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Dichlorobis(phthalazine)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.040
wR factor = 0.100
Data-to-parameter ratio = 15.4

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

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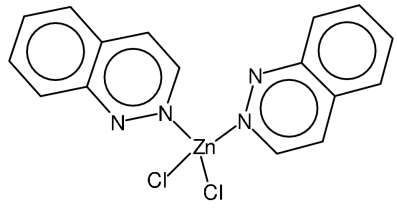
In the title compound, $[ZnCl_2(C_8H_6N_2)_2]$, the Zn^{II} atom is coordinated in a distorted tetrahedral environment by two Cl atoms and two N atoms from the phthalazine ligands. There is an intramolecular C—H···N interaction between the phthalazine ligands.

Comment

Phthalazine is a diazanaphthalene molecule with two adjacent N atoms and is also known as 2,3-benzodiazine. Phthalazines, like the other members of the isomeric benzodiazine series, have found wide application as therapeutic agents. At the same time, they are widely used in industry and pharmaceutical chemistry as intermediates in the syntheses of antimalarial drugs (Silva *et al.*, 1995; Tsoungas & Searcey, 2001, Sugihara *et al.*, 2000; Napoletano *et al.*, 2000; Sivakumar *et al.*, 2002). Various phthalazine compounds offer strong protection against acrolein-mediated toxicity in isolated hepatocytes (Burcham *et al.*, 2002).



(I)

The Zn atom in the title compound, (I), is coordinated tetrahedrally by two Cl atoms and two N atoms of the phthalazine ligands (Fig. 1 and Table 1). The Cl_2N_2 donor set defines a distorted tetrahedron, with angles ranging from 103.8 (1) to 114.96 (5)°. The range of these bond angles is

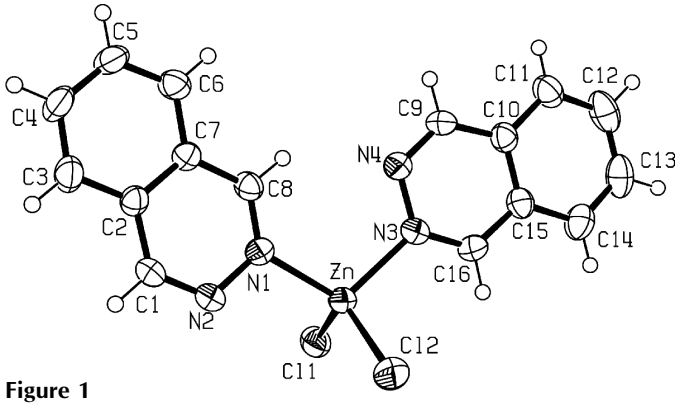


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

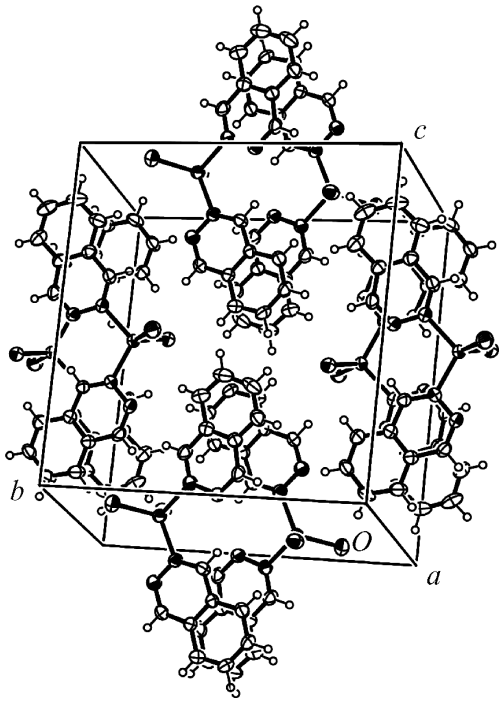


Figure 2
Packing diagram of (I).

comparable to those reported in other compounds: $ZnCl_2$(2-benzyl-1H benzimidazole)$_2$, 103.32 (7)–116.67 (7)° (Bei *et al.*, 2001); $ZnCl_2$(5,7-dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine)$_2$, 102.09 (9)–117.54 (4)° (Salas *et al.*, 1994); and $ZnCl_2$(purine)$_2$, 99.9 (1)–113.7 (1)° (Laity & Taylor, 1995).

