Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Dichlorodipyridazinezinc(II)

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Received 16 July 2004
Accepted 9 August 2004
Online 13 August 2004

In the title compound, $[ZnCl_2(C_4H_4N_2)_2]$, the tetrahedral coordination sphere of Zn^{II} is formed by two Cl ions and two pyridazine ligands. The rings of the two pyridazine ligands in the coordination sphere are almost perpendicular to each other. Each pyridazine is involved in one C—H···Cl interaction but only one chloride participates in these contacts.

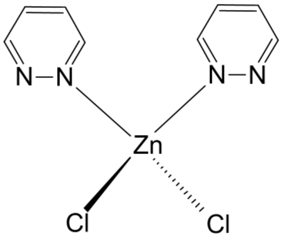
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.087
Data-to-parameter ratio = 26.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Transition metal complexes of pyridazine usually form polymeric chains with the central ions bridged by either N,N'-coordinated heterocyclic rings or inorganic anions. Typical formulae of the respective chloride coordination compounds are $[M^{I}(\mu\text{-pyridazine})(\mu\text{-Cl})]_n$ (M = Cu) (Kromp & Sheldrick, 1999) or $[M^{II}(\mu\text{-pyridazine})(\mu\text{-Cl})_2]_n$ (M = Mn, Fe, Co, Ni) (Masciocchi *et al.*, 1994). Monodentate complexation has been reported for only a few species, such as $[Co^{II}(\text{pyridazine})_4(NCS)_2]$ (Lloret *et al.*, 1998), $[Cu^{II}(\text{pyridazine})_x(NO_3)_y]^{n+}$ (x = 3–4, y = 1–3, $n = 2 - y$; Otieno *et al.*, 1995), $[Pt^{II}(\text{pyridazine})_4](ClO_4)_2$ (Kozmin *et al.*, 1993) and assumed, on the basis of spectroscopic methods, for $Zn(\text{pyridazine})_2Cl_2$ (Allan *et al.*, 1971; Child *et al.*, 1981). In this paper, we present the X-ray study of the latter compound, (I), which, to the best of our knowledge, is the first structurally characterized pyridazine complex of that composition with zinc triad metal.



(I)

In contrast to the Zn^{II} chloride complexes of other unsubstituted diazines (pyrazine and pyrimidine), which were polymers of the $[Zn^{II}(\mu\text{-pyrazine})(\mu\text{-Cl})_2]_n$ and $[Zn(\mu\text{-pyrimidine})(\mu\text{-Cl})_2]_n$ types (Pickardt & Staub, 1996), the structure of (I) is monomeric (Fig. 1), being similar to that of $[Zn(\text{pyridine})_2Cl_2]$ (Steffen & Palenik, 1976). The tetrahedral coordination sphere of Zn^{II} is formed by two Cl ions and two monodentately N-bonded pyridazine ligands. The coordination bond distances are typical (Table 1). The N1—Zn1—N11 and Cl1—Zn—Cl2 bond angles deviate most from ideal tetrahedral geometry with values of 98.78 (7) and 118.72 (3)°,

