

# catena-Poly[[*(dipyrido*[3,2-*a*:2',3'-*c*]-phenazine)cobalt(II)]- $\mu$ -biphenyl-2,2'-dicarboxylato]

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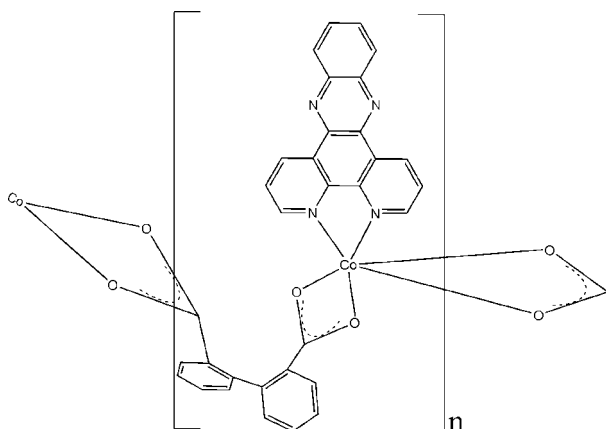
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.049;  $wR$  factor = 0.086; data-to-parameter ratio = 13.4.

In the title compound,  $[\text{Co}(\text{C}_{14}\text{H}_8\text{O}_4)(\text{C}_{18}\text{H}_{10}\text{N}_4)]_n$ , the  $\text{Co}^{\text{II}}$  atom is six-coordinated by four O atoms from two different biphenyl-2,2'-dicarboxylate ligands and two N atoms from the bidentate dipyrido[3,2-*a*:2',3'-*c*]phenazine ligand in a distorted octahedral geometry. The  $\text{Co}^{\text{II}}$  atoms are bridged by the biphenyl-2,2'-dicarboxylate ligands to form a one-dimensional chain structure.  $\pi$ - $\pi$  interactions between neighbouring chains result in a two-dimensional supramolecular network (centroid-to-centroid separation = 3.381 Å).

## Related literature

For related literature, see: Hao *et al.* (2004); Li *et al.* (2006); Noveron *et al.* (2002); Dickeson & Summers (1970); Li *et al.* (2007); Zhang *et al.* (2001).



## Experimental

### Crystal data

$[\text{Co}(\text{C}_{14}\text{H}_8\text{O}_4)(\text{C}_{18}\text{H}_{10}\text{N}_4)]$   
 $M_r = 581.43$   
 Monoclinic,  $P2_1/c$   
 $a = 9.311$  (4) Å  
 $b = 12.521$  (5) Å  
 $c = 21.831$  (10) Å  
 $\beta = 102.31^\circ$

$V = 2486.5$  (19) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.74$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.43 \times 0.11 \times 0.07$  mm

### Data collection

Bruker APEXII diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2002)  
 $T_{\text{min}} = 0.904$ ,  $T_{\text{max}} = 0.951$

13141 measured reflections  
 5022 independent reflections  
 1796 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.085$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.085$   
 $S = 0.87$   
 5022 reflections

370 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.92$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Co1—O3 <sup>i</sup>	2.087 (3)	Co1—N1	2.115 (4)
Co1—N2	2.093 (4)	Co1—O2	2.151 (3)
Co1—O1	2.105 (3)	Co1—O4 <sup>i</sup>	2.185 (3)
N2—Co1—O1	95.31 (15)	N2—Co1—O2	97.96 (13)
N2—Co1—N1	78.05 (16)	O1—Co1—O2	61.86 (10)
O1—Co1—N1	159.78 (13)	N1—Co1—O2	99.79 (13)

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

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL-Plus (Sheldrick, 2008); software used to prepare material for publication: SHELXTL-Plus.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2538).

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**supplementary materials**

*Acta Cryst.* (2008). E64, m379 [ doi:10.1107/S1600536808001827 ]

