

trans*-Bis[2-[(4-oxidobenzylideneamino)methyl]-phenolato]cobalt(II) monohydrate*Zhao-Di Liu**Department of Chemistry, Fuyang Normal
College, Fuyang Anhui 236041, People's
Republic of China

Correspondence e-mail: zhaodi_liu@163.com

The title compound, $[\text{Co}(\text{C}_{15}\text{H}_{14}\text{NO}_2)_2]\cdot\text{H}_2\text{O}$, is a mononuclear cobalt(II) compound. The Co^{II} atom, located on an inversion centre, is coordinated by two N atoms and two O atoms from two Schiff base ligands in a square-planar geometry. $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding involving the water molecule, located on a twofold axis, links the complex molecules into a three-dimensional network.

Received 23 October 2006

Accepted 31 October 2006

Key indicators

Single-crystal X-ray study

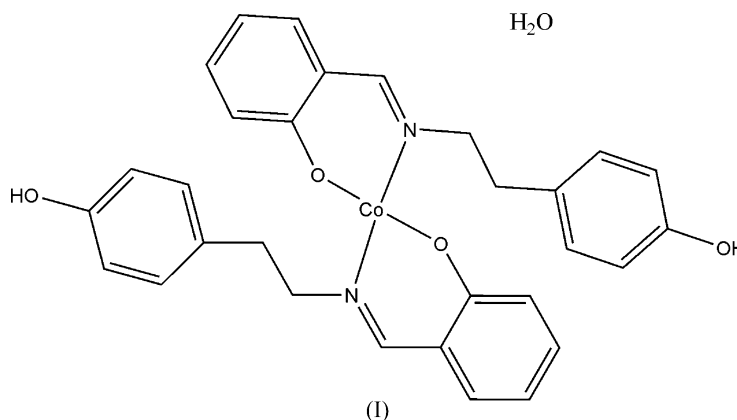
 $T = 292\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$ R factor = 0.054 wR factor = 0.170

Data-to-parameter ratio = 17.9

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

Comment

The crystal structure of *trans*-bis[2-[(4-hydroxyphenethyl-imino)methyl]phenolato]zinc(II) monohydrate has recently been reported (Xu *et al.*, 2006). The structure of the cobalt(II) analogue, (I), is reported here.



The asymmetric unit of (I) consists of half each of a mononuclear Co^{II} complex and a water molecule (Fig. 1). Atom $\text{Co}1$ of the complex molecule lies on an inversion centre, while the water atom $\text{O}1W$ lies on a twofold axis. The Co^{II} ion is four-coordinated by two O atoms and two N atoms from two Schiff base ligands. This CoO_2N_2 coordination forms a square-planar geometry (Table 1).

In the crystal structure, the O atoms of the Schiff base ligands and the water molecules contribute to hydrogen bonds, leading to the formation of a three-dimensional network (Fig. 2 and Table 2).

Experimental

4-(2-Aminoethyl)phenol and salicylaldehyde were available commercially and were used without further purification. 4-(2-Aminoethyl)phenol (0.2 mmol, 27.8 mg) and salicylaldehyde (0.2 mmol, 24.4 mg) were dissolved in methanol (15 ml) and the mixture was stirred for 1 h to give a clear orange solution of *L* (0.2 mmol), where *L* is 2-[(4-hydroxyphenethylimino)methyl]phenol.

To the solution of *L* was added a methanol solution (8 ml) of $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ (0.1 mmol, 24.9 mg) with stirring. After allowing the resulting solution to stand in air at room temperature for 7 d, red block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed with ethanol and dried.

Crystal data

$[\text{Co}(\text{C}_{15}\text{H}_{14}\text{NO}_2)_2] \cdot \text{H}_2\text{O}$	$Z = 4$
$M_r = 557.49$	$D_x = 1.400 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbcn</i>	Mo $K\alpha$ radiation
$a = 15.402 (3) \text{ \AA}$	$\mu = 0.69 \text{ mm}^{-1}$
$b = 11.022 (2) \text{ \AA}$	$T = 292 (2) \text{ K}$
$c = 15.585 (3) \text{ \AA}$	Block, red
$V = 2645.7 (9) \text{ \AA}^3$	$0.30 \times 0.20 \times 0.13 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	15703 measured reflections
φ and ω scans	3182 independent reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	2347 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.819$, $T_{\max} = 0.916$	$R_{\text{int}} = 0.063$
	$\theta_{\text{max}} = 28.4^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2 + 0.8044P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.170$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.91 \text{ e \AA}^{-3}$
3182 reflections	$\Delta\rho_{\text{min}} = -0.78 \text{ e \AA}^{-3}$
178 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

