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trans-Bis(methanol-κO)bis(2-quinolinecarboxylato-$\kappa^2 N,O$)zinc(II)

Zheng-Yu Yue,* Chao Cheng, Po Gao and Peng-Fei Yan

College of Chemistry and Chemical Engineering, Heilongjiang University, Harbin 150080, People's Republic of China

Correspondence e-mail: yuezhengyu@vip.sina.com

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Key indicators

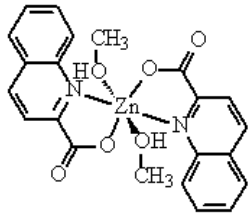
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.071
Data-to-parameter ratio = 14.2

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

The title complex, $[Zn(C_{10}H_6NO_2)_2(CH_3OH)_2]$, is a neutral mononuclear complex containing a Zn^{II} ion in a six-coordinate environment. The Zn^{II} center, located on a crystallographic center of symmetry, displays a distorted octahedral geometry, with two 2-quinolinecarboxylate and two methanol ligands, all in *trans* configurations. The complex molecules are linked together by O—H···O hydrogen bonds between methanol molecules and carboxylate groups to form a two-dimensional framework.

Comment

2-Quinolinecarboxylic acid (quinaldinic acid) is a metabolite of tryptophan and is known to be a potent chelator of transition metal ions (Martell & Smith, 1974). Crystal structures of quinaldinic acid complexes have been determined for several metal ions, including Mn^{II} (Haendler, 1996; Okabe & Koizumi, 1997), Fe^{II} (Okabe & Makino, 1998), Co^{II} (Okabe & Makino, 1999), Cu^{II} (Haendler, 1986) and Zn^{II} (Zevaco *et al.*, 1998); in most cases, the auxiliary ligand is a water molecule, except for the Zn^{II} complex, which contains a 1-methylimidazole molecule as ligand. Recently, we have carried out the structural analysis of a Zn^{II} complex, $[Zn(C_{10}H_6NO_2)_2(MeOH)_2]$, (I), with a methanol molecule as secondary ligand, and we report the result here.



(I)

As shown in Fig. 1, the molecule of (I) is centrosymmetric. The six-coordinate geometry found in this study is similar to those of the above-mentioned analogous complexes. The 2-quinolinecarboxylate ligand and the Zn^{II} ion form a five-membered chelating ring, which is also present in the reported Mn^{II}, Fe^{II}, Co^{II}, Cu^{II} and Zn^{II} complexes. The carboxyl group of the quinolinecarboxylate moiety is ionized and almost coplanar with the plane defined by the aromatic system [the dihedral angle is 2.01 (3)°]. This conformation differs from that in the analogous Zn^{II} complex [Zn(2-quinolinecarboxylato)$_2$(1-methylimidazole)$_2$] (Zevaco *et al.*, 1998), in which the carbonyl O atom points away from the aromatic plane, with an O—C—[C—C]$_{ar}$ torsion angle of ∼15.6°. This difference is a result of the presence of weak intermolecular hydrogen-

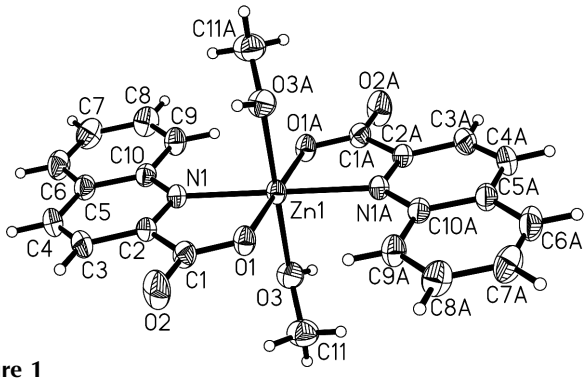


Figure 1
The molecular structure of the title complex, showing the atom-numbering scheme and 30% probability displacement ellipsoids. The suffix *A* corresponds to symmetry code (i) in Table 1.

