metal-organic papers

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Key indicators

Single-crystal X-ray study T = 293 K Mean σ (C–C) = 0.005 Å R factor = 0.032 wR factor = 0.086 Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e. In the title compound, $[ZnCl_2(C_{12}H_{12}N_2O_2)]$, Zn is tetrahedrally coordinated (N₂Cl₂), with N–Zn–N 81.92 (12)° and Cl–Zn–Cl 116.11 (4)°. The tetrahedron is slightly distorted by a weak interaction between Zn and one furaldehyde O

[N,N'-Bis(2-furylmethylene)ethylenediamine]-

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Comment

atom.

dichlorozinc(II)

Schiff base complexes are of great interest for inorganic and bioinorganic chemistry. These complexes exhibit high antitumour and antibacterial activity, and have also been extensively used in catalysis, because of their high activity and selectivity (Jones et al., 1979; Bush & Alcock, 1994). Zinc is considered to be an important inorganic element involved in various biological processes. It exists in many organs, such as the liver, kidney, brain and pancreas, and it plays an important role and has function within proteins, enzymes, etc. The ligand N, N'-bis(furaldehyde)ethylenediamine possesses a remarkable capacity for coordination with transition metals. From a chemical point of view, N, N'-bis(furaldehyde)ethylenediamine is considered to be a good type of chelating ligand, with extensive chemical properties; therefore this ligand can coordinate to transition metals as a bidentate, tridentate or quadridentate ligand, with consequent variable structural properties. In some cases, the O atom of the furaldehyde does not coordinate to the metal ion, such as in the title complex, (I), but it can slightly affect the configuration of the complex and may be a potential coordinating atom.



In the title complex, N,N'-bis(furaldehyde)ethylenediamine is coordinated in a bidentate fashion to Zn *via* two N atoms, and the tetrahedral coordination of Zn is completed by two Cl atoms (Fig. 1 and Table 1). The two furaldehyde moieties are almost coplanar, but are oriented differently so that one has its O atom in closer proximity to the Zn atom than the other. This gives rise to the possibility of a very weak bonding interaction between Zn and O1. This conjecture is supported by the observation that the N1–Zn–(Cl1,Cl2) angles are significantly larger than the N2–Zn–(Cl1,Cl2) angles (Table 1).

The Zn-N bond distances, with values 2.054 (3) and 2.100 (3) Å, are very similar to the Zn-N bond distances in trichloro(N,N-dimethylbiguanidium)zinc(II) (Zhu *et al.*, 2002). The Zn-Cl bond distances in the title compound are slightly less than those found in the morpholine biguanide Zn

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Figure 1

A view of the molecular structure of (I), with the atom-numbering scheme. A possible weak bonding interaction is shown as a dashed line. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

complex, $[ZnCl_3(C_6H_{14}N_5O)]$ [Yang & Zhu, 1991, 1992; 2.245 (1)–2.258 (1) Å].

Experimental

N, N'-Bis(furaldehyde)ethylenediamine was synthesized by following a procedure similar to that in the literature (Shukla et al., 1990). ZnCl₂ from Across was used without further purification. A ZnCl₂ solution was added slowly with stirring to a solution of the ligand, with a final ratio of 1:1(M:L). The yellow solution was filtered and the filtrate was left at room temperature, whereupon colourless crystals formed after a few days.

Crystal data

-	
$[ZnCl_2(C_{12}H_{12}N_2O_2)]$	$D_x = 1.608 \text{ Mg m}^{-3}$
$M_r = 352.51$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3019
a = 8.780 (11) Å	reflections
b = 14.461 (18) Å	$\theta = 2.7 - 25.8^{\circ}$
c = 11.495(15) Å	$\mu = 2.05 \text{ mm}^{-1}$
$\beta = 94.121 \ (18)^{\circ}$	T = 293 (2) K
$V = 1456 (3) \text{ Å}^3$	Block, colourless
Z = 4	$0.38 \times 0.31 \times 0.25 \ \mathrm{mm}$
Data collection	
Bruker SMART CCD	2562 independent reflections
diffractometer	1946 reflections with $I > 2\sigma(I)$
ω scans	$R_{\rm int} = 0.039$
Absorption correction: multi-scan	$\theta_{\rm max} = 25.0^{\circ}$
(SADABS; Sheldrick, 2000)	$h = -10 \rightarrow 9$
$T_{\rm min} = 0.460, T_{\rm max} = 0.567$	$k = -17 \rightarrow 14$
7218 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0476P)^2]$
$wR(F^2) = 0.086$	where $P = (F_o^2 + 2F_c^2)/3$
S = 0.98	$(\Delta/\sigma)_{\rm max} = 0.021$
2562 reflections	$\Delta \rho_{\rm max} = 0.29 \ {\rm e} \ {\rm \AA}^{-3}$
172 parameters	$\Delta \rho_{\rm min} = -0.34 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Zn-N1	2.054 (3)	Zn-Cl1	2.217 (3)
Zn-N2	2.100 (3)	$Zn \cdots O1$	2.882 (4)
Zn-Cl2	2.212 (2)		
N1-Zn-N2	81.92 (12)	N2-Zn-Cl1	110.27 (9)
N1-Zn-Cl2	115.11 (9)	Cl2-Zn-Cl1	116.11 (4)
N2-Zn-Cl2	112.07 (11)	Cl2-Zn-O1	86.59 (9)
N1-Zn-Cl1	116.28 (9)	Cl1-Zn-O1	82.41 (5)

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C-H distances ranging from 0.93 to 0.97 Å and $U_{iso}(H)$ values equal to $1.2U_{eq}$ of the parent C atom.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2000); program(s) used to refine structure: SHELXL97; molecular graphics: SHELXTL (Sheldrick, 1999); software used to prepare material for publication: SHELXTL.

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