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Aqua[*N*-(2-oxidophenylmethylimino)-3-azapentane-1,5-diamine]cobalt(II) chloride

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Key indicators

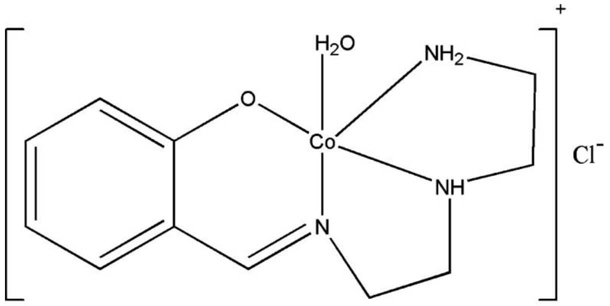
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.042
wR factor = 0.103
Data-to-parameter ratio = 17.2

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

The title compound, $[Co(C_{11}H_{16}N_3O)(H_2O)]Cl$, consists of a $[CoL]^+$ cation and a chloride anion, where *L* is the *N*-(2-oxidophenylmethylimino)-3-azapentane-1,5-diamine anion. In the complex cation, the Co atom is coordinated by three N and two O atoms from the ligand and an apical water molecule in a distorted square-pyramidal geometry. The crystal structure is stabilized by N—H···O, N—H···Cl, O—H···O and O—H···Cl hydrogen bonds.

Comment

Schiff base complexes are of great interest in coordination chemistry (Goswami & Eichhorn, 1999; Dominguez-Vera *et al.*, 1998; Bernardo *et al.*, 1996). In recent years, a few Schiff base complexes with the *N*-(2-hydroxyphenylmethylimino)-3-azapentane-1,5-diamine anion ($C_{11}H_{16}N_3O^-$) have been reported. Most of these compounds consist of a univalent mononuclear complex cation and a simple anion, such as Cl^-, Br^-, ClO_4^-, SCN^-, PF_6^- and $[B(Ph)_4]^-$ (Kratochvíl *et al.*, 1989, 1991; Liu *et al.*, 2004; Loub *et al.*, 1989.; Podlahová *et al.*, 1988; Cusmano Priolo *et al.*, 1983; Rotondo *et al.*, 1983; Zhu *et al.*, 2004). To date, there is only one dinuclear compound, ($C_{26}H_{44}Cd_2N_6O_4^{2+}\cdot 2ClO_4^-$), in which the two Cd atoms are connected by two O atoms of the hydroxyl group (Loub *et al.*, 1990). We report here the structure of another mononuclear Co compound, (I), which is isostructural with the copper analog $[Cu(C_{11}H_{16}N_3O)(H_2O)]Cl$ (Zhu *et al.*, 2004).



(I)

As shown in Fig. 1, the Co^{II} atom in (I) is in a distorted square-pyramidal geometry, being coordinated by three N atoms and one O atom from the ligand and one O atom from a water molecule (Table 1). The four coordinating atoms from the ligand constitute the basal plane, with a mean deviation from the plane of 0.079 Å, and the O atom from the water molecule occupies the apical position. The Co^{II} atom is displaced by 0.1779 (16) Å above the basal plane towards the water molecule. The three Co—N bonds represent the inter-

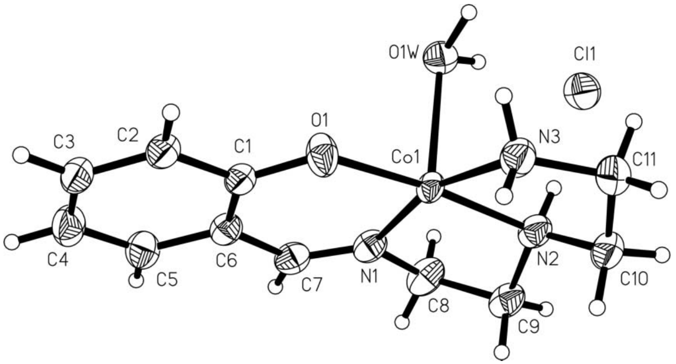


Figure 1
The structure of (I), showing 35% probability displacement ellipsoids (arbitrary spheres for the H atoms).

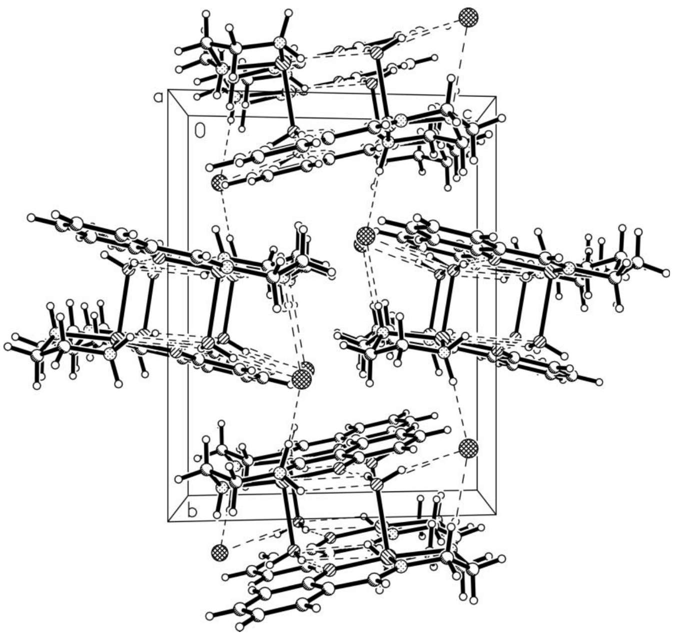


Figure 2
The packing of (I), showing hydrogen-bonded (dashed lines) layers in the *bc* plane.

action of the cobalt(II) centre with the primary amine, secondary amine and imine; they are in the normal bond-length ranges. The dihedral angle between the N1/N2/N3/O1 mean plane and the C1–C6 benzene ring mean plane is 11.90 (8)°.

