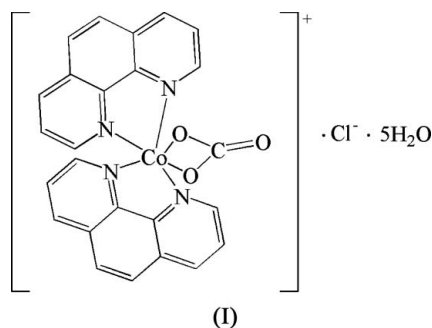


(Carbonato- κ^2O,O')bis(1,10-phenanthroline- κ^2N,N')cobalt(III) chloride pentahydrate**Xu-Cheng Fu,^{a,b} Xiao-Yan Wang,^b Ming-Tian Li,^a Cheng-Gang Wang^{a*} and Xiao-Tao Deng^a**^aDepartment of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China, and ^bChemistry and Biology Department, West Anhui University, Lu'an, Anhui 237000, People's Republic of ChinaCorrespondence e-mail:
wangcg23@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(C-C) = 0.004$ Å
Disorder in solvent or counterion
 R factor = 0.051
 wR factor = 0.130
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{Co}(\text{CO}_3)(\text{C}_{12}\text{H}_8\text{N}_2)_2]\text{Cl}\cdot 5\text{H}_2\text{O}$, contains $[\text{Co}(\text{CO}_3)(\text{phen})_2]^+$ cations (phen = 1,10-phenanthroline), chloride ions and five independent non-coordinated water molecules, four of which show positional disorder. The Co^{III} atom displays a distorted octahedral geometry, being coordinated by four N atoms of two 1,10-phenanthroline ligands and two O atoms of the bidentate chelating carbonate group. The crystal packing is consolidated by hydrogen bonds and aromatic π - π stacking interactions between neighboring phenanthroline rings.

Received 27 March 2006
Accepted 27 April 2006**Comment**

There has been considerable interest in the design and synthesis of transition metal complexes with carbonate ligands due to their use as models for metalloenzymes and in environmental chemistry (Steiner *et al.*, 1975; Kimura *et al.*, 2001; Behr *et al.*, 1988; Leitner *et al.*, 1996). The combination of cobalt(II) cations and carbonate ligands often results in Co^{III} -containing products as a result of an autoxidation reaction. Much of the previous work has been done to verify reaction mechanisms, and several crystal structures of Co^{III} complexes with carbonate ligands have been reported (Niederhoffer *et al.*, 1982; Guild *et al.*, 1980; Hennig *et al.*, 1980).



We describe here the synthesis and structure of the title compound, (I). The Co^{III} atom in the discrete $[\text{Co}(\text{CO}_3)(\text{phen})_2]^+$ cation (Fig. 1) displays a distorted octahedral geometry, being coordinated by four N atoms of two 1,10-phenanthroline ligands and two O atoms of the bidentate chelating carbonate group.

The charge-balancing chloride ion and four of the five non-coordinated water molecules are disordered over adjacent sites. This means that the network of $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2) should be regarded as rather uncertain. As shown in Fig. 2, the hydrogen bonds are supplemented by aromatic π - π stacking interactions of neighboring phenanthroline rings.

Experimental

To a solution containing $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.238 g, 1.0 mmol) and phen (0.396 g, 2.0 mmol) in water (20 ml), NaHCO_3 (0.336 g, 4.0 mmol) was added. The reaction mixture was stirred for 1 h at 323 K. The resulting solution was cooled to room temperature and filtered. The filtrate was left to stand in air for slow evaporation and red block-shaped single crystals of (I) were obtained after several months.

Crystal data

$[\text{Co}(\text{CO}_3)(\text{C}_{12}\text{H}_8\text{N}_2)_2]\text{Cl} \cdot 5\text{H}_2\text{O}$ $Z = 4$
 $M_r = 1191.74$ $D_x = 1.519 \text{ Mg m}^{-3}$
 Monoclinic, $C2/c$ $\text{Mo K}\alpha$ radiation
 $a = 27.526 (2) \text{ \AA}$ $\mu = 0.82 \text{ mm}^{-1}$
 $b = 13.5927 (12) \text{ \AA}$ $T = 292 (2) \text{ K}$
 $c = 14.2093 (13) \text{ \AA}$ Block, red
 $\beta = 101.505 (2)^\circ$ $0.36 \times 0.26 \times 0.20 \text{ mm}$
 $V = 5209.7 (8) \text{ \AA}^3$

