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catena-Poly[[(2,2′-bipyridine-*N*,*N*′)cobalt(II)]-*μ*-4,4′-oxydibenzoato-*O*,*O*′:*O*″,*O*‴]

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Key indicators

Single-crystal X-ray study
T = 302 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.135
Data-to-parameter ratio = 21.0

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

The title compound, $[Co(C_{14}H_8O_5)(C_{10}H_8N_2)]$, forms a polymeric chain *via* bidentate coordination of the carboxylate ligands from *μ*-4,4′-oxydibenzoate to the Co atoms. The chelating bipyridyl ligands stack with inverted forms along the [100] direction and are separated by 3.7952 (16) Å. The Co atom has a distorted octahedral geometry.

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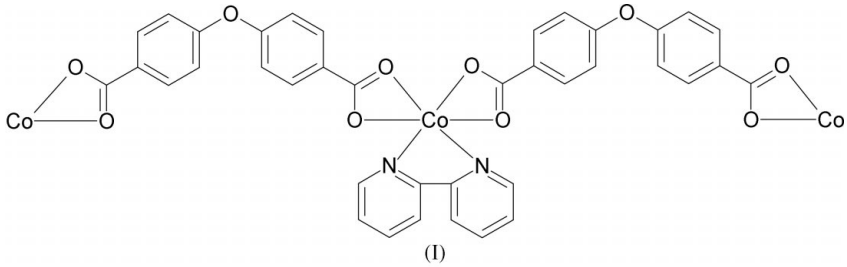
Comment

Coordination compounds crystallized from polyaromatic acids and metal ions are of interest for their polymeric network structures and their magnetic and porous properties (Yaghi *et al.*, 1995, 1996; Plater, Roberts & Howie, 1998; Plater, Roberts, Marr *et al.*, 1998; Plater *et al.*, 1999; Kepert & Rosseinsky, 1999). The title compound, (I) (Fig. 1), synthesized from cobalt acetate tetrahydrate, 4,4′-oxydibenzoic acid and 2,2-bipyridyl, forms such a one-dimensional polymer containing chains of Co atoms linked together by the carboxylate ligands (Fig. 2). These chains interact *via* *π*–*π* interactions between adjacent, inverted bipyridyl ligands stacking along [100].



(I)

The Co atom has a distorted octahedral environment (Table 1) formed from two N atoms from the chelating

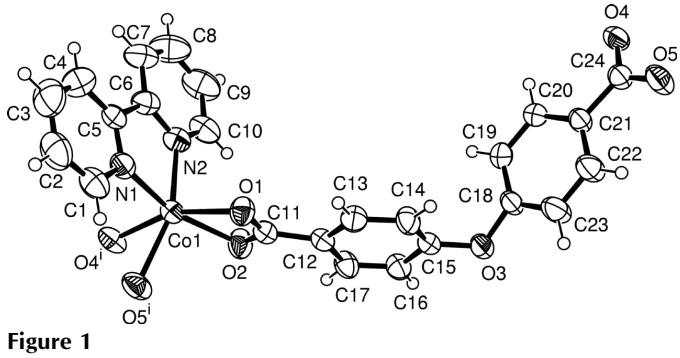


Figure 1
The title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $x+\frac{3}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.]

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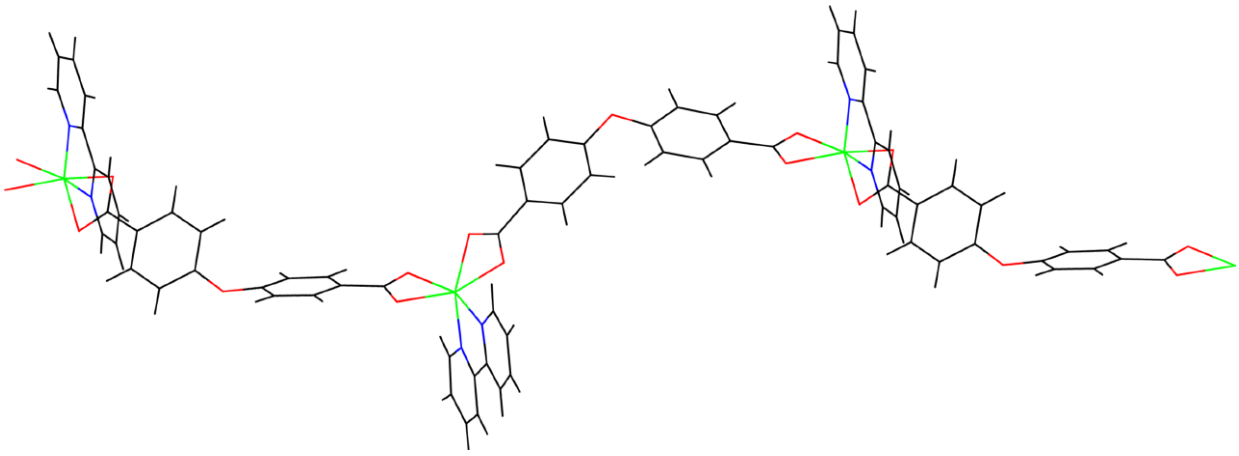

Figure 2
Formation of polymeric chains of Co atoms linked by the diacid.