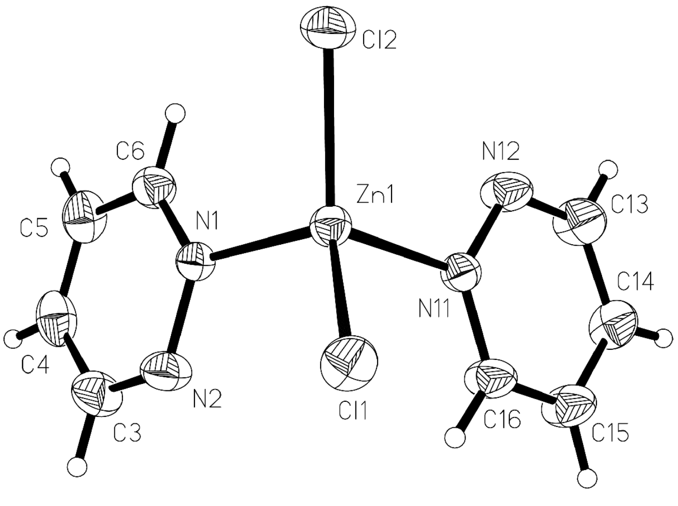


Figure 1
A view of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

respectively. The N—Zn1—Cl angles are in the range 103.82 (5)–113.21 (5)°. Slight geometry differences between both pyridazine ligands are observed but none are chemically significant. Their geometries are similar to that of unsubstituted pyridazine at 100 K (Blake & Rankin, 1991). The average values of chemically equivalent bonds and angles in the two pyridazine ligands in (I) are almost identical to those found in bridging *N,N*-bonded pyridazine ligands in the reported Cd^{II} and Hg^{II} complex structures (Pazderski *et al.*, 2004).

Each complex molecule forms two intermolecular C—H···Cl contacts involving only one chloride (Cl1), as well as both C4—H4 and C14—H14 groups of the pyridazines, the C4···Cl1(x, y, $z-1$) and C14···Cl1($x-1$, $\frac{3}{2}-y$, $z-\frac{1}{2}$) distances being 3.650 (3) and 3.485 (3) Å, respectively. This results in a slight elongation of the Zn—Cl1 bond compared to that of Zn—Cl2, as the second chloride (Cl2) does not participate in such interactions. The chain of complex molecules formed by the above contacts is approximately parallel to the [101] direction, *i.e.* the diagonal between the crystallographic x and z axes. Adjacent chains interact only by stacking interactions between the pyridazine rings.

The heterocyclic ligands are planar, with the r.m.s. deviations of fitted atoms being 0.002 (2) and 0.009 (2) Å for the N1—C6 and N11—C16 moieties, respectively. The dihedral angle between their least-squares planes is 86.59 (9)°. They are not coplanar with the Zn—N bonds and differ in the relative orientation. The deviations of the Zn atoms from the least-squares planes are 0.240 (3) and 0.030 (4) Å for the N1–C6 and N11–C16 moieties, respectively.

Experimental

The title compound was obtained as described previously (Allan *et al.*, 1971; Child *et al.*, 1981; Masciocchi *et al.*, 1994; Pazderski *et al.*, 2004). Colourless single crystals were obtained by slow evaporation of the ethanol solution remaining from the synthesis.

Crystal data

$[ZnCl_2(C_4H_4N_2)_2]$
$M_r = 296.45$
Monoclinic, $P2_1/c$
$a = 8.033$ (1) Å
$b = 17.034$ (2) Å
$c = 8.531$ (1) Å
$\beta = 96.09$ (1)°
$V = 1160.7$ (2) Å^3
$Z = 4$
$D_x = 1.696$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3552 reflections
$\theta = 2.6$–31.3°
$\mu = 2.55$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.29 × 0.25 × 0.11 mm

Data collection

Oxford Sapphire CCD diffractometer
$\theta/2\theta$ scans
Absorption correction: numerical (*CrysAlis RED*; Oxford Diffraction, 2000)
$T_{min} = 0.513$, $T_{max} = 0.743$
11321 measured reflections
3552 independent reflections
2894 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 31.3°$
$h = -8 \rightarrow 11$
$k = -24 \rightarrow 23$
$l = -12 \rightarrow 12$
1 frame standard reflection every every 50 frames reflections intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.087$
$S = 1.06$
3552 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.3919P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for (I).

Zn1—N1	2.0388 (17)	Zn1—Cl2	2.1949 (6)
Zn1—N11	2.0582 (17)	Zn1—Cl1	2.2029 (6)
N1—Zn1—N11	98.78 (7)	Cl2—Zn1—Cl1	118.72 (3)
N1—Zn1—Cl2	107.72 (5)	C6—N1—Zn1	123.81 (15)
N11—Zn1—Cl2	112.81 (5)	N2—N1—Zn1	114.75 (14)
N1—Zn1—Cl1	113.21 (5)	C16—N11—Zn1	121.16 (14)
N11—Zn1—Cl1	103.82 (5)	N12—N11—Zn1	118.08 (13)

H-atom positions were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 0.080$ Å^2.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2000); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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