filtrate was allowed to stand at room temperature for 40 days.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

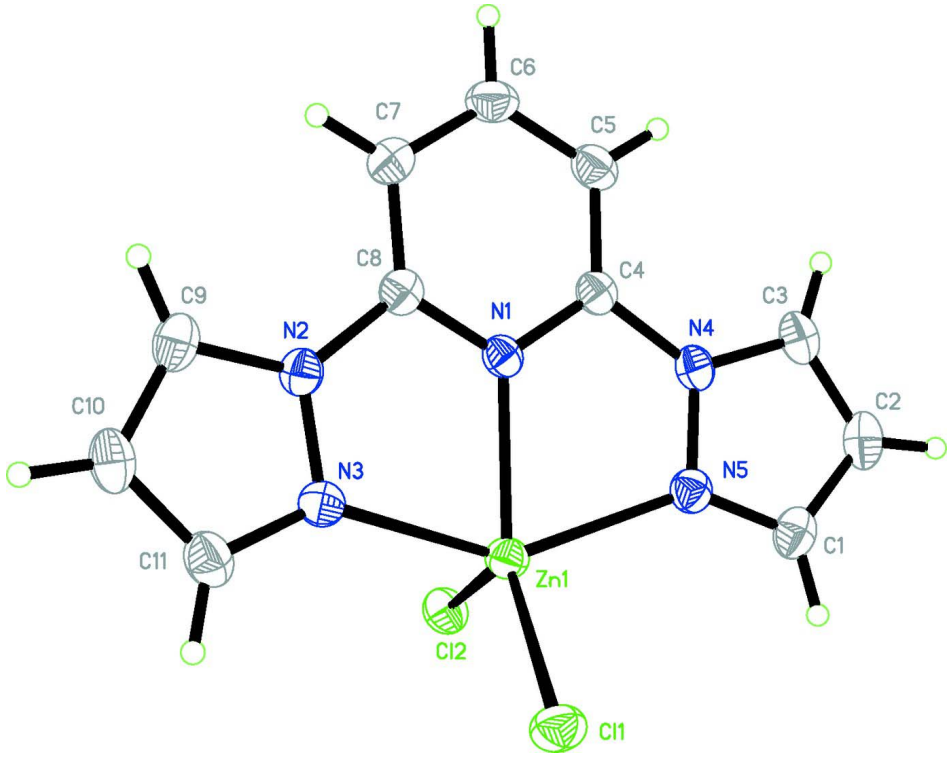

Figure 1

The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids.

Dichlorido(2,6-dipyrazol-1-ylpyridine)zinc(II)

Crystal data

$[ZnCl_2(C_{11}H_9N_5)]$
$M_r = 347.50$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.9630\ (17)$ Å
$b = 8.0263\ (13)$ Å
$c = 14.943\ (2)$ Å
$\beta = 93.079\ (2)°$
$V = 1313.0\ (4)$ Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.758$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3889 reflections
$\theta = 2.4–28.2°$
$\mu = 2.27$ mm^{-1}
$T = 298$ K
Block, colourless
0.48 × 0.42 × 0.29 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.409$, $T_{max} = 0.559$
7375 measured reflections
2848 independent reflections
2431 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.9°$
$h = -9\rightarrow14$
$k = -9\rightarrow10$
$l = -16\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.05$
2848 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.0869P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0167 (11)

