Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(1-acetophenone-1*H*-benzotriazole-κN^3)-dichlorozinc(II)

Fangfang Jian,* Hailian Xiao and Pingping Sun

New Materials and Function, Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China

Correspondence e-mail: ffj2003@163169.net

Corr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.045
wR factor = 0.110
Data-to-parameter ratio = 13.4

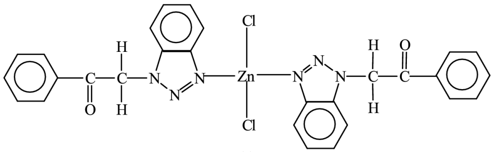
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 November 2003
Accepted 1 December 2003
Online 12 December 2003

In the title compound, $[ZnCl_2(C_6H_4N_3CH_2COPh)_2]$, the zinc ion is coordinated by two Cl^- anions and two N atoms of two triazole ligands, forming a distorted tetrahedral geometry. The molecular structure and packing are stabilized by van der Waals interactions.

Comment

Triazole nuclei appear frequently in the structures of various natural products and biologically active compounds, notably thiamine (vitamin B), penicillins and antibiotics such as micrococcin (James & Watson, 1966). Triazole derivatives have also attracted considerable attention in industry and agriculture because of their significant biological activities (Zhang *et al.*, 2002). Triazole acts as a ligand in transition metal compounds, and such compounds are increasingly being studied in the context of modeling biological systems (Pujar *et al.*, 1988). In this paper, we report the crystal structure of the title compound.



(I)

In the title complex, the Zn and methylene C atoms are coplanar with both benzotriazole ring systems, the planes forming a dihedral angle of 76.2 (2)°. The two independent acetophenone ligands are planar, forming with the benzotriazole planes a dihedral angle of 76.8 (1) Å for Cl-acetophenone with N1-benzotriazole, and 88.5 (1)° for C23-acetophenone with N4-benzotriazole.

The average Zn—Cl distance of 2.209 (1) Å is shorter than the average distances reported for related metal complexes with distorted ZnN_2Cl_2 tetrahedral environments (Salas *et al.*, 1994; Laity & Taylor, 1995; Bei *et al.*, 2001), but comparable to the value of 2.212 (4) Å in $ZnCl_2$(2,9-dimethyl-1,10-phenanthroline) (Preston & Dennard, 1969) and 2.209 (3) Å in $ZnCl_2$(4-vinylpyridine)$_2$ (Steffen & Palenik, 1977). The average Zn—N bond distance of 2.063 (4) Å is comparable to reported average values (Baenziger & Schultz, 1971), but longer than the average value of 2.039 (3) Å in $ZnCl_2$(5,7-dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine)$_2$ (Salas *et al.*, 1994) and 2.027 (3) Å in $ZnCl_2$[1-(5,6-dimethylbenzimidazoly)-3-benzimidazolyl-2-thiapropane] (Matthews *et al.*, 1998).

C—H$\cdots$*Y* (*Y* = O and Cl) interactions (Taylor & Kennard, 1982) are observed (Table 1), the intramolecular interactions co-operating to stabilize the conformation of the complex,

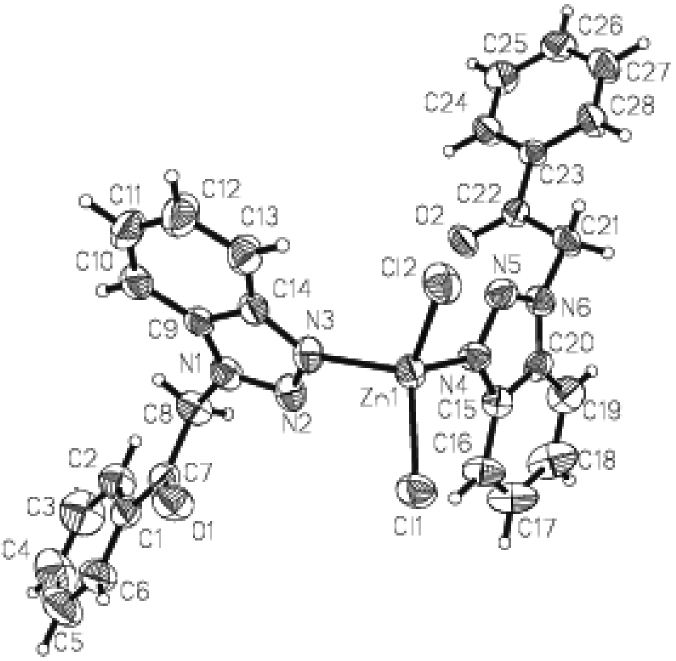


Figure 1

The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

while the intermolecular interactions influence molecular packing.

