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Key indicators

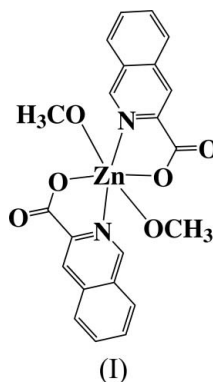
Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.033
 wR factor = 0.086
Data-to-parameter ratio = 16.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Bis(isoquinoline-3-carboxylato- $\kappa^2\text{N},\text{O}$)-
bis(methanol- κO)zinc(II)

In the crystal structure of the title complex, $[\text{Zn}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{CH}_3\text{OH})_2]$, the Zn atom at a center of inversion has distorted octahedral coordination geometry and is bonded to two quinoline N atoms, two carboxylate O atoms and two methanol O atoms. Two isoquinoline-3-carboxylate ligands lie in *trans* positions, forming the equatorial plane, and the two methanol ligands occupy the axial positions. The complex molecules are linked together by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between the methanol ligands and neighboring carboxylate groups.

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Comment

Transition metal ions are well known to have many biological functions, such as antimicrobial or fungicidal activity (Okide *et al.*, 2000; Patel *et al.*, 1999), or have redox activity such as Fenton-type reactions (Kasprzak, 2002) inducing toxicity or carcinogenesis. Zn^{II} is well known for its insulinomimetic activity (*e.g.* Matsumoto *et al.*, 2005). In previous papers, the crystal structures of the Fe^{II} (II), Co^{II} (III), Ni^{II} (IV) and Cu^{II} (V) complexes of isoquinoline-3-carboxylate have been reported (Okabe & Muranishi, 2003; Okabe *et al.*, 2004). We report here the structure of the corresponding Zn^{II} complex, (I).



The structure of (I) is shown in Fig. 1. It is isomorphous with the analogs (II)–(V), with the metal ion at a center of inversion and a distorted octahedral coordination geometry.

The two bidentate ligands lie *trans* to each other. They are coordinated to the central metal ion, through the isoquinoline N atoms and the carboxylate O atoms to form five-membered rings in the equatorial plane. Two O atoms of the methanol ligands complete the octahedron at the axial positions. The coordination bond distances of (I) are listed in Table 1, together with those of (II)–(V).

As shown in Table 1, coordination bond distances, $M-\text{N}$, decrease in the order (II) > (III) > (IV) > (V) < (I). The reverse of this order coincides well with the Irving–Williams

series, which indicates the general stability sequence of octahedral metal complexes in the order $\text{Fe} < \text{Co} < \text{Ni} < \text{Cu} > \text{Zn}$. The longest axial coordination bond distance ($M\text{—O1M}$) of (V) is explained by the Jahn–Teller effect.

The hydrogen-bonding parameters of (I)–(V) are listed in Table 2 for comparison. All structures are stabilized by a similar intermolecular $\text{O—H}\cdots\text{O}$ hydrogen-bonding pattern between methanol ligands and the neighboring carboxylate groups. A stacking interaction is also observed between the ligands with a mean distance of 3.366 (4) Å.

Experimental

Colorless plate-shaped crystals of (I) were obtained by slow evaporation of a methanol solution of a mixture of isoquinoline-3-carboxylic acid (5 mg) dissolved in methanol (3 ml) and ZnSO_4 (2.1 mg) dissolved in methanol (2 ml) (molar ratio 4:1) at room temperature.

Crystal data

$[\text{Zn}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{CH}_4\text{O})_2]$	$D_x = 1.577 \text{ Mg m}^{-3}$
$M_r = 473.79$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
$a = 10.672$ (1) Å	$\theta = 14.2\text{--}15.0^\circ$
$b = 6.301$ (2) Å	$\mu = 1.27 \text{ mm}^{-1}$
$c = 15.091$ (1) Å	$T = 296.2 \text{ K}$
$\beta = 100.567$ (9)°	Plate, colorless
$V = 997.6$ (3) Å ³	$0.40 \times 0.10 \times 0.10 \text{ mm}$
$Z = 2$	

Data collection

Rigaku AFC-5R diffractometer	$R_{\text{int}} = 0.025$
ω – 2θ scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 13$
$T_{\text{min}} = 0.858$, $T_{\text{max}} = 0.880$	$k = 0 \rightarrow 8$
2627 measured reflections	$l = -19 \rightarrow 19$
2288 independent reflections	3 standard reflections
1515 reflections with $I > 2\sigma(I)$	every 150 reflections
	intensity decay: 0.1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 0.6344P]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.086$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
2288 reflections	$\Delta\rho_{\text{min}} = -0.47 \text{ e \AA}^{-3}$
143 parameters	
H-atom parameters constrained	

Table 1

Comparative selected geometric parameters (Å, °).