***catena*-Poly[[*(dipyrido*[3,2-*a*:2',3'-*c*]phenazine)cobalt(II)]-*μ*-biphenyl-2,2'-dicarboxylato]**

**F. Wei, W.-J. Wang, X.-J. Jin, Z.-M. Mei and X.-P. Li**

**Comment**

Metal-organic hybrid compounds have attracted considerable interest and importance in recent years, not only due to their intriguing structural motifs but also their potential applications in areas such as catalysis, medicine and host-guest chemistry (Hao *et al.*, 2004). The chelating ligand 1,10-phenanthroline (phen) and its derivatives have been widely used in the construction of metal-organic coordination polymers (Li *et al.*, 2006). On the other hand, carboxylate ligands have already been proven to be efficient for the generation of a helical coordination polymer (Li *et al.*, 2007), so we reacted dipydo[3,2 - a:2',3'-c]phenazine with cobalt and biphenyl-2,2'-dicarboxylate, resulting in the title molecular complex, [Co(C<sub>14</sub>H<sub>8</sub>O<sub>4</sub>)(C<sub>18</sub>H<sub>10</sub>N<sub>4</sub>)]<sub>n</sub>, (I)

Compound (I) is a one-dimensional chain structure, which is constructed from one Co<sup>II</sup> atom, one *L* ligand and two biphenyl-2,2'-dicarboxylate dianion (Fig. 1). The Co<sup>II</sup> center is six-coordinated by two N atoms from the bidentate *L* ligand and four O atoms from two different 2,6'-biphenyl dicarboxylic acid ligands to result in a substantially distorted *cis*-CoN<sub>2</sub>O<sub>4</sub> octahedron. The mean Co—O and Co—N distances are 2.112 (3) and 2.104 (4) Å, respectively. The C—O bond lengths of the 2,6'-biphenyl dicarboxylic acid groups imply electronic delocalizations of the negative charges.

Neighboring Co<sup>II</sup> atoms are bridged by the biphenyl-2,2'-dicarboxylate ligands, forming a one-dimensional chain structure as shown in (Fig. 2). Then, neighbouring chains are connected by  $\pi$ - $\pi$  interactions, generating a two-dimensional supramolecular structure (Fig. 3). The  $\pi$ - $\pi$  stacking distances are 3.381 Å between *L* ligands. Similar values are seen in related structures (Noveron *et al.*, 2002).

**Experimental**

The *L* ligand was synthesized by the literature method of Dickeson & Summers (1970). A mixture of CoCl<sub>2</sub>·2H<sub>2</sub>O (0.3 mmol), *L* (0.1 mmol) and 2,6'-biphenyl dicarboxylic acid (0.3 mmol) in 30 ml of distilled water was stirred thoroughly for 1 h at ambient temperature. The pH value was adjusted to about 7.5 with NaOH aqueous solution. The suspension was sealed in a Teflon-lined stainless reaction vessel (40 ml) and heated at 443 K for 5 days. The vessel was cooled slowly to room temperature at a rate of 10 K h<sup>-1</sup> before opening and yellow crystals of (I) were collected.

**Refinement**

All H atoms were placed geometrically (C—H = 0.93 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ .

Figures

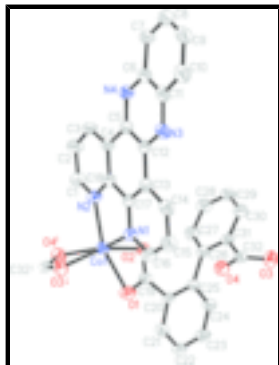


Fig. 1. The asymmetric unit of (I), together with additional atoms to complete the coordination of Co1 with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). Symmetry codes: (i)  $-x, -y + 1/2, -z + 1/2$ ; (ii)  $-x, y - 1/2, -z + 1/2$ .



Fig. 2. A view of the one-chain structure of (I). H atoms have been omitted for clarity.

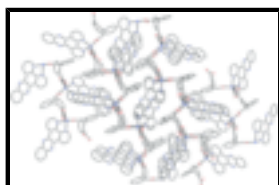


Fig. 3. View of the two-dimensional supramolecular structure of (I) generated by  $\pi$ - $\pi$  interactions. H atoms have been omitted for clarity.

**catena-Poly[[*(dipyrido*[3,2 - a:2',3'-c]*phenazine)cobalt(II)*]- $\mu$ -biphenyl-2,2'- dicarboxylato]**

*Crystal data*

[Co(C<sub>14</sub>H<sub>8</sub>O<sub>4</sub>)(C<sub>18</sub>H<sub>10</sub>N<sub>4</sub>)]

$M_r = 581.43$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 9.311\ (4)\ \text{\AA}$

$b = 12.521\ (5)\ \text{\AA}$

$c = 21.831\ (10)\ \text{\AA}$

$\beta = 102.31^\circ$

$V = 2486.5\ (19)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1188.0$

$D_x = 1.553\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2096 reflections

