

Wen-Bing Yuan, Ming Liu,
Shan-Shan Wu, Hai-Yang Wang
and Qi Zhang*Hainan Provincial Key Laboratory of Fine
Chemicals, Hainan University, Hainan 570228,
People's Republic of ChinaCorrespondence e-mail:
zhangqi_hainu@163.com

Key indicators

Single-crystal X-ray study
 $T = 153$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.022
 wR factor = 0.067
Data-to-parameter ratio = 14.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Diaquabis(isoquinoline-1-carboxylato- $\kappa^2\text{N},\text{O}$)-
manganese(II) dihydrate

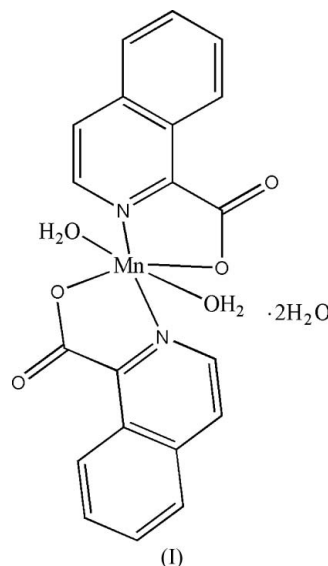
The centrosymmetric title complex, $[\text{Mn}(\text{C}_{10}\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, contains a six-coordinate Mn^{II} ion displaying distorted octahedral coordination geometry defined by the two isoquinoline N atoms, two O atoms of the carboxylate groups and two O atoms of the water molecules. The isoquinoline-1-carboxylate ligands lie in *trans* positions with the two water ligands occupying the axial positions. The complex molecules are linked together by intermolecular hydrogen bonds involving the uncoordinated water molecules.

Received 17 October 2006

Accepted 31 October 2006

Comment

Isoquinoline-1-carboxylic acid (IQCA) is a potent inhibitor of the copper enzyme dopamine β -hydroxylase (Townes *et al.*, 1990). To date, the crystal structures of the Cu^{II} (Tomas *et al.*, 1999), Sn^{IV} (Smith *et al.*, 1995), Co^{II} and Ni^{II} (Okabe & Muranishi, 2002), and Zn^{II} complexes (Okabe & Muranishi, 2003) of IQCA have been reported. Here, we have obtained crystals of the title compound, (I), and carried out the structural analysis of this Mn^{II} complex.



Complex (I) is hexacoordinate, with the Mn^{II} ion at a centre of symmetry, similar to the Co^{II} , Ni^{II} and Zn^{II} complexes. The two isoquinoline-1-carboxylate ligands chelate the metal through the N atom and one O atom to form the equatorial plane. Two water molecules are located at the axial positions and complete the octahedron. The isoquinoline-1-carboxylate and the Mn^{II} ion form a five-membered ring, which is also present in the other complexes. In this ring, the $\text{Mn}-\text{O}$ bond length is 2.1408 (8) Å and the $\text{Mn}-\text{N}$ bond length is 2.2196 (9) Å. The previously reported $M-\text{N}$ bond lengths are

2.096 (2) (Co^{II}), 2.039 (3) (Ni^{II}), 2.084 (3) (Zn^{II}), and 1.957 (3) and 1.969 (3) Å (Cu^{II}). These results indicate that the order of stability of these complexes corresponds to the well known Irving–Williams series, Mn^{II} < Co^{II} < Ni^{II} < Cu^{II} < Zn^{II}. These molecules are linked together by a hydrogen-bonding network involving the complex molecules and uncoordinated water molecules.

Experimental

Compound (I) was obtained by slow evaporation of a solution in methanol–water (50:50 v/v) of a mixture of isoquinoline-1-carboxylic acid and Mn(OAc)₂·2H₂O (molar ratio 2:1).

Crystal data

[Mn(C ₁₀ H ₆ NO ₂) ₂ (H ₂ O) ₂] ₂ ·2H ₂ O	Z = 2
<i>M_r</i> = 471.32	<i>D_x</i> = 1.592 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 12.4828 (3) Å	<i>μ</i> = 0.72 mm ⁻¹
<i>b</i> = 5.2252 (1) Å	<i>T</i> = 153 (2) K
<i>c</i> = 15.2252 (4) Å	Pillar, red
<i>β</i> = 98.057 (1)°	0.42 × 0.33 × 0.30 mm
<i>V</i> = 983.26 (4) Å ³	