Experimental

The title compound was prepared by the reaction of 1-acetophenone-1*H*-benzotriazole with $ZnCl_2$ in ethanol solution. Single crystals suitable for X-ray measurements were obtained by recrystallization from an ethanol solution at room temperature.

Crystal data

$[ZnCl_2(C_{14}H_{11}N_3O)_2]$
$M_r = 610.79$
Triclinic, $P\bar{1}$
$a = 9.4490 (19)$ Å
$b = 11.291 (2)$ Å
$c = 13.637 (3)$ Å
$\alpha = 111.70 (3)^\circ$
$\beta = 94.33 (3)^\circ$
$\gamma = 90.97 (3)^\circ$
$V = 1346.4 (6)$ Å^3

$Z = 2$
$D_x = 1.507$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 2$–11°
$\mu = 1.15$ mm^{-1}
$T = 293 (2)$ K
Pillar, colorless
0.35 × 0.25 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
$\theta/2\theta$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.714$, $T_{max} = 0.842$
5045 measured reflections
4729 independent reflections
2798 reflections with $I > 2\sigma(I)$

$R_{int} = 0.036$
$\theta_{max} = 25.3^\circ$
$h = 0 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.110$
$S = 1.05$
4729 reflections
352 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 0.4269P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Table 1

Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···O1	0.93	2.56	2.846 (8)	98
C13—H13A···Cl2	0.93	2.92	3.661 (6)	138
C16—H16A···Cl1	0.93	2.88	3.578 (6)	133
C24—H24A···O2	0.93	2.51	2.803 (6)	98
C10—H10A···O2^{i}	0.93	2.46	3.036 (7)	120
C21—H21A···Cl2^{ii}	0.97	2.78	3.716 (5)	163
C28—H28A···Cl1^{ii}	0.92	2.88	3.601 (6)	135

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $-x, 1-y, 2-z$.

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ of the parent atom.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Natural Science Foundation of Shandong Province (No. Y2002B06).

References

Baenziger, N. C. & Schultz, R. J. (1971). *Inorg. Chem.* **10**, 661–667.

Bei, F. L., Jian, F. F., Yang, X. J., Lu, L. D., Wang, X., Razak, I. A., Shanmuga Sundara Raj, & Fun, H.-K. (2001). *Acta Cryst.* C**57**, 45–46.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

James, M. N. G. & Watson, K. J. (1966). *J. Chem. Soc. C*, pp. 1361–1371.

Laity, H. L. & Taylor, M. R. (1995). *Acta Cryst.* C**51**, 1791–1793.

Matthews, C. J., Clegg, W., Heath, S. L., Martin, N. C., Hill, S. M. N. & Lockhart, J. C. (1998). *Inorg. Chem.* **37**, 199–207.

Preston, H. S. & Kennard, C. H. L. (1969). *J. Chem. Soc. A*, pp. 1956–1961.

Pujar, M. A., Bharamgoudar, T. D. & Sathyanarayana, D. N. (1988). *Transition Met. Chem.* **13**, 423–425.

Salas, J. M., Romero, M. A. & Rahmani, A. (1994). *Acta Cryst.* C**50**, 510–512.

Sheldrick, G. M. (1990). *SHELXTL-PC*. Siemens Analytical X-ray Instruments Inc. Madison, Wisconsin, USA.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Steffen, W. L. & Palenik, G. J. (1977). *Inorg. Chem.* **16**, 1119–1127.

Taylor, R. & Kennard, O. (1982). *J. Am. Chem. Soc.* **104**, 5063–5070.

Zhang, Y., Sun, X. W., Hui, X. P., Zhang, Z. X., Wang, Q. & Zhang, Q. (2002). *Chin. J. Chem.* **20**, 168–173.