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Key indicators

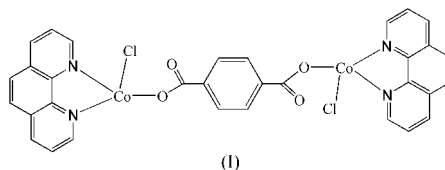
Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.011 \text{ \AA}$
R factor = 0.089
wR factor = 0.167
Data-to-parameter ratio = 12.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>. μ -Terephthalato-bis[chloro(1,10-phenanthroline)-cobalt(II)]

In the centrosymmetric title complex, $[\text{Co}_2\text{Cl}_2(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2]$, each Co atom is surrounded by one O atom from a terephthalate dianion, a Cl atom and two N atoms from a 1,10-phenanthroline heterocycle in a distorted square-planar arrangement. The terephthalate dianion lies on an inversion centre and bridges two Co atoms.

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Comment

Among the metal complexes of terephthalic acid (Deakin *et al.*, 1999; Fun *et al.*, 1999; Li *et al.*, 1998; Mori & Takamizawa, 2000), the copper-phenanthroline system has been well studied. There are at least five compounds that display structural diversity (Sun *et al.*, 2000, 2001; Xiao & Zhu, 2003; Zhu *et al.*, 2004). To our knowledge, the cobalt-phenanthroline system is less studied, having only one published structure of a polymeric compound, $[\text{Co}(\text{phen})(\text{ta})(\text{H}_2\text{O})]$ (phen is 1,10-phenanthroline and ta is terephthalate; Sun *et al.*, 2001). We report here the crystal structure of the title compound, (I).



In (I), the Co atom is surrounded by an O atom, a Cl atom and two N atoms from a phenanthroline heterocycle in a distorted square-planar arrangement (Fig. 1). Atoms Cl1, O1, N1 and N2 form the basal plane, with a mean deviation of 0.0023 Å. The benzene ring of the terephthalate is roughly perpendicular to the plane of the 1,10-phenanthroline heterocycle, the dihedral angle being 105.60 (2)°. The terephthalate dianion, which acts as a bridge between the two Co atoms, lies on an inversion centre. The Co1—O1 bond distance [1.917 (5) Å] is the shortest for reported terephthalate-bridged cobalt(II) complexes (Cano *et al.*, 1997; Kurmoo *et al.*, 2001; Sun *et al.*, 2001). The Co···Co distance [10.94 (7) Å]

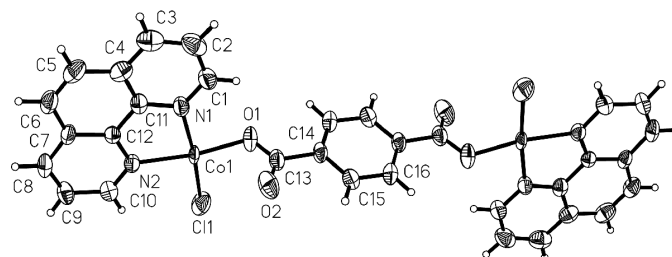


Figure 1

View of (I), with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

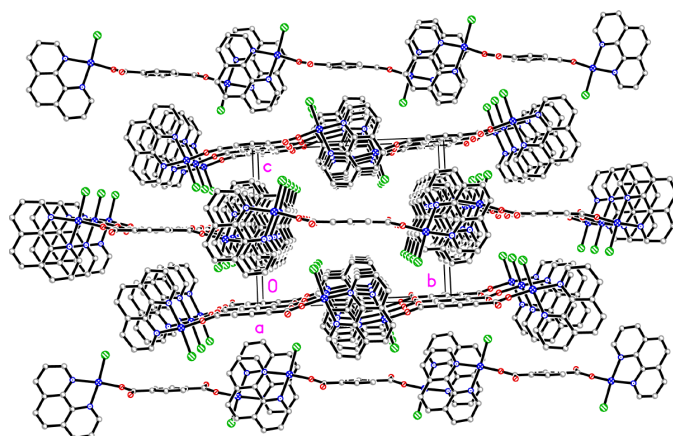


Figure 2
The crystal packing of (I), viewed down the *a* axis.

through the bridging terephthalate dianion is shorter than those for the reported terephthalate-bridged cobalt(II) complexes (Cano *et al.*, 1997; Sun *et al.*, 2001). Moreover, the 1,10-phenanthroline heterocycles of adjacent molecules are partially overlapped (Fig. 2), separated by 3.674 (3) Å, which suggests the existence of π - π stacking interactions.

Experimental

A solution (10 ml) of dimethylformamide containing CoCl₂·6H₂O (0.25 mmol, 0.119 g), Cu₂Cl₂·2H₂O (0.5 mol, 0.085 g) and terephthalic acid (0.5 mmol, 0.083 g) was added slowly to a solution (10 ml) of dimethylformamide containing 1,10-phenanthroline (0.5 mmol, 0.099 g). The mixture was stirred for 30 min and left to stand at room temperature for about a month, after which time violet crystals were obtained.

Crystal data

[Co ₂ Cl ₂ (C ₈ H ₄ O ₄)(C ₁₂ H ₈ N ₂) ₂]	$D_x = 1.744 \text{ Mg m}^{-3}$
$M_r = 713.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 648 reflections
$a = 7.5020$ (4) Å	$\theta = 2.4$ – 22.0°
$b = 14.6261$ (7) Å	$\mu = 1.47 \text{ mm}^{-1}$
$c = 12.4567$ (6) Å	$T = 293$ (2) K
$\beta = 96.295$ (2) $^\circ$	Prism, violet
$V = 1358.57$ (12) Å ³	$0.23 \times 0.21 \times 0.09 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	2396 independent reflections
φ and ω scans	2362 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$R_{\text{int}} = 0.028$
$T_{\text{min}} = 0.729$, $T_{\text{max}} = 0.879$	$\theta_{\text{max}} = 25.1^\circ$
7049 measured reflections	$h = -7 \rightarrow 8$
	$k = -17 \rightarrow 17$
	$l = -14 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0248P)^2 + 8.0871P]$
$R[F^2 > 2\sigma(F^2)] = 0.089$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.167$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.37$	$\Delta\rho_{\text{max}} = 0.73 \text{ e \AA}^{-3}$
2396 reflections	$\Delta\rho_{\text{min}} = -0.80 \text{ e \AA}^{-3}$
200 parameters	H-atom parameters constrained

Table 1

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

Co1—O1	1.917 (5)	Co1—N2	2.029 (6)
Co1—N1	2.023 (6)	Co1—Cl1	2.208 (2)
O1—Co1—N1	91.6 (3)	N1—Co1—Cl1	173.97 (18)
O1—Co1—N2	172.1 (3)	N2—Co1—Cl1	93.50 (18)
N1—Co1—N2	81.4 (2)	Cl1—O1—Co1	116.2 (5)
O1—Co1—Cl1	93.2 (2)		

All H atoms were positioned geometrically and allowed to ride on their parent atoms, at distances of 0.93 Å and with $U_{\text{iso}} = 1.2U_{\text{eq}}$ (parent atom).

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT (Bruker, 2000); program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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