

## Bis(benzoato- $\kappa^2O,O'$ )(2,9-dimethyl-1,10-phenanthroline- $\kappa^2N,N'$ )cobalt(II)

Pei-Zheng Zhao,\* Xiao-Peng Xuan and Qing-Hu Tang

College of Chemistry and Environmental Science, Henan Normal University, Xixiang 453007, People's Republic of China  
Correspondence e-mail: pz\_zhao@hotmail.com

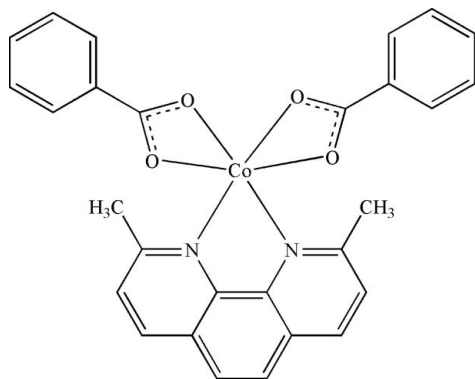
Received 14 November 2007; accepted 21 December 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.004$  Å; disorder in main residue;  $R$  factor = 0.041;  $wR$  factor = 0.111; data-to-parameter ratio = 12.5.

In the title compound,  $[Co(C_7H_5O_2)_2(C_{14}H_{12}N_2)]$ , the  $Co^{II}$  ion is located on a twofold rotation axis and is chelated by a 2,9-dimethyl-1,10-phenanthroline (dmphen) ligand and two benzoate anions in a distorted octahedral geometry. The crystal packing is stabilized by  $\pi-\pi$  interactions between parallel dmphen ligands of neighbouring molecules, with a face-to-face distance of 3.411 (2) Å.

### Related literature

For background information on cobalt coordination chemistry, see: Wang *et al.* (1996); Wall *et al.* (1999); Naing *et al.* (1995). For related structures, see: Wu *et al.* (2003); Su *et al.* (2005); Ding *et al.* (2006); Ren *et al.* (2007); Zhong *et al.* (2006); Li *et al.* (2007).



### Experimental

#### Crystal data

$[Co(C_7H_5O_2)_2(C_{14}H_{12}N_2)]$	$V = 2420.6$ (7) Å <sup>3</sup>
$M_r = 509.41$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 17.632$ (3) Å	$\mu = 0.75$ mm <sup>-1</sup>
$b = 14.410$ (2) Å	$T = 293$ (2) K
$c = 9.5282$ (15) Å	$0.30 \times 0.22 \times 0.22$ mm
$\beta = 90.796$ (2)°	

#### Data collection

Bruker SMART CCD area-detector diffractometer	8882 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	2253 independent reflections
$T_{min} = 0.805$ , $T_{max} = 0.856$	1840 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.026$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$	180 parameters
$wR(F^2) = 0.111$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{max} = 0.48$ e Å <sup>-3</sup>
2253 reflections	$\Delta\rho_{min} = -0.37$ e Å <sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Co1—N1	2.114 (2)	Co1—O2	2.154 (2)
Co1—O1	2.159 (2)		

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Financial support from the Science Fund of Henan Province for Distinguished Young Scholars (grant No. 074100510005) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2376).

### References

- Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2004). *SMART* (Version 5.624) and *SAINTE* (Version 7.12A). Bruker AXS Inc., Madison, Wisconsin, USA.
- Ding, C.-F., Zhang, M.-L., Li, X.-M. & Zhang, S.-S. (2006). *Acta Cryst.* **E62**, m2540–m2542.
- Li, Z.-G., Wang, G.-H., Niu, J.-J., Xu, J.-W. & Hu, N.-H. (2007). *Acta Cryst.* **C63**, m94–m96.
- Naing, K., Taniguchi, M., Takahashi, M. & Yamagishi, A. (1995). *Inorg. Chem.* **34**, 350–356.
- Ren, Y.-L., Liu, Y.-J. & Song, W.-D. (2007). *Acta Cryst.* **E63**, m1191–m1193.
- Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
- Su, J.-R., Gu, J.-M. & Xu, D.-J. (2005). *Acta Cryst.* **E61**, m1033–m1035.
- Wall, M., Linkletter, B., Williams, D., Lebus, A.-M., Hynes, R. C. & Chin, J. (1999). *J. Am. Chem. Soc.* **121**, 4710–4711.
- Wang, J., Cai, X., Rivas, G., Shiraishi, H., Farias, P. A. M. & Dontha, N. (1996). *Anal. Chem.* **68**, 2629–2634.
- Wu, Z.-Y., Xue, Y.-H. & Xu, D.-J. (2003). *Acta Cryst.* **E59**, m809–m811.
- Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2006). *Acta Cryst.* **E62**, m3330–m3332.