$\theta = 2.3\text{--}26.0^\circ$

$\mu = 0.74\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Block, amethyst

$0.44 \times 0.11 \times 0.07\ \text{mm}$

*Data collection*

Bruker APEXII  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 0 pixels  $\text{mm}^{-1}$

$T = 292\ (2)\ \text{K}$

not measured scans

5022 independent reflections

1796 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.085$

$\theta_{\text{max}} = 26.2^\circ$

$\theta_{\text{min}} = 1.9^\circ$

$h = -9 \rightarrow 11$

Absorption correction: multi-scan  
(SADABS; Bruker, 2002)  $k = -15 \rightarrow 15$   
 $T_{\min} = 0.904$ ,  $T_{\max} = 0.951$   $l = -27 \rightarrow 18$   
13141 measured reflections

### Refinement

Refinement on  $F^2$  Secondary atom site location: difference Fourier map  
Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites  
 $R[F^2 > 2\sigma(F^2)] = 0.048$  H-atom parameters constrained  
 $wR(F^2) = 0.085$   $w = 1/[\sigma^2(F_o^2) + (0.002P)^2]$   
 $S = 0.87$  where  $P = (F_o^2 + 2F_c^2)/3$   
5022 reflections  $(\Delta/\sigma)_{\max} = 0.001$   
370 parameters  $\Delta\rho_{\max} = 0.92 \text{ e } \text{\AA}^{-3}$   
Primary atom site location: structure-invariant direct methods Extinction correction: none  
 $\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.02037 (7)	0.27680 (5)	0.19183 (3)	0.0511 (2)
O1	0.1414 (3)	0.2191 (3)	0.27808 (13)	0.0644 (10)
O2	-0.0977 (3)	0.2343 (2)	0.26292 (13)	0.0526 (9)
N2	0.0064 (4)	0.1293 (3)	0.14589 (18)	0.0486 (11)
C5	-0.3420 (5)	0.1185 (4)	-0.0118 (2)	0.0458 (13)
N1	-0.1583 (4)	0.3017 (3)	0.11521 (17)	0.0496 (11)
C4	-0.3106 (5)	0.2151 (4)	0.0256 (2)	0.0455 (13)
C12	-0.2475 (5)	0.0282 (4)	0.0016 (2)	0.0449 (13)
N4	-0.4625 (4)	0.1169 (3)	-0.05836 (18)	0.0521 (12)
C13	-0.1245 (5)	0.0309 (4)	0.0561 (2)	0.0454 (13)
N3	-0.2692 (4)	-0.0605 (3)	-0.03208 (19)	0.0512 (11)
C18	-0.1927 (5)	0.2156 (4)	0.0769 (2)	0.0436 (12)
C17	-0.1001 (5)	0.1222 (4)	0.0925 (2)	0.0422 (13)
C19	0.0254 (5)	0.2107 (4)	0.2984 (2)	0.0457 (13)