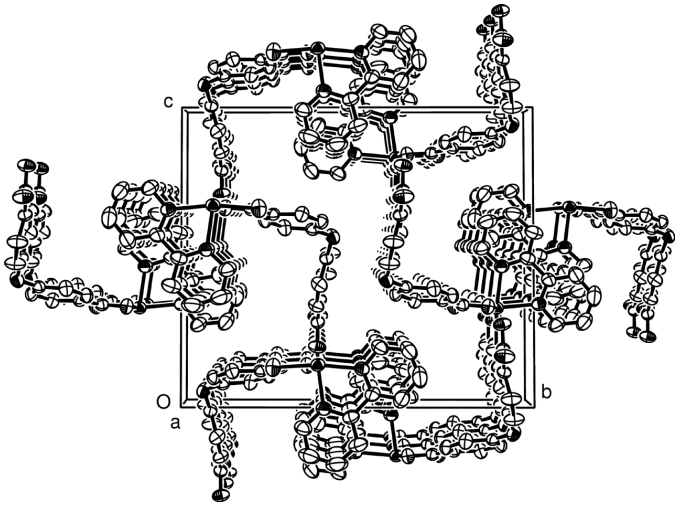

Figure 3
View of the packing of the structure within the unit cell, showing the 'square wave' diacid chains and the superposition of the bipyridyl ligands which lead to π–π interactions in the [100] direction.

bipyridyl and four carboxylate O atoms (two bidentate ligands). The aromatic rings in the diacid are oriented at 80.79 (9)° to one another, giving a 'square wave' shape to the chain (Fig. 3).

Experimental

Cobalt acetate tetrahydrate (102 mg, 0.410 mmol), 2,2′-bipyridyl (63 mg, 0.403 mmol), 4,4′-oxydibenzoic acid (105 mg, 0.407 mmol) and water (20 ml) were placed in a 45 ml bomb. After sealing, the bomb was heated at 100 K h^{-1} to 503 K; this temperature was maintained for 2 h, after which the bomb was cooled at 5 K h^{-1} to 453 K. After a further 6 h, the bomb was cooled at 5 K h^{-1} to 293 K. The bomb was opened and the resultant solid collected by filtration, washed with water and dried in air. Red needle-shaped crystals were selected for analysis.

Crystal data

$[Co(C_{14}H_8O_5)(C_{10}H_8N_2)]$	D_x = 1.497 Mg m^{-3}
M_r = 471.32	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 18 261 reflections
a = 7.8975 (4) Å	θ = 2.3–30.0°
b = 17.6323 (8) Å	μ = 0.86 mm^{-1}
c = 15.1057 (7) Å	T = 302 (2) K
β = 96.360 (1)°	Needle, red
V = 2090.54 (17) Å^3	0.4 × 0.1 × 0.1 mm
Z = 4	

Data collection

Bruker SMART 1000 area CCD diffractometer	6071 independent reflections
φ–ω scans	3584 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	R_{int} = 0.050
T_{min} = 0.816, T_{max} = 0.928	θ_{max} = 30.0°
18 261 measured reflections	$h = -10 \rightarrow 11$
	$k = -24 \rightarrow 22$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.075P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.135	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.94	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
6071 reflections	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
289 parameters	

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0885 (16)	Co1—O4^{i}	2.1203 (17)
Co1—N1	2.092 (2)	Co1—O5^{i}	2.1513 (18)
Co1—N2	2.103 (2)	Co1—O2	2.1837 (18)
O1—Co1—N1	101.21 (7)	N2—Co1—O5^{i}	156.61 (8)
O1—Co1—N2	99.95 (8)	O4^{i}—Co1—O5^{i}	61.62 (6)
N1—Co1—N2	77.94 (8)	O1—Co1—O2	61.65 (6)
O1—Co1—O4^{i}	159.03 (7)	N1—Co1—O2	161.10 (7)
N1—Co1—O4^{i}	95.15 (7)	N2—Co1—O2	96.39 (8)
N2—Co1—O4^{i}	96.20 (7)	O4^{i}—Co1—O2	103.43 (6)
O1—Co1—O5^{i}	103.38 (7)	O5^{i}—Co1—O2	96.11 (7)
N1—Co1—O5^{i}	95.75 (8)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2^{i}	0.93	2.58	3.317 (4)	136
C13—H13···O4^{ii}	0.93	2.45	3.201 (3)	137
C20—H20···O1^{iii}	0.93	2.53	3.419 (3)	159

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2000); software used to prepare material for publication: *SHELXL*97.

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