The Zn—Cl bond distances of 2.223 (1) and 2.229 (1) Å are nearly equal to the corresponding distances reported for other compounds, *viz.* 2.229 (2) Å in $ZnCl_2$(purine)$_2$ (Laity & Taylor, 1995), 2.224 (1) Å in $ZnCl_2$(5,7-dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine)$_2$ (Salas *et al.*, 1994), 2.212 (4) Å in $ZnCl_2$(2,9-dimethyl-1,10-phenanthroline) (Preston & Kennard, 1969) and 2.209 (3) Å in $ZnCl_2$(4-vinylpyridine)$_2$ (Steffen & Palenik, 1977), but shorter than the value of 2.255 (1) Å in $ZnCl_2$(1-[5,6-dimethylbenzimidazolyl]-3-benzimidazolyl-2-thiapropane) (Matthews *et al.*, 1998).

The Zn—N bond distances of 2.038 (3) (Zn—N1) and 2.068 (3) Å (Zn—N3) may be compared to the reported average values of 2.039 (3) Å in $ZnCl_2$(5,7-dimethyl-1,2,4-triazolo[1,5-*a*]) (Bei *et al.*, 2001), 2.05 (1) Å in $ZnCl_2$(1-methyltetrazole)$_2$ (Baenziger & Schultz, 1971), 2.059 (3) Å in $ZnCl_2$(1-methylcytosine)$_2$ (Beauchamp, 1984), 2.011 (9) Å in $ZnBr_2$(benzimidazole)$_2$ (Şahin *et al.*, 2002) and 2.027 (2) Å in $ZnCl_2$([1-dimethyl-benzimidazolyl]-3-benzimidazolyl-2-thiapropane) (Matthews *et al.*, 1998). The Zn—N bond lengths are nearly equal to those of 2.035 (6) and 2.048 (6) Å observed in $ZnBr_2$(phthalazine)$_2$ (Çelik *et al.*, 2004).

The dihedral angle between the least-squares planes through the phthalazine ligands is 4.34 (7)°. In the crystal structure, individual molecules are loosely associated into pairs *via* weak C—H···Cl interactions that occur between centrosymmetric pairs (Table 2, Fig. 2). In addition, there is a short intramolecular C8—H6···N4 hydrogen-bonding interaction.

Experimental

All chemicals were reagent grade (Sigma) and were used without further purification. The title compound was obtained by addition of phthalazine (261 mg, 2 mmol) to a saturated solution of $ZnCl_2$ (136 mg, 1 mmol) in hot ethanol. The mixture was allowed to stand for several weeks, and crystals of the title compound were deposited. Elemental analysis (found/calculated): C 48.30/48.48, H 3.05/3.03, N 14.85/14.14%.

Crystal data

$[ZnCl_2(C_8H_6N_2)_2]$
M_r = 396.6
Monoclinic, $P2_1/c$
a = 7.499 (1) Å
b = 14.525 (2) Å
c = 15.049 (1) Å
β = 101.15 (4)°
V = 1608.1 (4) Å^3
Z = 4
D_x = 1.638 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.8–26.3°
μ = 1.86 mm^{-1}
T = 293 (2) K
Prism, colourless
0.4 × 0.3 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.503, T_{max} = 0.688
3384 measured reflections
3258 independent reflections
1895 reflections with $I > 2\sigma(I)$
R_{int} = 0.04
θ_{max} = 26.3°
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 18$
3 standard reflections
frequency: 120 min
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 0.99
3258 reflections
212 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 2.0204P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—N1	2.038 (3)	Zn—Cl2	2.223 (1)
Zn—N3	2.068 (3)	Zn—Cl1	2.229 (1)
N1—Zn—N3	108.58 (13)	N1—Zn—Cl1	107.43 (10)
N1—Zn—Cl2	114.65 (10)	N3—Zn—Cl1	106.98 (10)
N3—Zn—Cl2	103.80 (10)	Cl2—Zn—Cl1	114.96 (5)
N1—Zn—N3—N4	−7.5 (3)	N3—Zn—N1—N2	−173.4 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H6···N4	0.93	2.43	3.185 (5)	139
C6—H5···Cl1^{i}	0.93	2.78	3.637 (5)	153

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

H atoms were included in the riding-model approximation, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1993); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *CAD*-4 *EXPRESS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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