## supplementary materials

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C6	-0.4883 (5)	0.0253 (5)	-0.0920 (2)	0.0519 (14)
C20	0.0350 (5)	0.1783 (3)	0.3653 (2)	0.0395 (12)
C31	-0.2806 (5)	0.0171 (4)	0.3290 (2)	0.0454 (13)
C26	-0.2356 (5)	0.1185 (4)	0.3516 (2)	0.0461 (13)
C11	-0.3907 (6)	-0.0624 (4)	-0.0800 (2)	0.0526 (14)
C23	0.0737 (5)	0.1393 (4)	0.4925 (2)	0.0661 (16)
H23A	0.0846	0.1279	0.5354	0.079*
C21	0.1700 (5)	0.1932 (3)	0.4056 (2)	0.0498 (14)
H21A	0.2490	0.2170	0.3894	0.060*
C3	-0.3955 (5)	0.3080 (4)	0.0141 (2)	0.0569 (15)
H3B	-0.4744	0.3108	-0.0201	0.068*
C25	-0.0827 (5)	0.1402 (4)	0.3883 (2)	0.0454 (13)
C24	-0.0610 (5)	0.1215 (4)	0.4522 (2)	0.0587 (15)
H24A	-0.1390	0.0963	0.4686	0.070*
C30	-0.4302 (6)	-0.0057 (4)	0.3079 (2)	0.0628 (16)
H30A	-0.4597	-0.0743	0.2944	0.075*
C7	-0.6179 (5)	0.0173 (4)	-0.1408 (2)	0.0602 (16)
H7A	-0.6833	0.0743	-0.1490	0.072*
C14	-0.0337 (5)	-0.0574 (4)	0.0756 (2)	0.0569 (15)
H14A	-0.0458	-0.1199	0.0520	0.068*
C27	-0.3441 (6)	0.1970 (4)	0.3493 (2)	0.0624 (15)
H27A	-0.3163	0.2656	0.3634	0.075*
C2	-0.3632 (5)	0.3954 (4)	0.0528 (2)	0.0692 (17)
H2B	-0.4201	0.4570	0.0460	0.083*
C16	0.0876 (5)	0.0434 (5)	0.1629 (2)	0.0578 (15)
H16A	0.1594	0.0471	0.1997	0.069*
C1	-0.2411 (5)	0.3880 (4)	0.1032 (2)	0.0574 (15)
H1B	-0.2174	0.4469	0.1294	0.069*
C10	-0.4203 (6)	-0.1538 (4)	-0.1182 (3)	0.0649 (16)
H10A	-0.3551	-0.2110	-0.1123	0.078*
C15	0.0737 (5)	-0.0517 (4)	0.1299 (3)	0.0635 (16)
H15A	0.1344	-0.1097	0.1438	0.076*
C22	0.1907 (5)	0.1739 (4)	0.4688 (2)	0.0571 (15)
H22A	0.2823	0.1840	0.4951	0.069*
C29	-0.5345 (6)	0.0734 (5)	0.3071 (2)	0.0678 (16)
H29A	-0.6337	0.0578	0.2932	0.081*
C28	-0.4916 (6)	0.1750 (5)	0.3267 (2)	0.0697 (17)
H28A	-0.5613	0.2287	0.3248	0.084*
C8	-0.6444 (6)	-0.0731 (5)	-0.1747 (2)	0.0716 (18)
H8A	-0.7299	-0.0790	-0.2055	0.086*
C9	-0.5458 (7)	-0.1579 (5)	-0.1642 (2)	0.0695 (17)
H9A	-0.5655	-0.2188	-0.1890	0.083*
C32	-0.1725 (6)	-0.0692 (4)	0.3244 (2)	0.0483 (14)
O3	-0.1965 (3)	-0.1613 (3)	0.34207 (15)	0.0616 (10)
O4	-0.0650 (3)	-0.0519 (2)	0.30026 (15)	0.0594 (10)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0506 (4)	0.0622 (5)	0.0386 (4)	-0.0010 (4)	0.0055 (3)	0.0012 (4)
O1	0.0366 (19)	0.114 (3)	0.044 (2)	0.004 (2)	0.0134 (17)	0.015 (2)
O2	0.0424 (19)	0.076 (2)	0.038 (2)	0.0024 (18)	0.0062 (16)	0.0077 (18)
N2	0.050 (3)	0.051 (3)	0.043 (3)	0.000 (2)	0.004 (2)	0.005 (2)