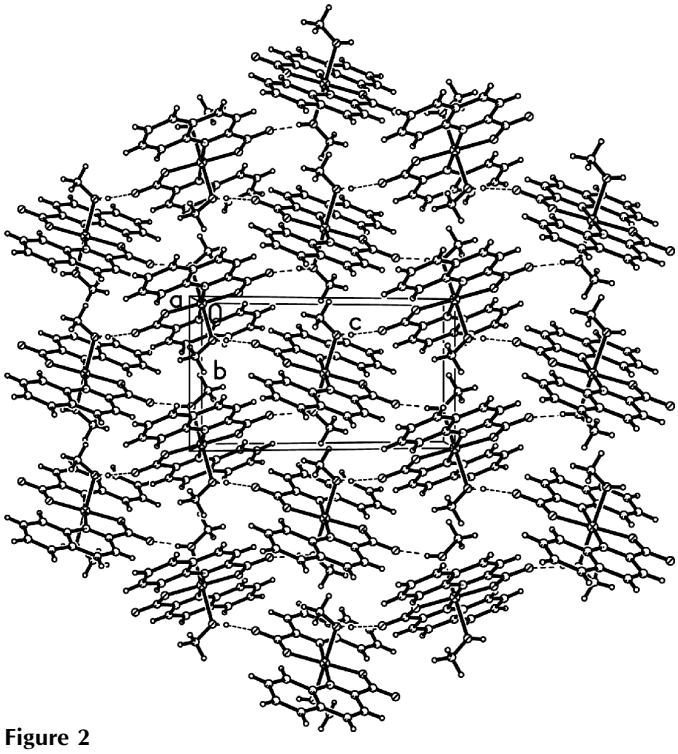


Figure 2
The two-dimensional hydrogen bonding, shown as dashed lines.

bonding interactions between adjacent molecules. In the crystal packing, the complex molecules are linked through O—H···O hydrogen-bonding interactions between the uncoordinated carboxyl O atoms and the coordinated methanol O atoms, thus forming a two-dimensional framework (Fig. 2). The O···O^{ii} and O^{ii}···H distances are 2.659 (3) and 1.87 (3) Å, respectively, and the O—H···O^{ii} angle is 168 (3)° [symmetry code: (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$].

Experimental

To a colorless solution of quinoline-2-carboxylic acid (0.4 mmol) dissolved in MeOH (25 ml) in the presence of Et_3N (two drops), a solution of $Zn(NO_3)_2{\cdot}6H_2O$ (0.2 mmol) in MeOH (25 ml) was added. The resulting solution was filtered and left to stand at room temperature. Crystals suitable for X-ray analysis were obtained after several days.

Crystal data

$[Zn(C_{10}H_6NO_2)_2(CH_4O)_2]$	$D_x = 1.574$ Mg m^{-3}
$M_r = 473.77$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 53 reflections
$a = 10.528$ (2) Å	$\theta = 3.2$–$27.5°$
$b = 7.377$ (5) Å	$\mu = 1.27$ mm^{-1}
$c = 13.551$ (5) Å	$T = 293$ (2) K
$\beta = 108.169$ (8)°	Cube, colorless
$V = 999.9$ (7) Å^3	0.20 × 0.20 × 0.20 mm
$Z = 2$	

Data collection

Rigaku Mercury/MSC CCD diffractometer	2075 independent reflections
ω scans	1803 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)	$R_{int} = 0.019$
$T_{min} = 0.615$, $T_{max} = 0.775$	$\theta_{max} = 27.5°$
4476 measured reflections	$h = -6 \rightarrow 13$
	$k = -8 \rightarrow 9$
	$l = -17 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 0.5647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.027$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.071$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.25$ e Å^{-3}
2075 reflections	
146 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1^{i}	2.003 (1)	Zn1—N1	2.231 (1)
Zn1—O3^{i}	2.170 (2)		
O1^{i}—Zn1—O1	180	O1—Zn1—N1	78.38 (5)
O1^{i}—Zn1—O3^{i}	90.76 (6)	O3^{i}—Zn1—N1	89.25 (6)
O1—Zn1—O3^{i}	89.24 (6)	O3—Zn1—N1	90.75 (6)
O1^{i}—Zn1—N1	101.62 (5)	N1—Zn1—N1^{i}	180

Symmetry codes: (i) $-x, -y, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{ii}	0.80 (3)	1.87 (3)	2.659 (5)	168 (3)

Symmetry code: (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

All H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and included as riding [with U_{iso}(H) = 1.5U_{eq}(C) (methyl H atoms) or 1.2U_{eq}(C) (other H atoms)], except for the methanol atom H3, which was located in a difference Fourier map and refined isotropically.

Data collection: *CrystalClear* (Molecular Structure Corporation/Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (1998). *SHELXTL.* Version 5.16. Bruker AXS Inc., Madison, Wisconsin, USA.
Haendler, H. M. (1986). *Acta Cryst.* C**42**, 147–149.
Haendler, H. M. (1996). *Acta Cryst.* C**52**, 801–803.
Martell, A. E. & Smith, R. M. (1974). *Critical Stability Constants*, Vol. 1, pp. 78, 372, Vol. 2, p. 219. New York: Plenum Press.
Molecular Structure Corporation/Rigaku (2000). *CrystalClear. d*TREK* Version 7.4SSI. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA, and Rigaku Corporation, 3-9-12 Akishima, Tokyo, Japan.
Okabe, N. & Koizumi, M. (1997). *Acta Cryst.* C**53**, 852–854.
Okabe, N. & Makino, T. (1998). *Acta Cryst.* C**54**, 1279–1280.
Okabe, N. & Makino, T. (1999). *Acta Cryst.* C**55**, 300–302.
Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Zevaco, T. A., Gorls, H. & Dinjus, E. (1998). *Inorg. Chim. Acta*, **269**, 283–286.