

Jin-Hua Cai,^{a*} Ying-Heng
Huang^a and Yi-Min Jiang^b^aDepartment of Chemistry and Life Science, Hechi University Yizhou, Guangxi 546300, People's Republic of China, and ^bCollege of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China

Correspondence e-mail: cjhzse@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.037
wR factor = 0.098
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Triaqua[*N*-(5-formylsalicylidene)glycinato(2-)- $\kappa^3\text{O},\text{N},\text{O}'$]zinc(II) monohydrate

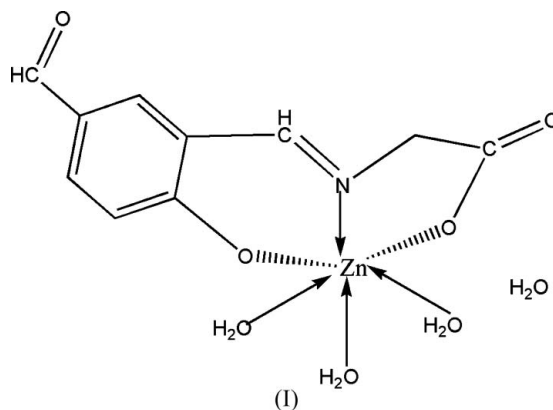
The title complex, $[\text{Zn}(\text{C}_{10}\text{H}_7\text{NO}_4)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$, is a mononuclear complex. The Zn^{II} atom is coordinated by one N and two O atoms from one Schiff base ligand, and by three O atoms from water molecules. In the crystal structure, the molecules are linked through intra- and intermolecular O—H...O hydrogen bonds, forming a three-dimensional framework.

Received 24 August 2006

Accepted 28 August 2006

Comment

Transition metal complexes containing Schiff bases have been of great interest for many years (Archer & Wang, 1990; Chang *et al.*, 1998). These complexes play an important role in the development of coordination chemistry, because of their catalytic activity in some industrial (Wu *et al.*, 2001) and biochemical processes (Kono & Fridovich, 1983; May *et al.*, 2004) and some polymerization reactions (Dutta & Das, 1988). In addition, transition metal complexes of salicylaldehyde-amino acid Schiff bases are found to behave analogously to those of pyridoxal-amino acid Schiff bases (Snell *et al.*, 1963). We thus focused our attention on the assembly of transition metal ions with flexible ligands, and the crystal structures of a few Schiff base complexes of the 5-formylsalicylaldehyde derivative have been reported from this laboratory (Zeng *et al.*, 2003; Liu *et al.*, 2006; Cai *et al.*, 2006). As an extension of the work on these complexes, the title zinc(II) complex, (I), is reported here.



The title compound is a mononuclear zinc(II) complex (Fig. 1) consisting of an (*N*-5-formylsalicylidene)glycinato-*N,O,O*)triqua- Zn^{II} unit and a solvent water molecule. The Zn^{II} atom is coordinated by the imine N, the phenolate O and one carboxylate O atom of the tridentate Schiff base ligand. The octahedral geometry is completed by the three O atoms of the coordinated water molecules. The equatorial plane is

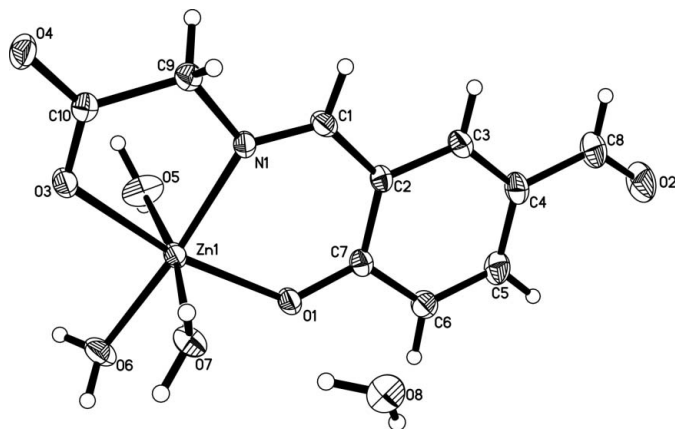


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

formed by four O atoms (O1, O5, O3, O7), while the axial sites are occupied by O6 and N1. The Zn–O and Zn–N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base zinc(II) complexes (Garcia-Raso *et al.*, 2000; Hermann *et al.*, 2002). In the crystal structure, the molecules are linked through intermolecular O–H...O hydrogen bonds (Table 2), forming a three-dimensional network structure.

It is interesting to note that, since 5-formylsalicylaldehyde has two aldehyde groups, a double Schiff base ligand should form from the reaction of glycine and 5-formylsalicylaldehyde. However, Fig. 1 shows that there is only one imine group in the complex. This is because, in the case of the imine ortho to the hydroxyl, the imino N, hydroxy O and Ni atoms can form a six-membered chelate ring stabilizing the imine, whereas this is not possible in the other imine. As a result, the C=N double bond is broken down by attack by water.