<i>M</i>	(II) ^a	(III) ^b	(IV) ^b	(V) ^b	(I)
<i>M</i> –O1	2.050 (2)	2.050 (2)	2.036 (2)	1.963 (2)	2.060 (2)
<i>M</i> –O1 <i>M</i>	2.196 (2)	2.149 (2)	2.116 (2)	2.516 (2)	2.214 (2)
<i>M</i> –N1	2.167 (2)	2.110 (2)	2.049 (2)	1.979 (2)	2.096 (2)
N1–C1	1.372 (4)	1.376 (3)	1.369 (3)	1.372 (3)	1.370 (4)
N1–C9	1.315 (4)	1.314 (3)	1.314 (3)	1.315 (3)	1.313 (3)
C1–C2	1.366 (4)	1.357 (3)	1.357 (3)	1.361 (3)	1.363 (3)
C2–C3	1.414 (4)	1.413 (3)	1.412 (3)	1.412 (3)	1.407 (4)
C3–C8	1.415 (5)	1.416 (3)	1.416 (4)	1.418 (3)	1.416 (4)
C8–C9	1.416 (4)	1.415 (3)	1.417 (3)	1.414 (3)	1.419 (4)
O1– <i>M</i> –O1 <i>M</i>	89.97 (9)	89.65 (6)	90.81 (7)	90.41 (7)	89.73 (7)
O1– <i>M</i> –N1	78.86 (9)	80.21 (6)	81.63 (7)	83.77 (7)	80.67 (8)
O1 <i>M</i> – <i>M</i> –N1	92.43 (9)	87.44 (7)	92.55 (7)	88.14 (7)	87.78 (7)

Notes: (a) Okabe & Muranishi (2003c); (b) Okabe *et al.* (2004).

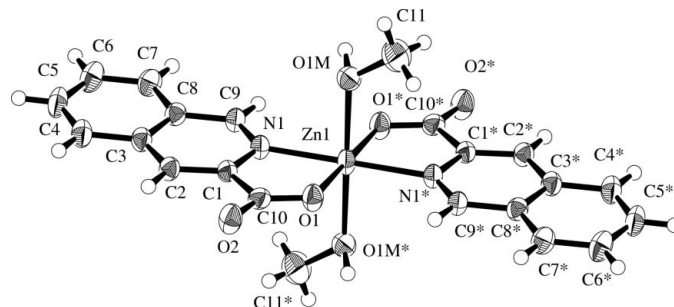


Figure 1

ORTEP (Johnson, 1976) drawing of (I), with the atomic numbering scheme. Displacement ellipsoids for non-H atoms correspond to 50% probability. Atoms labeled with an asterisk are at the symmetry position $-x, 1 - y, 1 - z$.

Table 2

Hydrogen-bonding geometry (Å, °).

	<i>D</i> – <i>H</i> ⋯ <i>A</i>	<i>D</i> – <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> – <i>H</i> ⋯ <i>A</i>
(I)	O1 <i>M</i> –H1 <i>M</i> ⋯O2 ⁱ	0.93	1.75	2.613 (3)	153
(II) ^a	O1 <i>M</i> –H1 <i>M</i> ⋯O2 ⁱⁱ	0.97	1.66	2.617 (3)	170
(III) ^b	O1 <i>M</i> –H1 <i>M</i> ⋯O2 ⁱⁱ	0.96	1.65	2.604 (2)	172
(IV) ^b	O1 <i>M</i> –H1 <i>M</i> ⋯O2 ⁱⁱ	0.90	1.70	2.600 (3)	178
(V) ^b	O1 <i>M</i> –H1 <i>M</i> ⋯O2 ⁱⁱ	0.82	1.86	2.679 (3)	175

Symmetry code: (i) $x, 1 + y, z$; (ii) $-x, -1 - y, -z$. Notes: (a) Okabe & Muranishi (2003c); (b) Okabe *et al.* (2004).

All H atoms were located in difference Fourier maps, and then were regenerated at ideal positions [$\text{C–H} = 0.96$ (methyl), 0.93 \AA (other H atoms); $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{methyl C})$ and $1.2U_{\text{eq}}(\text{other C})$]. The weighting schemes for both structures were optimized.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2000); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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