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Dichloro(*N*,*N*′-dibenzylethane-1,2-diamine-κ^2N,*N*)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.029
wR factor = 0.071
Data-to-parameter ratio = 16.3

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

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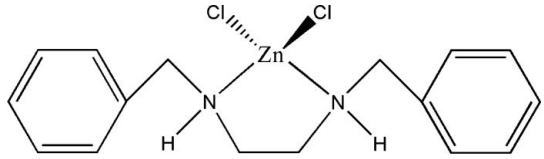
In the title compound, $[ZnCl_2(C_{16}H_{20}N_2)]$, the Zn cation is coordinated by two Cl anions and two N atoms of *N*,*N*′-dibenzylethane-1,2-diamine in a distorted tetrahedral geometry. The molecules are linked into dimers by N—H···Cl and C—H···Cl hydrogen bonds; neighboring dimers are linked into a sheet by C—H··· Cl hydrogen bonds.

Comment

Ethane-1,2-diamine derivatives are effective bidentate organic ligands. As part of our investigation of the reactions between diamine derivatives with metals, we report here the crystal structure of the title complex, (I) (Fig. 1). In (I), the Zn^{II} center is tetracoordinated by two N atoms of chelating *N*,*N*′-dibenzylethane-1,2-diamine ligands and two Cl^- anions.



(I)

In the crystal structure of (I), the molecules are linked into dimers. Atom Cl2 acts as a bifurcated acceptor, and atoms C9 and N1 in the molecule at (*x*, *y*, *z*) both act as hydrogen-bond donors to atom Cl2 in the molecule at (1 − *x*, 1 − *y*, 1 − *z*), generating an $R_2^1(6)$ ring (Fig. 2). Neighboring dimers are linked by C—H···Cl into sheets (Fig. 3), and neighboring sheets are connected by a pair of N—H···Cl hydrogen bonds, generating an $R_2^2(8)$ ring, resulting in a three-dimensional network (Fig. 4).

Experimental

A solution of *N*,*N*′-dibenzylethane-1,2-diamine (1 mmol) in ethanol (20 ml) and a solution of zinc chloride (1 mmol) in ethanol (10 ml)

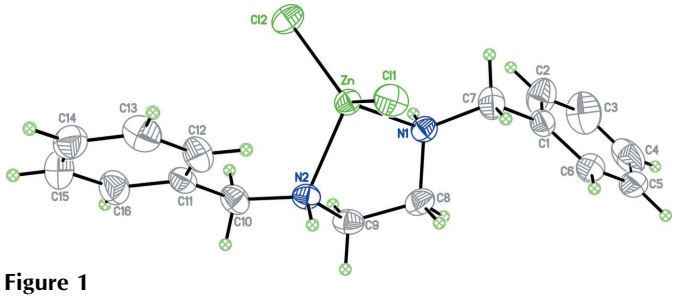


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

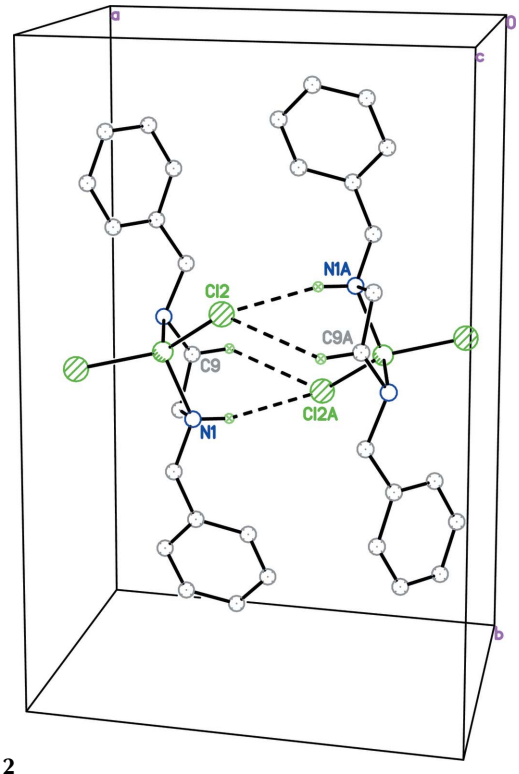


Figure 2
The formation of a hydrogen-bonded dimer built from C—H···Cl and N—H···Cl interactions. Dashed lines indicate hydrogen bonds. For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry code: (A) $1-x, 1-y, 1-z$.]