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	0.47097 (18)	0.3058 (2)	0.04770 (16)	0.0447 (5)
H1	0.4465	0.3525	0.1008	0.054*
C2	0.40961 (19)	0.3275 (3)	−0.03549 (17)	0.0478 (5)
H2	0.3389	0.3891	−0.0481	0.057*
C3	0.47479 (18)	0.2396 (2)	−0.09475 (16)	0.0440 (5)
H3	0.4572	0.2292	−0.1561	0.053*
C4	0.66172 (17)	0.0609 (2)	−0.07399 (13)	0.0349 (4)
C5	0.66885 (19)	0.0026 (3)	−0.16015 (14)	0.0448 (5)
H5	0.6147	0.0387	−0.2062	0.054*
C6	0.7591 (2)	−0.1111 (3)	−0.17553 (16)	0.0487 (5)
H6	0.7663	−0.1533	−0.2330	0.058*
C7	0.8394 (2)	−0.1637 (3)	−0.10659 (15)	0.0442 (5)
H7	0.8998	−0.2423	−0.1160	0.053*
C8	0.82578 (17)	−0.0944 (2)	−0.02369 (14)	0.0357 (4)
C9	0.99689 (18)	−0.2410 (2)	0.06325 (16)	0.0454 (5)
H9	1.0275	−0.3088	0.0192	0.054*
C10	1.0387 (2)	−0.2314 (3)	0.14943 (17)	0.0502 (6)
H10	1.1036	−0.2903	0.1767	0.060*
C11	0.9647 (2)	−0.1152 (3)	0.18931 (17)	0.0491 (6)
H11	0.9730	−0.0837	0.2492	0.059*
Cl1	0.65199 (5)	0.06053 (7)	0.25184 (4)	0.05045 (17)
Cl2	0.83525 (5)	0.37392 (6)	0.12155 (4)	0.04545 (15)
N1	0.74008 (13)	0.01621 (18)	−0.00710 (10)	0.0327 (3)

N2	0.90163 (15)	−0.13336 (19)	0.05243 (12)	0.0374 (4)
N3	0.88095 (15)	−0.0554 (2)	0.13084 (11)	0.0417 (4)
N4	0.57069 (14)	0.1699 (2)	−0.04655 (11)	0.0366 (4)
N5	0.56823 (14)	0.2105 (2)	0.04169 (11)	0.0385 (4)
Zn1	0.73202 (2)	0.13073 (3)	0.121755 (15)	0.03696 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0377 (11)	0.0347 (10)	0.0624 (14)	−0.0040 (8)	0.0090 (10)	−0.0009 (10)
C2	0.0347 (10)	0.0363 (10)	0.0721 (16)	−0.0005 (9)	−0.0004 (10)	0.0102 (10)
C3	0.0360 (10)	0.0439 (11)	0.0512 (13)	−0.0045 (9)	−0.0066 (9)	0.0124 (9)
C4	0.0329 (10)	0.0332 (9)	0.0386 (11)	−0.0072 (7)	0.0014 (8)	0.0020 (8)
C5	0.0441 (11)	0.0538 (12)	0.0361 (11)	−0.0052 (10)	−0.0025 (9)	0.0023 (9)
C6	0.0539 (13)	0.0570 (13)	0.0357 (12)	−0.0052 (10)	0.0062 (10)	−0.0076 (10)
C7	0.0428 (12)	0.0470 (11)	0.0435 (12)	0.0032 (9)	0.0071 (9)	−0.0029 (9)
C8	0.0338 (10)	0.0337 (9)	0.0400 (11)	−0.0062 (8)	0.0054 (8)	0.0026 (8)
C9	0.0392 (11)	0.0374 (11)	0.0599 (15)	0.0031 (9)	0.0064 (10)	0.0053 (9)
C10	0.0414 (11)	0.0469 (12)	0.0613 (15)	0.0030 (9)	−0.0047 (10)	0.0154 (11)
C11	0.0458 (12)	0.0549 (13)	0.0460 (14)	0.0010 (10)	−0.0036 (10)	0.0090 (10)
Cl1	0.0523 (3)	0.0611 (4)	0.0389 (3)	−0.0069 (2)	0.0112 (2)	−0.0012 (2)
Cl2	0.0431 (3)	0.0428 (3)	0.0500 (3)	−0.0086 (2)	−0.0017 (2)	−0.0035 (2)
N1	0.0309 (8)	0.0332 (8)	0.0338 (9)	−0.0042 (6)	0.0000 (7)	0.0014 (7)
N2	0.0348 (9)	0.0376 (9)	0.0400 (10)	0.0006 (6)	0.0034 (7)	0.0025 (7)
N3	0.0413 (9)	0.0486 (10)	0.0351 (9)	0.0030 (8)	0.0022 (7)	0.0011 (7)
N4	0.0316 (8)	0.0370 (8)	0.0407 (10)	−0.0038 (7)	−0.0015 (7)	0.0037 (7)
N5	0.0359 (9)	0.0376 (9)	0.0419 (10)	−0.0029 (7)	0.0022 (7)	−0.0007 (7)
Zn1	0.03632 (16)	0.04045 (17)	0.03418 (17)	−0.00377 (9)	0.00263 (10)	−0.00260 (9)

