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Diaquabis(4-chlorobenzoato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II)

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In the title complex, $[Co(C_7H_4ClO_2)_2(C_{12}H_8N_2)(H_2O)_2]$, the Co^{II} atom is six-coordinated in a distorted octahedral geometry by two O atoms from two 4-chlorobenzoate ligands, two N atoms from one 1,10-phenanthroline ligand and two water molecules. The molecules form O—H···O hydrogen-bonded centrosymmetric dimers that are extended by additonal intra- and intermolecular hydrogen-bonding interactions to form infinite chains of dimers parallel to the *a* axis.

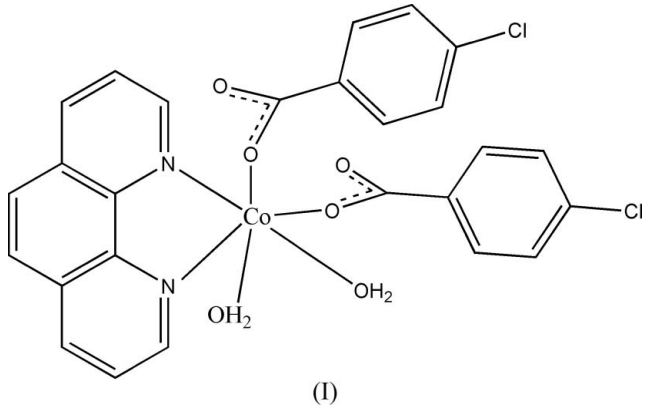
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.120
Data-to-parameter ratio = 14.2

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

Comment

The molecular self-assembly of supramolecular architectures has received much attention during recent decades (Tao *et al.*, 2000; Choi & Jeon, 2003). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metal ions and the bridging building blocks, as well as on the influence of weaker non-covalent interactions, such as hydrogen bonds and π–π stacking interactions. As a building block, 4-chlorobenzoic acid is a potential candidate for the construction of supramolecular complexes. Recently, we obtained the title mononuclear cobalt(II) complex, (I), by the reaction of cobalt nitrate, 4-chlorobenzoic acid and 1,10-phenanthroline in an aqueous solution, and its crystal structure is reported here.



(I)

The Co^{II} centre in (I) has a distorted octahedral geometry (Fig. 1) defined by two O atoms from two 4-chlorobenzoate ligands, two N atoms from one 1,10-phenanthroline ligand and two water molecules. The coordination bond lengths and angles at the Co^{II} atom are given in Table 1.

Via hydrogen bonding of their water molecules, pairs of molecules form centrosymmetric dimers with an $R_2^2(8)$ graph-set motif (Bernstein *et al.*, 1995). These dimers exhibit additional intra- and intermolecular O—H···O···H—O hydrogen bonds [graph-set motif $C_2^1(6)$] to form an infinite hydrogen-

bonded double chain of molecules parallel to the *a* axis of the unit cell (Fig. 2 and Table 2).

Experimental

The title complex was prepared by the addition of stoichiometric amounts of cobalt(II) nitrate (20 mmol) and 1,10-phenanthroline (20 mmol) to a hot aqueous solution (30 ml) of 4-chlorobenzoic acid (20 mmol). The pH was then adjusted to 7.0–8.0 with NaOH (30 mmol). The resulting solution was filtered and orange single crystals of (I) were obtained at room temperature after several days (yield 58%).

