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Key indicators

Single-crystal X-ray study T = 173 K Mean σ (C–C) = 0.008 Å R factor = 0.063 wR factor = 0.190 Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e. Received 10 February 2006

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µ-Oxalato-bis[chlorotripyridinecobalt(II)] pyridine disolvate

The Co complex of the title compound, $[Co_2(C_2O_4)Cl_2-(C_5H_5N)_6]\cdot C_5H_5N$, is located on a crystallographic centre of inversion. The solvent pyridine molecules are located on general positions. The Co centre is octahedrally coordinated by three pyridine ligands, one Cl atom and a chelating oxalate anion which bridges two Co centres.

Comment

Oxalate-bridged polynuclear metal complexes have been the focus of intensive research due to their interesting magnetic properties. The latter are highly dependent on the nature of the metal ion and the peripheral ligands (Castillo *et al.*, 2003). The ability of the oxalate moiety to connect to metal ions as a bis-bidentate bridging ligand enables the formation of diverse assemblies. The crystal structure determination of the title compound, (I), has been carried out in order to obtain information about the configuration and conformation of the reaction product.

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 5.27 plus one update; *MOGUL* Version 1.1; Allen, 2002). The Co atoms are octahedrally coordinated by three pyridine ligands, one chlorine atom and a chelating oxalate anion which bridges two Co centres. The three Co–N bonds are significantly different. Those that are mutually *trans* are longer than the one which is *trans* to a Co– O bond (Table 1). The two Co–O bonds have the same length. The space between the complexes is filled by solvent pyridine molecules.



Experimental



Crystal data

$Co_2(C_2O_4)Cl_2(C_5H_5N)_6] \cdot 2C_5H_5N$	$D_x = 1.421 \text{ Mg m}^{-3}$
$M_r = 909.58$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 12780
a = 9.5335 (19) Å	reflections
b = 10.518 (2) Å	$\theta = 2.2-25.3^{\circ}$
c = 21.205 (4) Å	$\mu = 0.96 \text{ mm}^{-1}$
$\beta = 91.78 \ (3)^{\circ}$	T = 173 (2) K
V = 2125.3 (7) Å ³	Thick plate, colourless
Z = 2	$0.28 \times 0.22 \times 0.12 \text{ mm}$

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Data collection

Stoe IPDS-II two-circle	3906 independent reflections
diffractometer	2545 reflections with $I > 2\sigma(I)$
ω scans	$R_{\rm int} = 0.089$
Absorption correction: multi-scan	$\theta_{\rm max} = 25.4^{\circ}$
(MULABS; Spek, 2003; Blessing,	$h = -11 \rightarrow 11$
1995)	$k = -12 \rightarrow 12$
$T_{\min} = 0.775, T_{\max} = 0.894$	$l = -23 \rightarrow 25$
24340 measured reflections	

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.063$ $wR(F^2) = 0.190$ S = 0.943906 reflections 263 parameters H-atom parameters constrained

Table 1

Selected bond lengths (Å).

 $w = 1/[\sigma^2(F_o^2) + (0.1345P)^2]$

 $(\Delta/\sigma)_{\rm max} < 0.001$

 $\Delta \rho_{\rm max} = 1.61 \text{ e Å}$

 $\Delta \rho_{\rm min} = -0.62 \text{ e} \text{ Å}^{-3}$

where $P = (F_0^2 + 2F_c^2)/3$

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Extinction correction: SHELXL97

Extinction coefficient: 0.014 (2)

Symmetry code: (i) -x + 1, -y + 1, -z + 2.

H atoms were located in a difference map, but were positioned geometrically (C-H = 0.95 Å) and refined with fixed individual displacement parameters $[U(H) = 1.2U_{eq}(C)]$ using a riding model. The largest positive residual peak (1.6 eÅ⁻³) is located at 1.52 Å from atom Cl1.

Data collection: X-AREA (Stoe & Cie, 2001); cell refinement: X-AREA; data reduction: X-AREA; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL-Plus (Sheldrick, 1991); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2003).

I thank Dr A. Mohamed, University of Frankfurt, Germany, for providing the sample.



Figure 1

Perspective view of the title compound with the atom numbering scheme; displacement ellipsoids are drawn at the 50% probability level. Atoms with the suffix A are generated by the symmetry operator 1 - x, 1 - y, 2 - z.

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