C5	0.039 (3)	0.064 (4)	0.036 (3)	-0.006 (3)	0.013 (3)	0.007 (3)
N1	0.048 (3)	0.059 (3)	0.040 (3)	0.005 (2)	0.006 (2)	0.000 (2)
C4	0.036 (3)	0.060 (4)	0.040 (3)	-0.003 (3)	0.006 (2)	0.002 (3)
C12	0.043 (3)	0.056 (4)	0.038 (3)	-0.008 (3)	0.013 (3)	0.004 (3)
N4	0.046 (3)	0.072 (3)	0.039 (3)	-0.008 (2)	0.009 (2)	0.001 (2)
C13	0.042 (3)	0.054 (4)	0.042 (3)	-0.003 (3)	0.014 (3)	0.006 (3)
N3	0.051 (3)	0.060 (3)	0.045 (3)	-0.013 (2)	0.015 (2)	-0.006 (2)
C18	0.040 (3)	0.056 (4)	0.036 (3)	-0.005 (3)	0.012 (2)	0.001 (3)
C17	0.039 (3)	0.051 (4)	0.039 (3)	-0.005 (3)	0.014 (3)	0.007 (3)
C19	0.047 (3)	0.046 (3)	0.043 (3)	-0.002 (3)	0.007 (3)	-0.005 (3)
C6	0.051 (4)	0.066 (4)	0.040 (4)	-0.015 (3)	0.014 (3)	-0.002 (3)
C20	0.038 (3)	0.047 (3)	0.031 (3)	0.001 (3)	0.001 (2)	0.000 (2)
C31	0.039 (3)	0.062 (4)	0.035 (3)	-0.001 (3)	0.008 (3)	0.002 (3)
C26	0.039 (3)	0.066 (4)	0.037 (3)	0.003 (3)	0.014 (3)	0.009 (3)
C11	0.060 (4)	0.063 (4)	0.041 (4)	-0.022 (3)	0.025 (3)	-0.004 (3)
C23	0.063 (4)	0.097 (5)	0.035 (3)	0.011 (4)	0.003 (3)	0.007 (3)
C21	0.049 (3)	0.060 (4)	0.041 (3)	-0.003 (3)	0.012 (3)	-0.005 (3)
C3	0.042 (3)	0.072 (4)	0.052 (4)	0.004 (3)	0.001 (3)	0.004 (3)
C25	0.040 (3)	0.055 (3)	0.041 (3)	0.003 (3)	0.005 (3)	0.001 (3)
C24	0.049 (3)	0.084 (4)	0.043 (4)	-0.005 (3)	0.011 (3)	0.004 (3)
C30	0.056 (4)	0.076 (4)	0.056 (4)	-0.003 (3)	0.010 (3)	0.004 (3)
C7	0.052 (4)	0.084 (5)	0.043 (4)	-0.016 (3)	0.009 (3)	0.004 (3)
C14	0.053 (3)	0.062 (4)	0.060 (4)	-0.010 (3)	0.022 (3)	-0.002 (3)
C27	0.053 (4)	0.069 (4)	0.067 (4)	0.003 (3)	0.018 (3)	0.002 (3)
C2	0.066 (4)	0.069 (4)	0.065 (4)	-0.002 (3)	-0.003 (3)	-0.011 (4)
C16	0.051 (3)	0.072 (4)	0.048 (4)	0.005 (3)	0.007 (3)	0.008 (4)
C1	0.058 (4)	0.057 (4)	0.055 (4)	0.011 (3)	0.009 (3)	-0.014 (3)
C10	0.076 (4)	0.068 (4)	0.058 (4)	-0.015 (3)	0.029 (3)	-0.010 (3)
C15	0.062 (4)	0.061 (4)	0.068 (4)	0.001 (3)	0.016 (3)	0.001 (4)
C22	0.047 (3)	0.074 (4)	0.046 (4)	0.002 (3)	-0.001 (3)	-0.002 (3)
C29	0.037 (3)	0.103 (5)	0.062 (4)	-0.004 (4)	0.006 (3)	0.006 (4)
C28	0.048 (4)	0.091 (5)	0.073 (4)	0.011 (4)	0.019 (3)	0.007 (4)
C8	0.074 (5)	0.097 (5)	0.044 (4)	-0.028 (4)	0.011 (3)	0.004 (4)
C9	0.090 (5)	0.079 (5)	0.042 (4)	-0.034 (4)	0.019 (4)	-0.016 (3)
C32	0.052 (4)	0.056 (4)	0.032 (3)	-0.001 (4)	-0.002 (3)	-0.007 (3)
O3	0.066 (2)	0.057 (2)	0.070 (3)	0.004 (2)	0.032 (2)	0.006 (2)
O4	0.050 (2)	0.068 (3)	0.063 (2)	0.003 (2)	0.019 (2)	0.004 (2)