Geometric parameters (Å, º)

C1—N5	1.319 (3)	C8—N1	1.325 (2)
C1—C2	1.392 (3)	C8—N2	1.408 (3)
C1—H1	0.9300	C9—C10	1.346 (3)
C2—C3	1.364 (3)	C9—N2	1.358 (2)
C2—H2	0.9300	C9—H9	0.9300
C3—N4	1.362 (2)	C10—C11	1.391 (3)
C3—H3	0.9300	C10—H10	0.9300
C4—N1	1.332 (2)	C11—N3	1.323 (3)
C4—C5	1.376 (3)	C11—H11	0.9300
C4—N4	1.405 (2)	Cl1—Zn1	2.2470 (6)
C5—C6	1.374 (3)	Cl2—Zn1	2.2564 (6)
C5—H5	0.9300	N1—Zn1	2.1397 (16)
C6—C7	1.385 (3)	N2—N3	1.358 (2)
C6—H6	0.9300	N3—Zn1	2.2117 (17)
C7—C8	1.374 (3)	N4—N5	1.360 (2)
C7—H7	0.9300	N5—Zn1	2.1988 (16)

Cg1···Cg2^{i}	3.4087 (12)	Cg2···Cg3^{i}	3.6253 (13)
N5—C1—C2	111.4 (2)	C11—C10—H10	127.1
N5—C1—H1	124.3	N3—C11—C10	111.1 (2)
C2—C1—H1	124.3	N3—C11—H11	124.4
C3—C2—C1	105.67 (19)	C10—C11—H11	124.4
C3—C2—H2	127.2	C8—N1—C4	118.37 (17)
C1—C2—H2	127.2	C8—N1—Zn1	121.33 (13)
N4—C3—C2	106.6 (2)	C4—N1—Zn1	120.23 (13)
N4—C3—H3	126.7	C9—N2—N3	110.69 (17)
C2—C3—H3	126.7	C9—N2—C8	130.90 (18)
N1—C4—C5	122.93 (18)	N3—N2—C8	118.41 (16)
N1—C4—N4	112.86 (17)	C11—N3—N2	105.09 (18)
C5—C4—N4	124.19 (18)	C11—N3—Zn1	140.30 (16)
C6—C5—C4	117.4 (2)	N2—N3—Zn1	114.53 (12)
C6—C5—H5	121.3	N5—N4—C3	111.07 (17)
C4—C5—H5	121.3	N5—N4—C4	118.92 (16)
C5—C6—C7	120.8 (2)	C3—N4—C4	129.90 (18)
C5—C6—H6	119.6	C1—N5—N4	105.25 (17)
C7—C6—H6	119.6	C1—N5—Zn1	140.46 (15)
C8—C7—C6	116.84 (19)	N4—N5—Zn1	113.56 (11)
C8—C7—H7	121.6	N1—Zn1—N5	72.99 (6)
C6—C7—H7	121.6	N1—Zn1—N3	72.49 (6)
N1—C8—C7	123.55 (19)	N5—Zn1—N3	143.97 (6)
N1—C8—N2	113.06 (17)	N1—Zn1—Cl1	135.05 (4)
C7—C8—N2	123.38 (18)	N5—Zn1—Cl1	101.44 (5)
C10—C9—N2	107.3 (2)	N3—Zn1—Cl1	95.67 (5)
C10—C9—H9	126.3	N1—Zn1—Cl2	108.99 (4)
N2—C9—H9	126.3	N5—Zn1—Cl2	98.18 (5)
C9—C10—C11	105.8 (2)	N3—Zn1—Cl2	102.45 (5)
C9—C10—H10	127.1	Cl1—Zn1—Cl2	115.93 (2)
N5—C1—C2—C3	−0.1 (2)	C5—C4—N4—N5	175.69 (18)
C1—C2—C3—N4	−0.1 (2)	N1—C4—N4—C3	−178.85 (18)
N1—C4—C5—C6	2.3 (3)	C5—C4—N4—C3	−0.2 (3)
N4—C4—C5—C6	−176.27 (18)	C2—C1—N5—N4	0.2 (2)
C4—C5—C6—C7	−0.2 (3)	C2—C1—N5—Zn1	169.07 (15)
C5—C6—C7—C8	−1.3 (3)	C3—N4—N5—C1	−0.3 (2)
C6—C7—C8—N1	0.9 (3)	C4—N4—N5—C1	−176.86 (16)
C6—C7—C8—N2	−178.97 (18)	C3—N4—N5—Zn1	−172.54 (12)
N2—C9—C10—C11	0.3 (2)	C4—N4—N5—Zn1	10.85 (19)
C9—C10—C11—N3	0.0 (3)	C8—N1—Zn1—N5	−173.52 (14)
C7—C8—N1—C4	1.0 (3)	C4—N1—Zn1—N5	9.64 (13)
N2—C8—N1—C4	−179.07 (15)	C8—N1—Zn1—N3	−4.01 (13)
C7—C8—N1—Zn1	−175.88 (15)	C4—N1—Zn1—N3	179.15 (15)
N2—C8—N1—Zn1	4.0 (2)	C8—N1—Zn1—Cl1	−84.26 (14)
C5—C4—N1—C8	−2.7 (3)	C4—N1—Zn1—Cl1	98.90 (13)
N4—C4—N1—C8	176.00 (15)	C8—N1—Zn1—Cl2	93.49 (13)