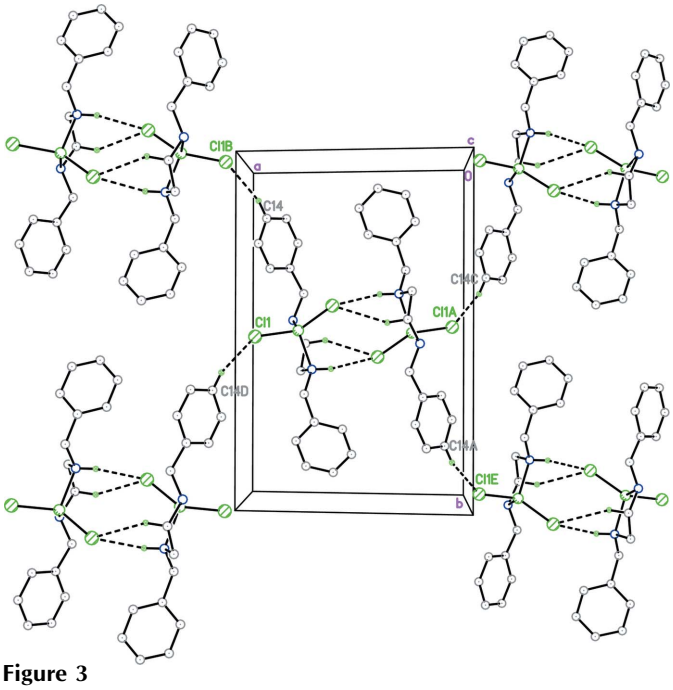


Figure 3
The formation of a hydrogen-bonded sheet built from C—H···Cl interactions. Dashed lines indicate hydrogen bonds. For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry codes: (A) $1-x, 1-y, 1-z$; (B) $2-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (C) $-1+x, \frac{1}{2}-y, -\frac{1}{2}+z$; (D) $2-x, \frac{1}{2}+y, \frac{3}{2}-z$; (E) $-1+x, \frac{3}{2}-y, -\frac{1}{2}+z$.]

were mixed. The reaction mixture was stirred for 2 h at room temperature and then filtered. X-ray quality crystals of (I) were obtained by evaporation of a solution in ethanol.

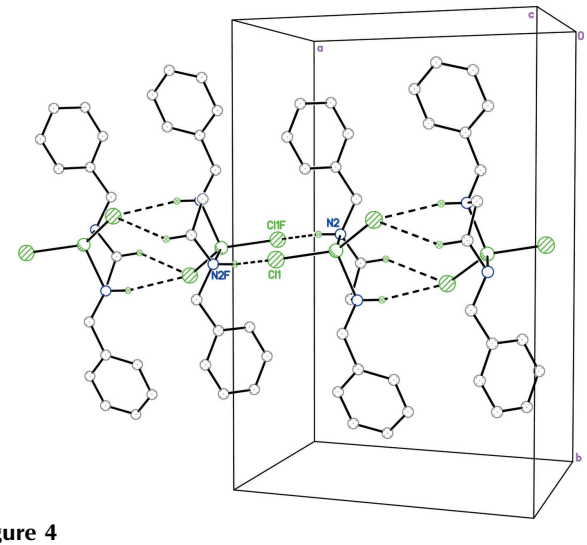


Figure 4
The crystal structure of (I). Neighboring sheets are connected by a pair of N—H···Cl hydrogen bonds (dashed lines), resulting in a three-dimensional network. [Symmetry code: (F) $2-x, 1-y, 1-z$.]

Crystal data

$[ZnCl_2(C_8H_{10}N)_2]$
$M_r = 376.61$
Monoclinic, $P2_1/c$
$a = 10.760$ (3) Å
$b = 16.179$ (4) Å
$c = 10.261$ (3) Å
$\beta = 98.783$ (3)°
$V = 1765.4$ (8) Å^3
$Z = 4$
$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.69$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.36 × 0.28 × 0.15 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.582$, $T_{max} = 0.786$
9067 measured reflections
3096 independent reflections
2232 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.071$
$S = 1.04$
3096 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.5191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl1^{i}	0.91	2.53	3.361 (2)	152
C14—H14···Cl1^{ii}	0.93	2.91	3.788 (4)	158
C9—H9A···Cl2^{iii}	0.97	2.90	3.699 (3)	140
N1—H1···Cl2^{iii}	0.91	2.50	3.363 (2)	159

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

All H atoms were located in a difference Fourier map and then treated as riding atoms, with C—H = 0.93–0.97 Å and N—H = 0.91 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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