Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{2-[2-(1*H*-Benzimidazol-2-yl)ethyliminomethyl]-4-bromophenolato}chlorozinc(II) methanol solvate

Xiao-Hang Qiu* and Xiao-Lan Tong

Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: qiuxh@nankai.edu.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.038
wR factor = 0.096
Data-to-parameter ratio = 17.0

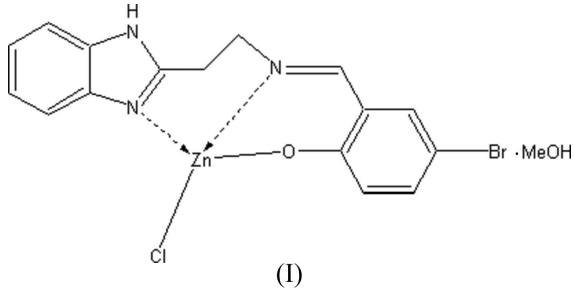
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 September 2005
Accepted 11 October 2005
Online 15 October 2005

The title compound, $[Zn(C_{16}H_{13}BrN_3)Cl]\cdot CH_4O$, has been prepared by the reaction of 2-[2-(1*H*-benzimidazol-2-yl)ethyliminomethyl]-4-bromophenol with zinc(II) chloride. The central Zn atom is coordinated by two N atoms and one O atom from the phenolate ligand, along with a Cl^- anion, which provide a distorted tetrahedral enviroment. Intermolecular O—H···O and N—H···O hydrogen bonds link two Zn complex molecules and two methanol solvent molecules into a centrosymmetric cluster. The crystal packing is further stabilized by weak C—H···Cl hydrogen bonds.

Comment

Benzimidazole and its derivatives have attracted a great deal of attention in recent years due to their biological activites and their strong coordination abilities as multidentate ligands, which provide metal complexes having a broad scope of properties (Carcanagne *et al.*, 2002). Zinc is an essential element for all forms of life, because of its presence at the active sites of various enzymes (Lipscomb & Straeter, 1996). Zinc complexes may be found in numerous biological systems. They function not only as catalytic centres in enzymes, but also as structural elements supporting three-dimensional protein structure (Vallee & Auld, 1990). In this work, we present the crystal structure of a new zinc(II) benzimidazole complex, the title compound, (I) (Fig. 1).



(I)

In (I), the Zn^{II} centre has a distorted tetrahedral coordination, formed by two N atoms and one O atom from the ligand and one Cl^- anion. The Zn—O and Zn—N bond distances (Table 1) correspond to those reported in the literature (Xiao *et al.*, 2004). The Zn1—Cl1 bond distance of 2.1985 (11) Å is smaller than that in a reported benzimidazole zinc complex (Lin *et al.*, 2004). The N2—Zn1—N1 and O1—Zn1—Cl1 bond angles of 93.55 (12) and 108.21 (9)°, respectively, indicate a large distortion of the tetrahedral coordination.

Intermolecular O—H···O and N—H···O hydrogen bonds (Table 2) link two Zn complexes and two methanol molecules

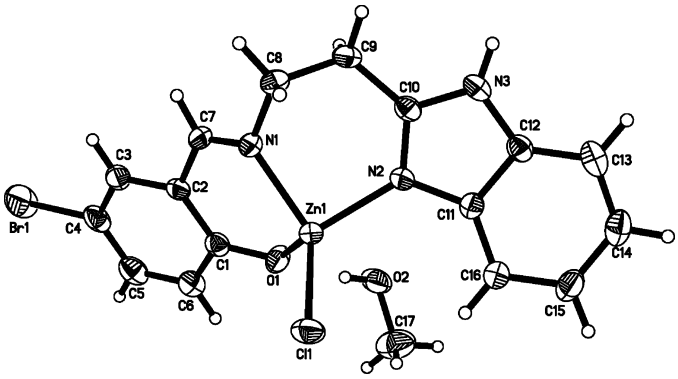


Figure 1
A view of (I), with the atom-labelling scheme and 30% probabilty displacement ellipsoids.