C5—C4—N1—Zn1	174.24 (14)	C4—N1—Zn1—Cl2	−83.35 (13)
N4—C4—N1—Zn1	−7.1 (2)	C1—N5—Zn1—N1	−178.6 (2)
C10—C9—N2—N3	−0.4 (2)	N4—N5—Zn1—N1	−10.30 (11)
C10—C9—N2—C8	179.88 (19)	C1—N5—Zn1—N3	164.27 (19)
N1—C8—N2—C9	178.77 (18)	N4—N5—Zn1—N3	−27.46 (18)
C7—C8—N2—C9	−1.3 (3)	C1—N5—Zn1—Cl1	47.6 (2)
N1—C8—N2—N3	−0.9 (2)	N4—N5—Zn1—Cl1	−144.18 (11)
C7—C8—N2—N3	179.04 (18)	C1—N5—Zn1—Cl2	−71.1 (2)
C10—C11—N3—N2	−0.3 (2)	N4—N5—Zn1—Cl2	97.15 (12)
C10—C11—N3—Zn1	−176.68 (16)	C11—N3—Zn1—N1	179.3 (2)
C9—N2—N3—C11	0.4 (2)	N2—N3—Zn1—N1	3.17 (12)
C8—N2—N3—C11	−179.84 (17)	C11—N3—Zn1—N5	−163.4 (2)
C9—N2—N3—Zn1	177.92 (12)	N2—N3—Zn1—N5	20.38 (19)
C8—N2—N3—Zn1	−2.4 (2)	C11—N3—Zn1—Cl1	−45.1 (2)
C2—C3—N4—N5	0.2 (2)	N2—N3—Zn1—Cl1	138.76 (12)
C2—C3—N4—C4	176.33 (18)	C11—N3—Zn1—Cl2	73.1 (2)
N1—C4—N4—N5	−3.0 (2)	N2—N3—Zn1—Cl2	−103.08 (12)

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