Crystal data

$[Co(C_7H_4ClO_2)_2(C_{12}H_8N_2)(H_2O)_2]$
M_r = 586.27
Triclinic, $P\overline{1}$
a = 7.7228 (2) Å
b = 9.0264 (2) Å
c = 18.0710 (4) Å
α = 96.427 (1)°
β = 94.887 (1)°
γ = 102.763 (1)°
V = 1212.99 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 293 (2) K
0.25 × 0.15 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.793, T_{max} = 0.868
16932 measured reflections
4731 independent reflections
3818 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.07
4731 reflections
334 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O3	2.070 (2)	Co1—N1	2.129 (2)
Co1—O1	2.1008 (19)	Co1—N2	2.144 (2)
Co1—O1*W*	2.118 (2)	Co1—O2*W*	2.1491 (18)
O3—Co1—O1	85.77 (8)	O1*W*—Co1—N2	171.32 (9)
O3—Co1—O1*W*	92.24 (9)	N1—Co1—N2	77.68 (9)
O1—Co1—O1*W*	86.14 (8)	O3—Co1—O2*W*	88.20 (8)
O3—Co1—N1	168.95 (9)	O1—Co1—O2*W*	171.01 (7)
O1—Co1—N1	99.01 (8)	O1*W*—Co1—O2*W*	87.45 (7)
O1*W*—Co1—N1	98.00 (9)	N1—Co1—O2*W*	88.11 (8)
O3—Co1—N2	92.70 (9)	N2—Co1—O2*W*	99.82 (8)
O1—Co1—N2	87.12 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H2*W*···O2*W*^{i}	0.82	1.93	2.751 (3)	177
O2*W*—H3*W*···O4	0.84	1.76	2.585 (3)	168
O1*W*—H1*W*···O2	0.82	1.93	2.713 (3)	160
O2*W*—H4*W*···O2^{ii}	0.84	1.87	2.690 (3)	165

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$.

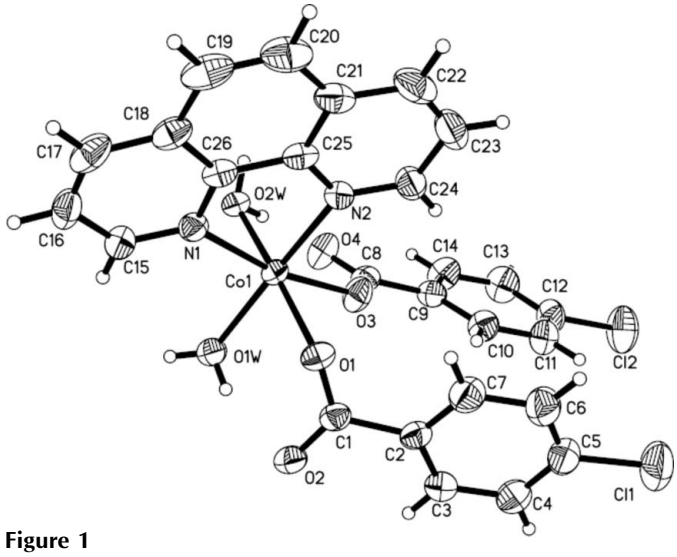


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

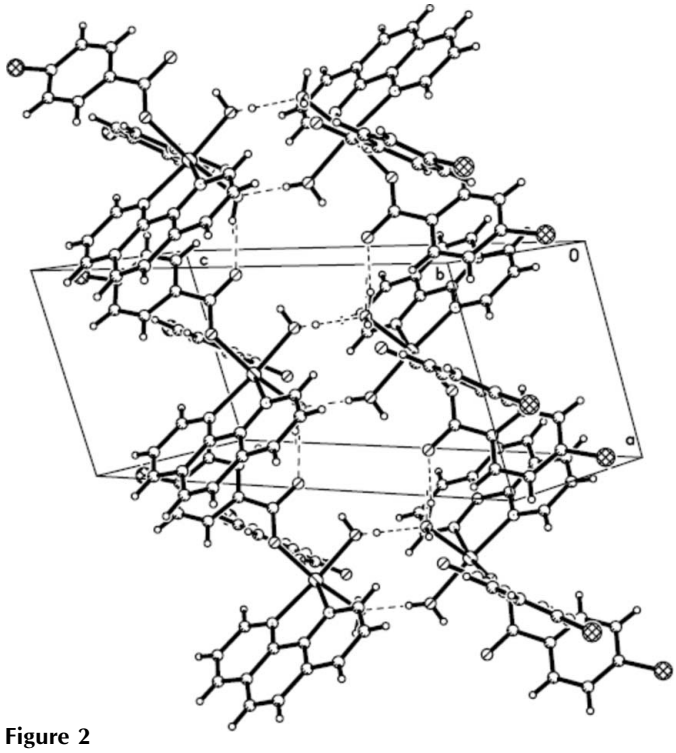


Figure 2
A packing view of (I), showing the intermolecular hydrogen bonds (dashed lines).

The aqua H atoms were located in a difference Fourier map and then refined as riding in their as-found relative positions, with $U_{iso}(H) = 1.2U_{eq}(O)$. The remaining H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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