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

Co1—O1	1.8297 (19)	Co1—N1	1.948 (2)
O1 ⁱ —Co1—O1	180	O1—Co1—N1 ⁱ	89.77 (9)
O1—Co1—N1	90.23 (9)	N1—Co1—N1 ⁱ	180

Symmetry code: (i) $-x, -y + 2, -z + 1$.

Table 2

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

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O1W—H1 ⁱⁱ —O1 ⁱⁱ	0.831 (10)	1.934 (11)	2.764 (3)	176 (4)
O2—H2 ⁱⁱⁱ —O1W	0.82	1.99	2.793 (4)	167

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

The water H atom was located in a difference map and was refined with an O—H distance restraint of 0.84 (1) \AA . The remaining H atoms were placed in idealized positions (O—H = 0.82 \AA and C—H = 0.93 or 0.97 \AA) and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H})$ values of $1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: *SHELXL97*.

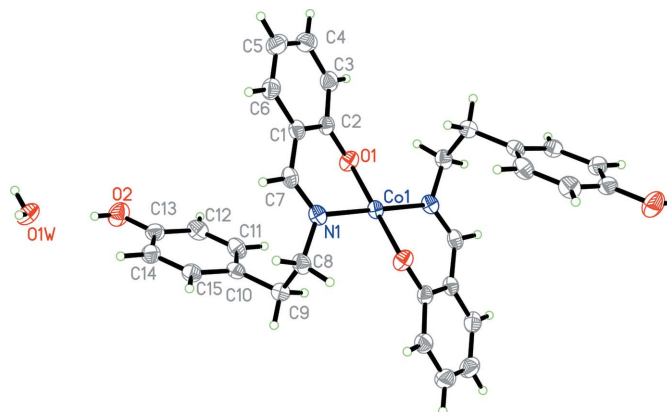


Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operation $(-x, 2 - y, 1 - z)$.

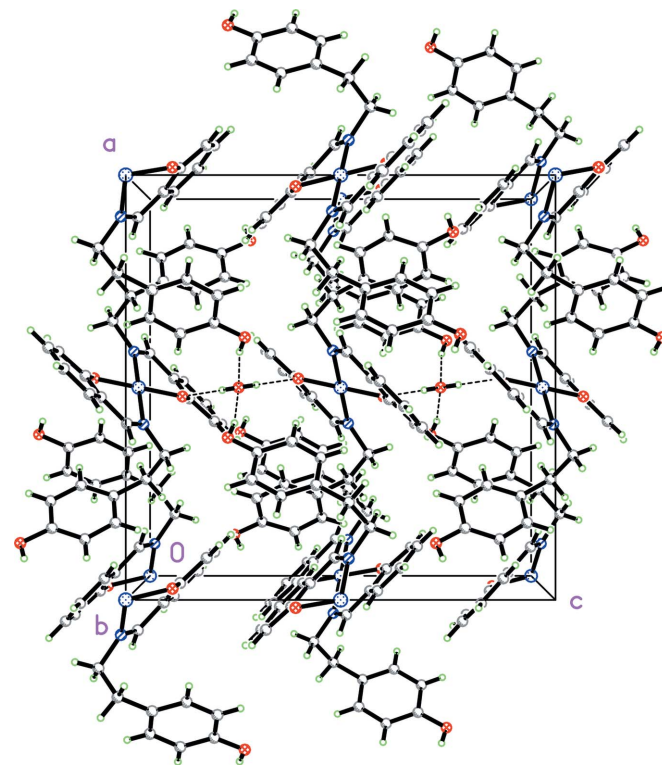


Figure 2

The packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

The author thanks Fuyang Normal College, China, for research grant No. 2005LQ06.

References

- 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.
 Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-Ray Instruments Inc., Madison, Wisconsin, USA.
 Xu, H.-J., Liu, Z.-D. & Sheng, L.-Q. (2006). *Acta Cryst.* **E62**, m2695–m2697.