Data collection

Rigaku R-AXIS RAPID diffractometer	9138 measured reflections
<i>ω</i> scans	2253 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2159 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T_{min}</i> = 0.751, <i>T_{max}</i> = 0.805	<i>R_{int}</i> = 0.013
	<i>θ_{max}</i> = 27.5°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.4716P]$
$R[F^2 > 2\sigma(F^2)] = 0.022$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.067$	(Δ/σ) _{max} = 0.001
<i>S</i> = 0.98	$\Delta\rho_{max} = 0.38 \text{ e } \text{Å}^{-3}$
2253 reflections	$\Delta\rho_{min} = -0.26 \text{ e } \text{Å}^{-3}$
159 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.031 (2)

Table 1

Hydrogen-bond geometry (Å, °).

D–H...A	D–H	H...A	D...A	D–H...A
O3–H3A...O4	0.831 (9)	1.973 (9)	2.8038 (12)	178.6 (18)
O3–H3B...O1 ⁱ	0.828 (9)	1.957 (10)	2.7728 (11)	168.6 (19)
O4–H4A...O2 ⁱⁱ	0.821 (9)	1.882 (10)	2.6980 (12)	171.9 (18)
O4–H4B...O4 ⁱⁱⁱ	0.816 (9)	2.108 (10)	2.9038 (9)	165.1 (18)

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

The H atoms of water molecules were found in a difference Fourier map and restrained with an O–H distance of 0.82 Å. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances of 0.95 Å and with $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$.

Data collection: RAPID-AUTO (Rigaku, 2004); cell refinement: RAPID-AUTO; data reduction: RAPID-AUTO; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

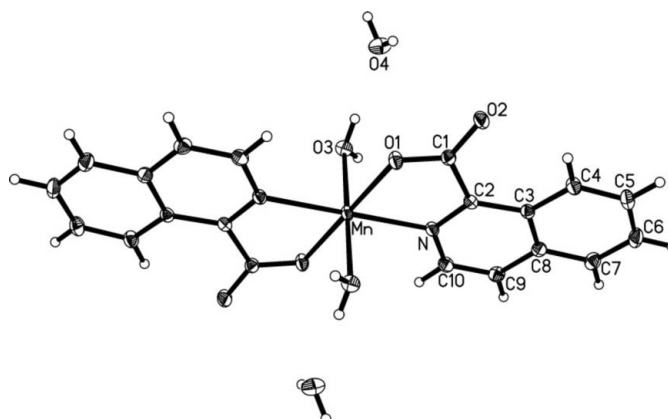


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry code $(-x + 1, -y + 1, -z + 1)$.

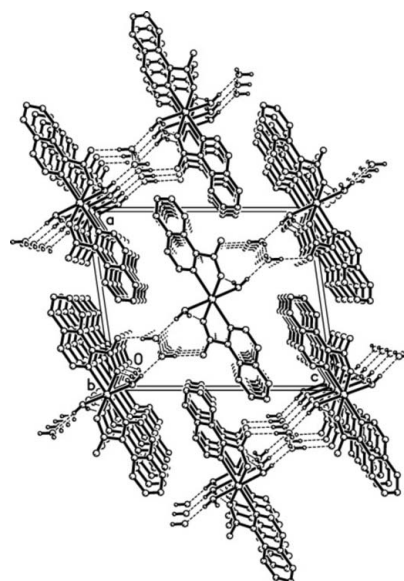


Figure 2

The crystal packing of the title complex (I), viewed along the *a* axis. In the crystal structure, the molecules stack along the *a* axis. Dashed lines indicate hydrogen bonds.

We thank the Open Fund (grant No. HNF2006005) of Hainan Provincial Key Laboratory of Fine Chemicals for financial support.

References

- Okabe, N. & Muranishi, Y. (2002). *Acta Cryst.* **C58**, m578–m580.
- Okabe, N. & Muranishi, Y. (2003). *Acta Cryst.* **E59**, m247–m248.
- Rigaku (2004). *RAPID AUTO*. Version 3.0. Manual No. MJ13159A01. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Smith, F. E., Khoo, L. E., Chia, L. S. & Hynes, R. C. (1995). *Can. J. Chem.* **73**, 1436–1443.
- Tomas, O. P. A., Viossat, B., Bachet, B. & Nguyen-Huy, D. (1999). *Z. Kristallogr. New Cryst. Struct.* **214**, 61–62.
- Townes, S., Titone, S. & Rosenberg, R. C. (1990). *Biochim. Biophys. Acta*, **1037**, 240–247.