Except for the imine N atom, all the other coordinating atoms and the uncoordinated chloride anion contribute to the formation of a hydrogen-bond network. The hydrogen bonds (Table 2) join two neighbouring cations to form a dimer. Further hydrogen bonds between the chloride ion and atoms O1*W*, N2, and N3 connect the dimers, forming a two-dimensional network in the *bc* plane, as shown in Fig. 2.

Experimental

A mixture of diethylenetriamine (1 mmol, 103 mg), salicylaldehyde (1 mmol, 122 mg) and $CoCl_2 \cdot 6H_2O$ (1 mmol, 238 mg) was stirred in ethanol (10 ml) for 1 h. The precipitate was recrystallized from acetonitrile, and red blocks of (I) were filtered off and washed with MeCN and EtOH. Analysis found: C 41.40, H 5.72, N 13.23%; calculated for $C_{11}H_{18}ClCoN_3O_2$: C 41.46, H 5.69, N 13.19%.

Crystal data

$[Co(C_{11}H_{16}N_3O)(H_2O)]Cl$
$M_r = 318.66$
Monoclinic, $P2_1/c$
$a = 9.047$ (4) Å
$b = 13.633$ (5) Å
$c = 10.754$ (5) Å
$\beta = 101.87$ (1)°
$V = 1298.0$ (10) Å^3
$Z = 4$
$D_x = 1.631$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.53$ mm^{-1}
$T = 293$ (2) K
Block, red
0.28 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.675$, $T_{max} = 0.750$
2993 measured reflections
2820 independent reflections
2276 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.103$
$S = 1.08$
2820 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 2.5584P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0105 (12)

Table 1
Selected bond lengths (Å).

Co1—O1	1.900 (3)	Co1—N3	2.007 (3)
Co1—N1	1.923 (3)	Co1—O1*W*	2.300 (3)
Co1—N2	1.994 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N*B*···O1*W*^{i}	0.92	2.42	3.096 (4)	130
N3—H3N*A*···Cl1^{ii}	0.98	2.38	3.330 (4)	162
N2—H2N···Cl1	0.90	2.35	3.241 (3)	170
O1*W*—H1*WB*···Cl1	0.91	2.23	3.117 (3)	165
O1*W*—H1*WA*···O1^{i}	1.01	1.69	2.665 (4)	163

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

All the H atoms, except for H1*WA* and H1*WB* attached to O1*W*, H3N*A* and H3N*B* attached to N3, were placed in idealized positions (C—H = 0.96 Å, N—H = 0.90–0.98 Å and O—H = 0.91 and 1.01 Å) and refined as riding with U_{iso}(H) values fixed at 0.08 Å^2 (C-bound H atoms) and 0.05 Å^2 (N- and O-bound H atoms). Atoms H1*WA*, H1*WB*, H3N*A* and H3N*B* were located from a difference Fourier map and it was allowed to attached atom during the final cycles of refinement.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

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SHELXTL (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

References

Bernardo, K., Leppard, S., Robert, A., Commenges, G., Dahan, F. & Meunier, B. (1996). *Inorg. Chem.* **35**, 387–396.

Bruker (2001). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cusmano Priolo, F., Rotondo, E., Rizzardi, G., Bruno, G. & Bombieri, G. (1983). *Acta Cryst.* C**39**, 550–552.

Dominguez-Vera, J. M., Camara, F., Moreno, J. M., Colacio, E. & Stoeckli-Evans, H. (1998). *Inorg. Chem.* **37**, 3046–3050.

Goswami, N. & Eichhorn, D. M. (1999). *Inorg. Chem.* **38**, 4329–4333.

Kratochvíl, B., Nováková, M., Haber, V., Ondrácek, J. & Hájek, B. (1989). *Acta Cryst.* C**45**, 403–405.

Kratochvíl, B., Ondraćek, J., Novotný, J. & Haber, V. (1991). *Acta Cryst.* C**47**, 2207–2209.

Liu, G.-X., Ren, X.-M., Xu, H., Tang, C.-Y., Wu, G.-H. & Chen, Y.-C. (2004). *Chin. Chem. Lett.* **15**, 1105–1108.

Loub, J., Podlahová, J., Haber, V., Kopf, J. & Weiss, E. (1990). *Acta Cryst.* C**46**, 596–598.

Loub, J., Podlahová, J., Kopf, J. & Weiss, E. (1989). *Acta Cryst.* C**45**, 406–407.

Podlahová, J., Knízek, K., Loub, J. & Hasek, J. (1988). *Acta Cryst.* C**44**, 631–633.

Rotondo, E., Cusmano Priolo, F., Romeo, M., Bruno, G. & Bombieri, G. (1983). *Acta Cryst.* C**39**, 1525–1527.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Zhu, H.-L., Li, S.-Y., Wang, Z.-D. & Yang, F. (2004). *J. Chem. Crystallogr.* **34**, 203–206.

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