Data collection

Bruker SMART CCD 17359 measured reflections
 diffractometer 5947 independent reflections
 ω scans 4423 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan $R_{\text{int}} = 0.036$
 (SADABS; Bruker, 2000) $\theta_{\text{max}} = 27.5^\circ$
 $T_{\text{min}} = 0.758, T_{\text{max}} = 0.854$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 2.6301P]$
 $R[F^2 > 2\sigma(F^2)] = 0.051$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.130$ $(\Delta/\sigma)_{\text{max}} = 0.001$
 $S = 1.03$ $\Delta\rho_{\text{max}} = 0.39 \text{ e \AA}^{-3}$
 5947 reflections $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
 429 parameters
 H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected bond lengths (\AA).

Co1—O2	1.8871 (18)	Co1—N1	1.939 (2)
Co1—O1	1.8885 (18)	Co1—N2	1.947 (2)
Co1—N4	1.925 (2)	Co1—N3	1.956 (2)
O2—Co1—O1	69.39 (8)	N4—Co1—N3	83.88 (9)
N1—Co1—N2	84.01 (9)		

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O5—H5A \cdots O7'	0.82 (2)	1.94 (3)	2.694 (10)	153 (6)
O5—H5A \cdots O7	0.82 (2)	1.96 (2)	2.782 (14)	176 (5)
O5—H5B \cdots O3	0.82 (2)	2.12 (3)	2.881 (4)	154 (5)
O6—H6B \cdots O5'	0.85 (2)	2.21 (6)	2.975 (8)	150 (11)
O6—H6A \cdots O1	0.83 (2)	2.09 (4)	2.876 (6)	158 (11)
O4'—H4C \cdots Cl1'	0.83 (2)	2.45 (4)	3.253 (8)	165 (12)
O4'—H4D \cdots O8'	0.81 (2)	2.20 (7)	2.918 (12)	147 (13)
O8'—H8D \cdots O4'	0.80 (2)	2.30 (3)	2.918 (12)	134 (3)

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

The water H atoms were located in a difference map and their positional parameters were refined, with O—H distances restrained

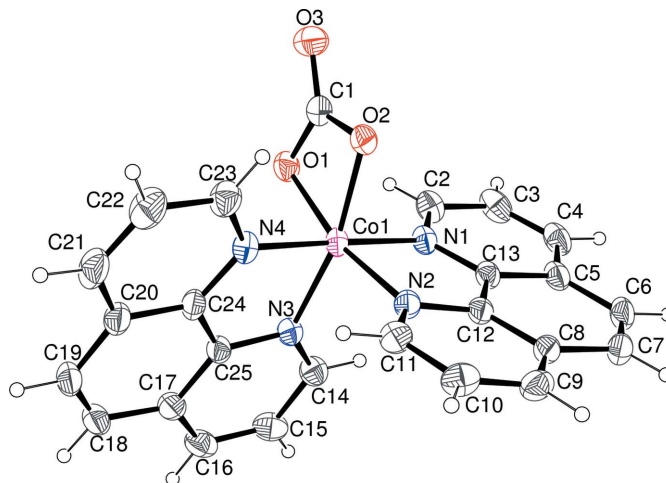


Figure 1

The structure of the cation of (I), showing displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms)

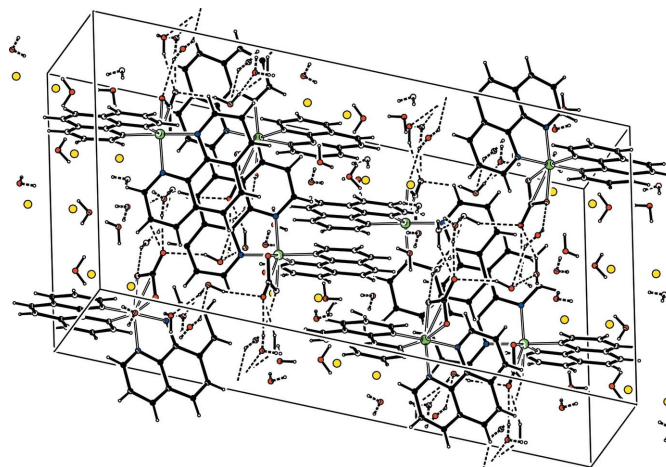


Figure 2

The packing of (I), with hydrogen bonds shown as dashed lines.

to 0.82 (2) \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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, 1997); software used to prepare material for publication: SHELXTL.

The authors thank the Education Office of Anhui Province, People's Republic of China, for research grant No. 200161.

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