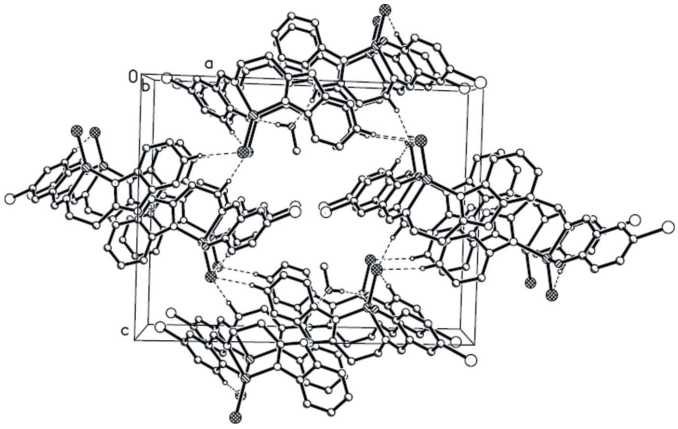


Figure 2
A packing diagram, viewed down the *b* axis. H atoms not participating in the intermolecular hydrogen bonds (dashed lines) have been omitted for clarity.

into a centrosymmetric cluster. The crystal packing (Fig. 2) is further stabilized by weak C—H···Cl hydrogen bonds (Table 2).

Experimental

The title compound was prepared by adding a methanol solution (5 ml) of zinc chloride (0.1 mmol) to a methanol solution (10 ml) of *N*-(5-bromosalicylidine)-2-aminoethylbenzimidazole (0.1 mmol; Das & Dash, 1995) neutralized with triethylamine (0.1 mmol). The mixture was stirred for about 2 h and then filtered. The filtrate was slowly evaporated at room temperature to yield colourless crystals of (I) suitable for X-ray analysis. Analysis, calculated for $C_{17}H_{17}ClBrZnN_3O_2$: C 42.88, H 3.60, N 8.83%; found: C 42.36, H 3.52,*N* 9.01%.

Crystal data

$[Zn(C_{16}H_{13}BrN_3O)Cl]\cdot CH_4O$
M_r = 476.07
Monoclinic, $P2_1/c$
a = 7.4425 (17) Å
b = 13.989 (3) Å
c = 18.936 (4) Å
β = 105.739 (8)°
V = 1897.6 (7) Å^3
Z = 4
D_x = 1.666 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2554 reflections
θ = 2.3–23.5°
μ = 3.56 mm^{-1}
T = 294 (2) K
Block, colourless
0.22 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.495, T_{max} = 0.653
10548 measured reflections
3864 independent reflections
2350 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 26.4°
$h = -9 \rightarrow 7$
$k = -17 \rightarrow 9$
$l = -22 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.096
S = 1.02
3864 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.893P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.940 (3)	Zn1—N1	2.018 (3)
Zn1—N2	2.002 (3)	Zn1—Cl1	2.1985 (12)
O1—Zn1—N2	120.83 (12)	C1—O1—Zn1	122.2 (3)
O1—Zn1—N1	92.78 (12)	C7—N1—Zn1	123.0 (3)
N2—Zn1—N1	93.55 (12)	C8—N1—Zn1	116.9 (3)
O1—Zn1—Cl1	108.21 (9)	C10—N2—Zn1	125.3 (3)
N2—Zn1—Cl1	112.08 (9)	C11—N2—Zn1	128.0 (2)
N1—Zn1—Cl1	129.27 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.84	2.655 (4)	172
N3—H3A···O2^{ii}	0.86	1.88	2.716 (4)	163
C6—H6···Cl1^{iii}	0.93	2.83	3.600 (5)	141
C8—H8B···Cl1^{iv}	0.97	2.88	3.589 (4)	131
C14—H14···Cl1^{v}	0.93	2.82	3.698 (4)	159

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

H atoms were included in calculated positions and refined as riding, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2–1.5U_{eq} of the parent atom.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-NT* (Bruker, 1998); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 1998); software used to prepare material for publication: *SHELXTL-NT*.

This work was supported by the Innovation Foundation of Nankai University.

References

Bruker (1998). *SMART-NT* (Version 5.1), *SAINT-NT* (Version 5.1) and *SHELXTL-NT* (Version 5.1). Bruker AXS, Madison, Wisconsin, USA.
Carcanagne, D., Shue, Y.-K., Shue, M. A., Wuonola, M. A. & Uria-Nickelsen, M. (2002). *J. Med. Chem.* **45**, 4300–4309.
Das, N. N. & Dash, A. C. (1995). *Polyhedron*, **14**, 1221–1227.

Lin, X.-J., Shen, Z. & Xu, H.-J. (2004). *Inorg. Chem. Commun.* **7**, 1167–1169.
Lipscomb, W. N. & Straeter, N. (1996). *Chem. Rev.* **96**, 2375–2434.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Vallee, B. L. & Auld, D. S. (1990). Biochemistry, 29, 5647–5659.
Xiao, B., Han, H.-Y. & Meng, X.-R. (2004). *Inorg. Chem. Commun.* **7**, 378–381.