## supplementary materials

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### *Geometric parameters (Å, °)*

Co1—O3 <sup>i</sup>	2.087 (3)	C23—C22	1.372 (5)
Co1—N2	2.093 (4)	C23—C24	1.388 (5)
Co1—O1	2.105 (3)	C23—H23A	0.9300
Co1—N1	2.115 (4)	C21—C22	1.374 (5)
Co1—O2	2.151 (3)	C21—H21A	0.9300
Co1—O4 <sup>i</sup>	2.185 (3)	C3—C2	1.376 (5)
Co1—C19	2.460 (5)	C3—H3B	0.9300
Co1—C32 <sup>i</sup>	2.463 (6)	C25—C24	1.386 (5)
O1—C19	1.256 (4)	C24—H24A	0.9300
O2—C19	1.274 (4)	C30—C29	1.384 (6)
N2—C16	1.322 (5)	C30—H30A	0.9300
N2—C17	1.363 (5)	C7—C8	1.346 (6)
C5—N4	1.344 (5)	C7—H7A	0.9300
C5—C12	1.424 (6)	C14—C15	1.381 (6)
C5—C4	1.454 (6)	C14—H14A	0.9300
N1—C1	1.322 (5)	C27—C28	1.384 (6)
N1—C18	1.360 (5)	C27—H27A	0.9300
C4—C18	1.391 (5)	C2—C1	1.406 (5)
C4—C3	1.398 (5)	C2—H2B	0.9300
C12—N3	1.323 (5)	C16—C15	1.383 (5)
C12—C13	1.465 (5)	C16—H16A	0.9300
N4—C6	1.355 (5)	C1—H1B	0.9300
C13—C17	1.384 (6)	C10—C9	1.369 (6)
C13—C14	1.402 (6)	C10—H10A	0.9300
N3—C11	1.367 (5)	C15—H15A	0.9300
C18—C17	1.450 (6)	C22—H22A	0.9300
C19—C20	1.501 (6)	C29—C28	1.374 (6)
C6—C11	1.414 (6)	C29—H29A	0.9300
C6—C7	1.432 (6)	C28—H28A	0.9300
C20—C25	1.384 (5)	C8—C9	1.390 (6)
C20—C21	1.385 (5)	C8—H8A	0.9300
C31—C26	1.394 (6)	C9—H9A	0.9300
C31—C30	1.400 (5)	C32—O4	1.246 (5)
C31—C32	1.494 (6)	C32—O3	1.252 (5)
C26—C27	1.403 (5)	C32—Co1 <sup>ii</sup>	2.463 (6)
C26—C25	1.502 (5)	O3—Co1 <sup>ii</sup>	2.087 (3)
C11—C10	1.409 (6)	O4—Co1 <sup>ii</sup>	2.185 (3)
O3 <sup>i</sup> —Co1—N2	97.50 (14)	C31—C26—C27	117.8 (5)
O3 <sup>i</sup> —Co1—O1	97.66 (12)	C31—C26—C25	122.2 (5)
N2—Co1—O1	95.31 (15)	C27—C26—C25	119.0 (5)
O3 <sup>i</sup> —Co1—N1	102.12 (13)	N3—C11—C10	119.5 (6)
N2—Co1—N1	78.05 (16)	N3—C11—C6	121.5 (5)
O1—Co1—N1	159.78 (13)	C10—C11—C6	119.0 (5)
O3 <sup>i</sup> —Co1—O2	155.35 (12)	C22—C23—C24	119.6 (5)



