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Dichlorodiquinoxalinezinc(II)

Brian M. E. Markowitz,[a] Mark M. Turnbull[a]* and Firas F. Awwadi[b]‡

[a]Carlson School of Chemistry and Biochemistry, Clark University, 950 Main Street, Worcester, MA 01610, USA, and [b]Department of Chemistry, Washington State University, Pullman, WA 99164-4630, USA

‡ Present address: Department of Applied Chemistry, Jordan University of Science and Technology, Irbid, Jordan.

Correspondence e-mail: mturnbull@clarku.edu

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Key indicators

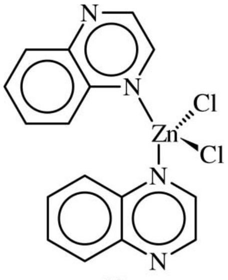
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.027
wR factor = 0.072
Data-to-parameter ratio = 13.0

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

In the title molecular structure, $[ZnCl_2(C_8H_6N_2)_2]$, two quinoxaline ligands are mono-coordinated to a Zn^{II} atom. With two chloride ions, they form a distorted tetrahedral coordination geometry. The combination of π stacking interactions between inversion-related quinoxaline ligands and the coordination to zinc creates layers parallel to the *bc* plane.

Comment

We are interested in the design and synthesis of low-dimensional coordination polymers to study their magnetic properties. We have examined two copper(II) complexes of quinoxaline (quinox) and found that Cu(quinox)Cl_2 and Cu(quinox)Br_2 occur as both structural and magnetic ladders with the rungs of the ladder formed by bridging halide ions and the rails formed by bridging quinoxaline molecules (Lindroos & Lumme, 1990; Landee *et al.*, 2003). A diamagnetic analogue of these materials would be useful for specific heat, neutron scattering and percolation experiments. Hence we attempted the preparation of the corresponding zinc(II) complexes. Reaction of $ZnCl_2$ with quinoxaline, even at high zinc-to-quinoxaline ratios, gave Zn(quinox)Cl_2, (I).



(I)

The title complex (Fig. 1) has distorted tetrahedral coordination geometry with both the Cl1—Zn—Cl2 and the N1—Zn1—N11 angles expanded, nearly equally, to a mean value of 120.52 (3)° (Turnbull *et al.*, 2005). This is in contrast to the corresponding bis-pyridine complex (Steffen & Palenik, 1976) where only the Cl—Zn—Cl [120.9 (1)°] angle is enlarged relative to the ideal value (109.5°) for a tetrahedron, although the Zn—Cl bond lengths are comparable. Even the close structural analogue Zn(quinoline)Cl_2 (Cui *et al.*, 1998) shows expansion of only the Cl—Zn—Cl angle [115.47 (5)°], while the N—Zn—N angle is virtually undistorted [109.3 (1)°]. The two quinoxaline ligands are nearly planar but show a slight folding. The mean deviation from planarity for the N1-containing quinoxaline is 0.0132 Å and the angle between the normals to the two component rings is 1.3 (1)°; the compar-

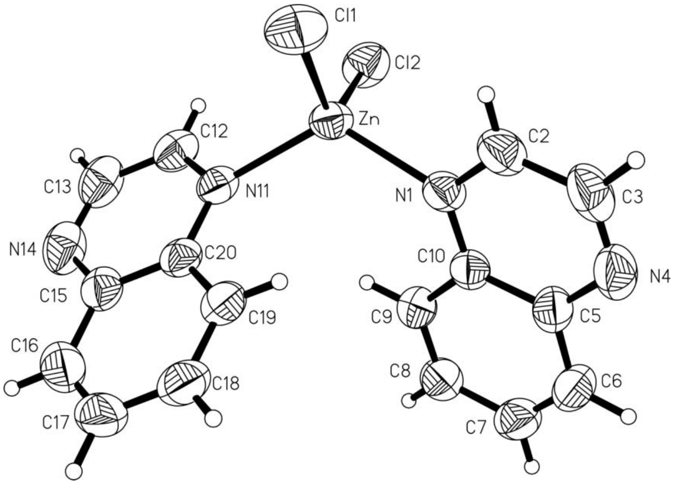


Figure 1
Molecular structure of (I), showing 50% probability displacement ellipsoids.

