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## Key indicators

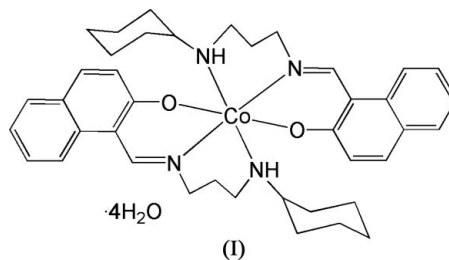
Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
Some non-H atoms missing  
 $R$  factor = 0.069  
 $wR$  factor = 0.188  
Data-to-parameter ratio = 16.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis{1-[3-(cyclohexylamino)propyliminomethyl]-  
naphth-2-olato}cobalt(II) tetrahydrate

In the title centrosymmetric mononuclear cobalt(II) complex,  $[\text{Co}(\text{C}_{20}\text{H}_{25}\text{N}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$ , the  $\text{Co}^{\text{II}}$  atom is six-coordinated by two O and four N atoms from the two Schiff base ligands, forming a very slightly distorted octahedral coordination.

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## Comment

Recently, we have reported the structures of a few Schiff base metal complexes (You, Wang & Han, 2006; You, Han *et al.*, 2006; You & Niu, 2006). As an extension of our work on the structural characterization of these complexes, the crystal structure of the title cobalt(II) complex, (I), is reported here.



In the molecular structure of complex (I) (Fig. 1), in addition to the centrosymmetric  $[\text{Co}(\text{C}_{20}\text{H}_{25}\text{N}_2\text{O})_2]$  complex there are four solvent water molecules. Only three of these water molecules were located (see *Experimental*). The  $\text{Co}^{\text{II}}$  atom is six-coordinated by two O and four N atoms from the two Schiff base ligands, forming a slightly distorted octahedral coordination. The Co—O and Co—N bond lengths (Table 1) are comparable with the corresponding values observed in the structures of similar Schiff base cobalt(II) complexes (You, 2005; Iyere *et al.*, 2004; Elerman *et al.*, 1996; Akitsu *et al.*, 2004). The three *trans* angles at the  $\text{Co}^{\text{II}}$  centre are  $180^\circ$ , by symmetry, and all other angles are close to  $90^\circ$ , ranging from  $89.50$  (13) to  $90.50$  (13) $^\circ$ .

## Experimental

All reagents were of commercially available grade and were used without further purification. 2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.3 mg) and *N*-cyclohexyl-1,3-diaminopropane (0.2 mmol, 31.1 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear red solution. To this solution was added an aqueous solution (3 ml) of  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (0.1 mmol, 23.8 mg) with stirring. The mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 12 d, red block-shaped crystals of (I) were formed. Analysis, found: C 64.23, H 7.82, N 7.54, O 12.68%; calculated for  $\text{C}_{40}\text{H}_{56}\text{CoN}_4\text{O}_5$ : C 65.65, H 7.71, N 7.66, O 10.93%; calculated for  $\text{C}_{40}\text{H}_{58}\text{CoN}_4\text{O}_6$ : C 64.07, H 7.80, N 7.47, O 12.80%.

## Crystal data

[Co(C<sub>20</sub>H<sub>25</sub>N<sub>2</sub>O)<sub>2</sub>]<sub>2</sub>·4H<sub>2</sub>O*M<sub>r</sub>* = 749.83

Monoclinic, C2/c

*a* = 21.192 (4) Å*b* = 9.115 (2) Å*c* = 22.426 (5) Å

β = 116.939 (4)°

*V* = 3861.9 (14) Å<sup>3</sup>*Z* = 4*D<sub>x</sub>* = 1.290 Mg m<sup>-3</sup>

Mo Kα radiation

μ = 0.50 mm<sup>-1</sup>*T* = 298 (2) K

Block, red

0.23 × 0.21 × 0.20 mm

## Data collection

Bruker SMART 1000 CCD area-detector diffractometer

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

*T<sub>min</sub>* = 0.895, *T<sub>max</sub>* = 0.908

10625 measured reflections

3871 independent reflections

2573 reflections with *I* > 2σ(*I*)*R<sub>int</sub>* = 0.046θ<sub>max</sub> = 26.5°

## Refinement

Refinement on *F*<sup>2</sup>*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.069*wR* (*F*<sup>2</sup>) = 0.188*S* = 1.02

3871 reflections

241 parameters

H atoms treated by a mixture of independent and constrained refinement

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.1043*P*)<sup>2</sup>]  
where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3(Δ/σ)<sub>max</sub> < 0.001Δρ<sub>max</sub> = 1.47 e Å<sup>-3</sup>Δρ<sub>min</sub> = -0.30 e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Co1—O1	1.886 (2)	Co1—N2	2.013 (3)
Co1—N1	1.921 (3)		
O1 <sup>i</sup> —Co1—O1	180	N1—Co1—N2 <sup>i</sup>	90.50 (13)
O1—Co1—N1 <sup>i</sup>	89.77 (12)	O1—Co1—N2	90.35 (12)
O1—Co1—N1	90.23 (12)	N1—Co1—N2	89.50 (13)
N1 <sup>i</sup> —Co1—N1	180	N2 <sup>i</sup> —Co1—N2	180
O1—Co1—N2 <sup>i</sup>	89.65 (12)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2A...O3 <sup>ii</sup>	0.84 (3)	2.20 (2)	3.003 (11)	162 (2)

Symmetry code: (ii)  $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 1$ .

Atoms H2, H2A, H3A and H3B were located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å, the O—H distance restrained to 0.85 (1) Å and the H...H distances restrained to 1.37 (2) Å, and with *U*<sub>iso</sub>(H) values fixed at 0.08 Å<sup>2</sup>. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with *U*<sub>iso</sub>(H) set to 1.2*U*<sub>eq</sub>(C). From the calculated and found elemental analysis it appears that the structure may contain additional solvent water. This is supported by

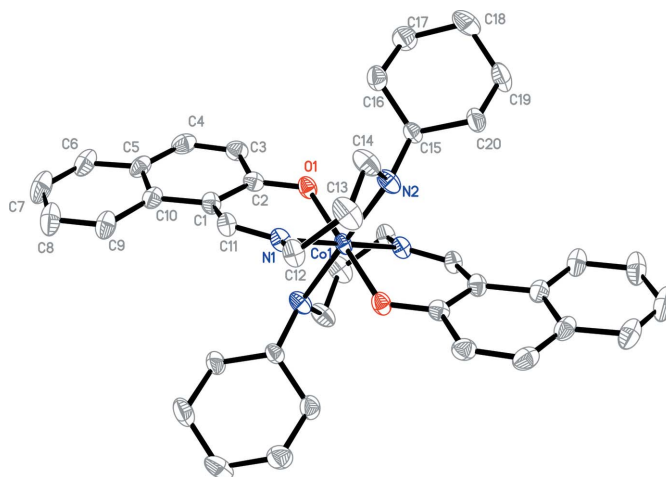


Figure 1

The structure of compound (I), showing 30% probability displacement ellipsoids. Unlabelled atoms are at the symmetry position ( $\frac{1}{2} - x, \frac{1}{2} - y, -z$ ). Water molecules and H atoms have been omitted.

the presence of solvent-accessible voids of 46 Å<sup>3</sup> (PLATON; Spek, 2003) and the fact that not all H atoms of the located water atom O3 have acceptor atoms. In accordance with the elemental analysis, one additional water atom has been included in the empirical formula. This additional solvent water molecule is suspected to be highly disordered within the void and hence 'invisible' in Fourier maps. An unassigned maximum residual electron density was observed 2.96 Å from atom H13A.

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.

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