N2—Co1—O2	97.96 (13)	C22—C23—H23A	120.2
O1—Co1—O2	61.86 (10)	C24—C23—H23A	120.2
N1—Co1—O2	99.79 (13)	C22—C21—C20	121.8 (5)
O3 <sup>i</sup> —Co1—O4 <sup>i</sup>	60.87 (12)	C22—C21—H21A	119.1
N2—Co1—O4 <sup>i</sup>	153.61 (14)	C20—C21—H21A	119.1
O1—Co1—O4 <sup>i</sup>	102.11 (12)	C2—C3—C4	120.6 (5)
N1—Co1—O4 <sup>i</sup>	91.27 (14)	C2—C3—H3B	119.7
O2—Co1—O4 <sup>i</sup>	107.67 (12)	C4—C3—H3B	119.7
O3 <sup>i</sup> —Co1—C19	127.04 (14)	C20—C25—C24	117.8 (4)
N2—Co1—C19	98.21 (15)	C20—C25—C26	127.0 (4)
O1—Co1—C19	30.71 (11)	C24—C25—C26	115.1 (4)
N1—Co1—C19	130.56 (15)	C25—C24—C23	121.9 (5)
O2—Co1—C19	31.16 (11)	C25—C24—H24A	119.0
O4 <sup>i</sup> —Co1—C19	106.91 (14)	C23—C24—H24A	119.0
O3 <sup>i</sup> —Co1—C32 <sup>i</sup>	30.54 (13)	C29—C30—C31	120.3 (5)
N2—Co1—C32 <sup>i</sup>	126.93 (16)	C29—C30—H30A	119.9
O1—Co1—C32 <sup>i</sup>	100.54 (13)	C31—C30—H30A	119.9
N1—Co1—C32 <sup>i</sup>	98.65 (15)	C8—C7—C6	119.6 (5)
O2—Co1—C32 <sup>i</sup>	134.08 (15)	C8—C7—H7A	120.2
O4 <sup>i</sup> —Co1—C32 <sup>i</sup>	30.36 (12)	C6—C7—H7A	120.2
C19—Co1—C32 <sup>i</sup>	120.29 (15)	C15—C14—C13	120.0 (5)
C19—O1—Co1	90.5 (3)	C15—C14—H14A	120.0
C19—O2—Co1	87.9 (3)	C13—C14—H14A	120.0
C16—N2—C17	117.1 (4)	C28—C27—C26	121.7 (5)
C16—N2—Co1	127.6 (4)	C28—C27—H27A	119.2
C17—N2—Co1	115.3 (3)	C26—C27—H27A	119.2
N4—C5—C12	121.5 (5)	C3—C2—C1	117.6 (5)
N4—C5—C4	118.2 (5)	C3—C2—H2B	121.2
C12—C5—C4	120.3 (5)	C1—C2—H2B	121.2
C1—N1—C18	118.4 (4)	N2—C16—C15	124.8 (5)
C1—N1—Co1	127.2 (4)	N2—C16—H16A	117.6
C18—N1—Co1	114.3 (3)	C15—C16—H16A	117.6
C18—C4—C3	117.4 (5)	N1—C1—C2	123.3 (5)
C18—C4—C5	119.0 (5)	N1—C1—H1B	118.3
C3—C4—C5	123.5 (4)	C2—C1—H1B	118.3
N3—C12—C5	122.5 (5)	C9—C10—C11	119.5 (5)
N3—C12—C13	118.1 (5)	C9—C10—H10A	120.2
C5—C12—C13	119.3 (5)	C11—C10—H10A	120.2
C5—N4—C6	116.5 (4)	C14—C15—C16	117.5 (5)
C17—C13—C14	117.5 (5)	C14—C15—H15A	121.2
C17—C13—C12	119.3 (5)	C16—C15—H15A	121.2
C14—C13—C12	123.0 (5)	C23—C22—C21	118.9 (4)
C12—N3—C11	116.3 (4)	C23—C22—H22A	120.6
N1—C18—C4	122.7 (5)	C21—C22—H22A	120.6
N1—C18—C17	116.4 (4)	C28—C29—C30	120.1 (5)
C4—C18—C17	120.9 (5)	C28—C29—H29A	119.9

## supplementary materials

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N2—C17—C13	123.1 (5)	C30—C29—H29A	119.9
N2—C17—C18	115.9 (5)	C29—C28—C27	119.7 (5)
C13—C17—C18	121.0 (5)	C29—C28—H28A	120.1
O1—C19—O2	119.7 (4)	C27—C28—H28A	120.1
O1—C19—C20	119.3 (4)	C7—C8—C9	121.0 (6)
O2—C19—C20	120.9 (4)	C7—C8—H8A	119.5
O1—C19—Co1	58.8 (2)	C9—C8—H8A	119.5
O2—C19—Co1	60.9 (2)	C10—C9—C8	121.5 (6)
C20—C19—Co1	175.4 (3)	C10—C9—H9A	119.2
N4—C6—C11	121.6 (5)	C8—C9—H9A	119.2
N4—C6—C7	119.1 (5)	O4—C32—O3	120.2 (5)
C11—C6—C7	119.3 (5)	O4—C32—C31	121.1 (5)
C25—C20—C21	119.9 (4)	O3—C32—C31	118.6 (5)
C25—C20—C19	124.0 (4)	O4—C32—Co1 <sup>ii</sup>	62.4 (3)
C21—C20—C19	116.0 (4)	O3—C32—Co1 <sup>ii</sup>	57.9 (3)
C26—C31—C30	120.3 (5)	C31—C32—Co1 <sup>ii</sup>	172.7 (3)
C26—C31—C32	121.8 (5)	C32—O3—Co1 <sup>ii</sup>	91.6 (3)
C30—C31—C32	117.9 (5)	C32—O4—Co1 <sup>ii</sup>	87.3 (3)

Symmetry codes: (i)  $-x, y+1/2, -z+1/2$ ; (ii)  $-x, y-1/2, -z+1/2$ .