Experimental

All reagents were of commercially available grade and were used without further purification. A mixture of 5-formylsalicylaldehyde (0.1 mmol, 0.134 g), glycine (0.2 mmol, 0.15 g) and KOH (0.2 mmol, 0.112 g) were dissolved in aqueous methanol (80% 20 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added an aqueous solution (10 ml) of $\text{ZnCl}_2 \cdot 7\text{H}_2\text{O}$ (0.2 mmol, 0.520 g), with stirring. The mixture was stirred and refluxed at 323 K for 4 h, and then cooled to room temperature. After filtration, the filtrate was left to stand at room temperature. Yellow crystals suitable for X-ray diffraction were obtained in a yield of 42%. Analysis found: C 35.15, H 4.42, N 4.16%; calculated for $\text{C}_{10}\text{H}_{13}\text{NO}_8\text{Zn}$: C 35.19, H 4.43, N 4.14%.

Crystal data

$[\text{Zn}(\text{C}_{10}\text{H}_7\text{NO}_4)(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$	$Z = 8$
$M_r = 342.60$	$D_x = 1.686 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 11.232(4) \text{ \AA}$	$\mu = 1.86 \text{ mm}^{-1}$
$b = 7.759(3) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 30.973(11) \text{ \AA}$	Block, yellow
$V = 2699.3(16) \text{ \AA}^3$	$0.15 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	12398 measured reflections
φ and ω scans	2947 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2270 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.768$, $T_{\max} = 0.866$	$R_{\text{int}} = 0.042$
	$\theta_{\max} = 27.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.3452P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.05$	$\Delta\rho_{\max} = 0.44 \text{ e \AA}^{-3}$
2947 reflections	$\Delta\rho_{\min} = -0.75 \text{ e \AA}^{-3}$
213 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1–O1	2.028 (2)	Zn1–O3	2.137 (2)
Zn1–N1	2.080 (2)		
O1–Zn1–N1	88.74 (8)	N1–Zn1–O3	78.31 (9)
O1–Zn1–O3	166.54 (8)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O8–H8B...O7	0.85 (2)	1.99 (2)	2.838 (4)	175 (6)
O7–H7B...O4 ⁱ	0.837 (17)	1.917 (18)	2.754 (3)	178 (3)
O5–H5A...O8 ⁱⁱ	0.865 (18)	1.85 (2)	2.675 (4)	159 (4)
O5–H5B...O1 ⁱⁱⁱ	0.843 (18)	1.91 (2)	2.740 (3)	169 (4)
O6–H6A...O4 ^{iv}	0.830 (17)	1.848 (19)	2.669 (3)	170 (3)
O6–H6B...O4 ^v	0.830 (18)	2.22 (3)	2.977 (3)	152 (3)
O7–H7A...O3 ^{iv}	0.827 (17)	1.928 (19)	2.748 (3)	171 (3)

Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, z$; (ii) $x, y - 1, z$; (iii) $-x + \frac{1}{2}, y - \frac{1}{2}, z$; (iv) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (v) $x - \frac{1}{2}, y, -z + \frac{1}{2}$.

The coordinated and uncoordinated water H atoms were located in a difference Fourier map and refined isotropically, with the O–H distances restrained to 0.83 (3) and 0.86 (2) \AA , and refined as riding in their as-found relative positions. The C-bound H atoms were placed in calculated positions, with aryl C–H = 0.93 \AA and methylene C–H = 0.97 \AA , and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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*.

This work was supported by the Natural Science Foundation of the Guangxi Chuang Autonomous Region of the People's Republic of China (grant No. 0339034) and the Science Research Foundation of Guangxi Universities of the People's Republic of China.

References

- Archer, R. D. & Wang, B. (1990). *Inorg. Chem.* **29**, 39–43.
- Bruker (1998). *SMART* (Version 5.628) and *SAINTE* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Cai, J.-H., Huang, Y.-H. & Jiang, Y.-M. (2006). *Acta Cryst. E* **62**, m2064–m2066.
- Chang, S., Jones, L., Wang, C. M., Henling, L. M. & Grubbs, R. H. (1998). *Organometallics*, **17**, 3460–3465.
- Dutta, R. L. & Das, B. R. (1988). *J. Sci. Ind. Res.* **47**, 547–551.
- Garcia-Raso, A., Fiol, J. J., Lopez-zafra, A., Mata, Z., Espinosa, E. & Molins, E. (2000). *Polyhedron*, **19**, 673–677.
- Hermann, J., Schumacher, D. & Erxleben, A. (2002). *Eur. J. Inorg. Chem.* pp. 2276–2280.
- Kono, Y. & Fridovich, I. (1983). *J. Biol. Chem.* **258**, 6015–6020.
- Liu, X.-H., Cai, J.-H., Jiang, Y.-M., Huang, Y.-H. & Yin, X.-J. (2006). *Acta Cryst. E* **62**, m2119–m2121.
- May, J. P., Ting, R., Lermer, L., Thomas, J. M., Roupioz, Y. & Perrin, D. M. (2004). *J. Am. Chem. Soc.* **126**, 4145–4156.
- 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.
- Snell, E. E., Fasella, P. M., Braunstein, A. & Rossi-Fanelli, A. (1963). *Chemical and Biological Aspects of Pyridoxal Catalysis*, pp. 121–128. New York: McMillan.
- Wu, Z. Y., Xu, D. J. & Feng, Z. X. (2001). *Polyhedron*, **20**, 281–284.
- Zeng, J.-L., Jiang, Y.-M. & Yu, K.-B. (2003). *Acta Cryst. E* **59**, m1137–m1139.