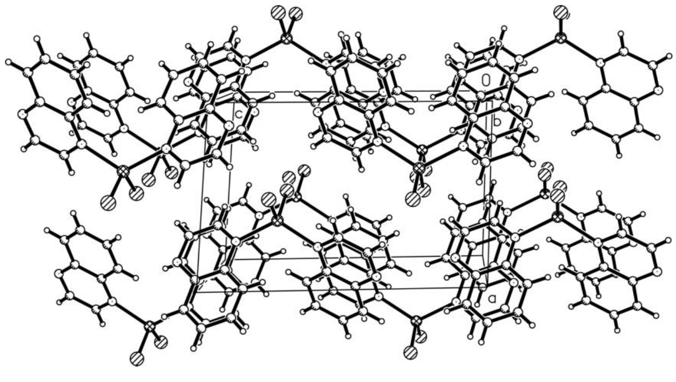


Figure 2
Packing of (I), viewed parallel to the *b* axis, showing the layer structure.

able values for the N11 ligand are 0.0104 Å and 1.1 (1)°. The two quinoxaline groups are canted 64.8 (1)° with respect to each other.

The bond lengths and angles within the quinoxaline ring systems are the same within experimental error and agree with those values seen in similar mono-coordinated complexes such as $[Cu(quinox)_2(H_2O)_3](ClO_4)_2$ (Lumme *et al.*, 1988) and $[Cu(quinox)_2(C_2N_3)_2]$ (Luo *et al.*, 2004), except that the N1—C2/N11—C12 and C3—N4/C13—N14 bonds are lengthened by roughly 0.010 Å and the C—N—C bond angles are opened correspondingly (1–2°).

The compound packs in the crystal structure such that π stacking is observed between inversion-related quinoxaline ligands, generating layers parallel to the *bc* plane (Fig. 2). The ring overlap occurs between successive nitrogen-containing rings. The interplanar distance between the stacked N1 rings is 3.22 (1) Å and the displacement angle (defined as the angle between the mean plane of the ring and the line connecting the ring centroids) is 18.8 (1)°, while for the stacked N11 rings the distance is 3.30 (1) Å and the displacement angle is 18.5 (1)°.

Experimental

A solution of quinoxaline (1.32 g, 10 mmol) in absolute ethanol (10 ml) was added to a solution of $ZnCl_2$ (1.37 g, 10 mmol) in absolute ethanol (10 mol), yielding a pale-orange solution. The flask was wrapped in aluminum foil and fitted with a drying tube ($CaCl_2$). Beige crystals of (I) were collected *via* filtration after two days, washed with cold ethanol and allowed to air-dry (yield 0.41 g, 24%).

Crystal data

$[ZnCl_2(C_8H_6N_2)_2]$
$M_r = 396.57$
Triclinic, $P\overline{1}$
$a = 8.1097$ (10) Å
$b = 8.6533$ (8) Å
$c = 12.2541$ (12) Å
$\alpha = 81.017$ (8)°
$\beta = 86.018$ (8)°
$\gamma = 73.294$ (9)°
$V = 813.27$ (15) Å^3
$Z = 2$
$D_x = 1.619$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.84$ mm^{-1}
$T = 295$ (2) K
Chunk, colorless
0.5 × 0.4 × 0.3 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: ψ scan
(*SHELXTL*; Siemens, 1990)
$T_{min} = 0.429$, $T_{max} = 0.568$
3340 measured reflections
2707 independent reflections
2417 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 24.5°$
3 standard reflections
every 97 reflections
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.072$
$S = 1.06$
2707 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 0.1923P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—N1	2.0836 (19)	Zn—Cl1	2.2237 (8)
Zn—N11	2.077 (2)	Zn—Cl2	2.2274 (7)
N11—Zn—N1	120.41 (8)	N11—Zn—Cl2	103.34 (6)
N11—Zn—Cl1	104.61 (6)	N1—Zn—Cl2	104.84 (6)
N1—Zn—Cl1	104.18 (6)	Cl1—Zn—Cl2	120.63 (3)

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

Data collection: *XSCANS* (Siemens, 1992); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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