Fig. 1

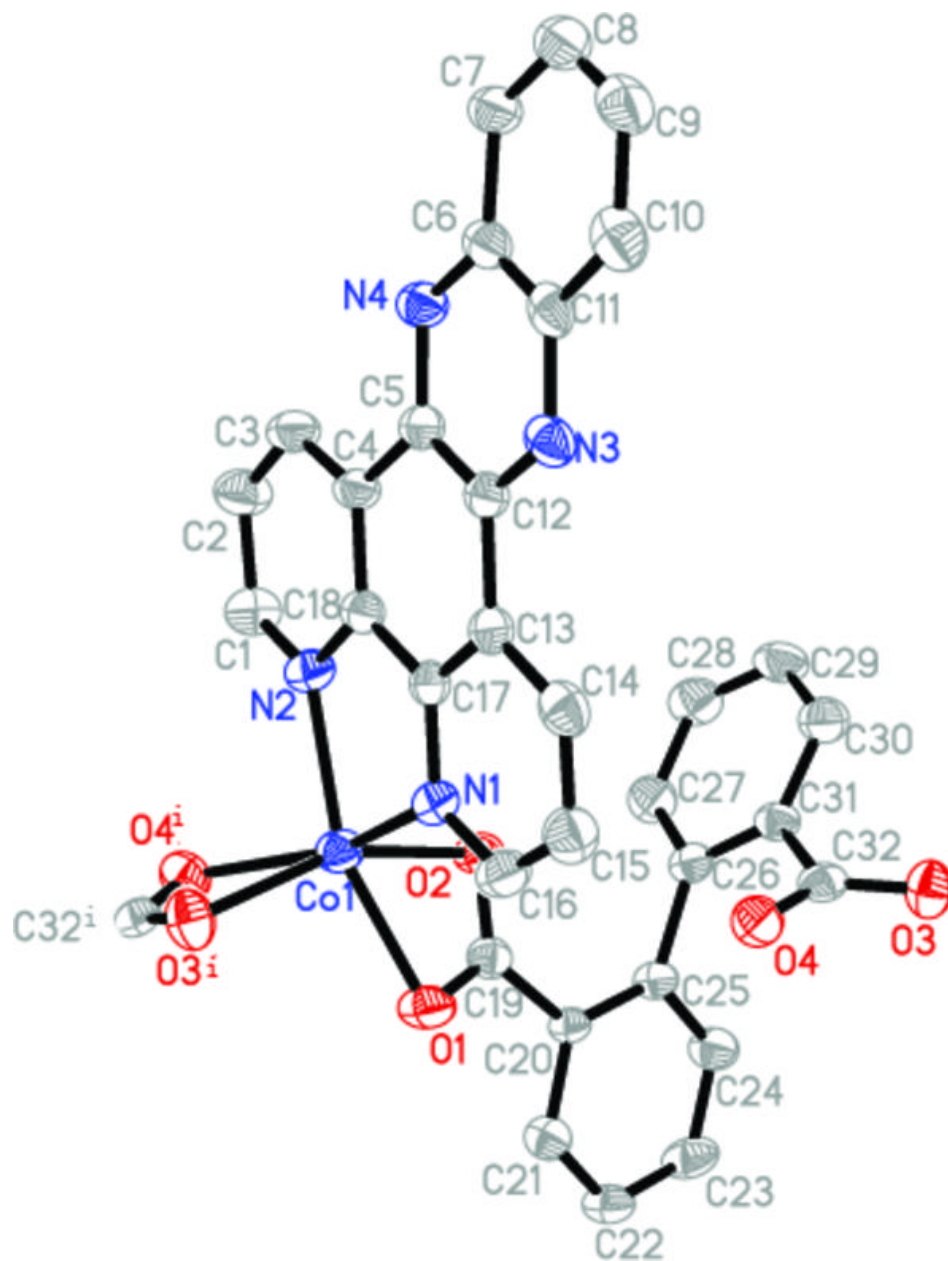


Fig. 2

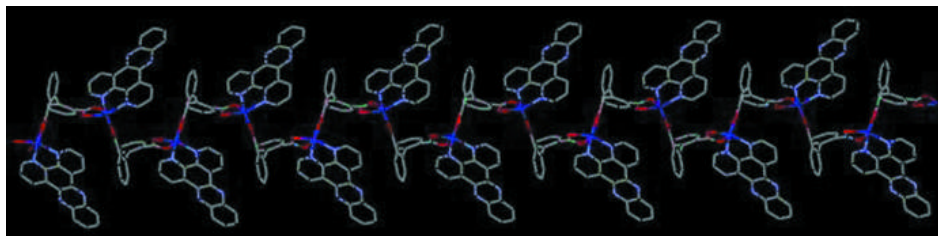


Fig. 3