**supplementary materials**

*Acta Cryst.* (2008). E64, m327 [ doi:10.1107/S1600536807068080 ]

## Bis(benzoato- $\kappa^2O,O'$ )(2,9-dimethyl-1,10-phenanthroline- $\kappa^2N,N'$ )cobalt(II)

P.-Z. Zhao, X.-P. Xuan and Q.-H. Tang

### Comment

Metal-phenanthroline complexes and their derivatives have attracted much attention because of their peculiar features during recent decades (Wang *et al.*, 1996; Wall *et al.*, 1999; Naing *et al.*, 1995). A number of Co(II) complexes have been synthesized and structures determined (Wu *et al.*, 2003; Su *et al.*, 2005; Ding *et al.*, 2006; Ren *et al.*, 2007; Zhong *et al.*, 2006; Li *et al.*, 2007). The title complex, (I), was recently prepared and its crystal structure is reported here.

Each Co<sup>II</sup> ion is located on a twofold rotation axis and six-coordinated by two N atoms from a dmphen ligand and four carbonyl O atoms from two benzoate ligands (Fig. 1) with a distorted octahedral geometry (Table 1).

In the crystal structure, molecules are linked into a one dimensional network by  $\pi$ - $\pi$  interactions between the dmphen ring systems (Fig. 2). These intermolecular interaction occur between the parallel rings within offset face-to-face packing. The face-to-face distance of neighboring parallel rings is 3.411 (2) Å.

### Experimental

Sodium benzoate (0.1455 g, 1 mmol) and Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (0.1456 g, 0.5 mmol) were dissolved in distilled water (15 ml). This solution was added to a solution of 2,9-dimethyl-1,10-phenanthroline hemihydrate (C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>·0.5H<sub>2</sub>O, 0.1090 g, 0.5 mmol) in ethanol (10 ml). The mixture was refluxed for 4 h. After cooling to room temperature the mixture was filtered. Brown single crystals were obtained by slow evaporation at room temperature after 1 d.

### Refinement

The benzene ring of benzoate ligand is disordered over two positions, site occupancy factors were refined and converged to 0.452 (14) and 0.548 (14), respectively. H atoms were placed in calculated positions and refined in riding model approximation, with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic, and 0.96 Å,  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl.

### Figures

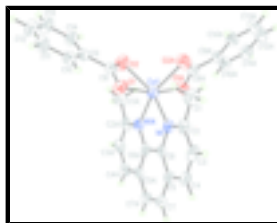


Fig. 1. The molecular structure of the title complex with 30% probability displacement ellipsoids, one disordered component has been omitted for clarity. Symmetry code: (A)  $-x + 1, y, -z + 3/2$ .

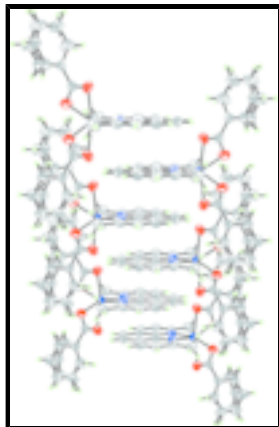


Fig. 2. The  $\pi$ - $\pi$  interaction between the dmphen rings of neighboring molecules in the crystal structure.

**Bis(benzoato- $\kappa^2O,O'$ )(2,9-dimethyl-1,10-phenanthroline- $\kappa^2N,N'$ )cobalt(II)**

*Crystal data*

[Co(C<sub>7</sub>H<sub>5</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>)]

$M_r = 509.41$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 17.632\ (3)\ \text{\AA}$

$b = 14.410\ (2)\ \text{\AA}$

$c = 9.5282\ (15)\ \text{\AA}$

$\beta = 90.796\ (2)^\circ$

$V = 2420.6\ (7)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1052$

$D_x = 1.398\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

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

Cell parameters from 2433 reflections

$\theta = 2.3\text{--}22.5^\circ$

$\mu = 0.75\ \text{mm}^{-1}$

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

Block, brown

$0.30 \times 0.22 \times 0.22\ \text{mm}$

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

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

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2004)

$T_{\min} = 0.805$ ,  $T_{\max} = 0.856$

8882 measured reflections

2253 independent reflections

1840 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 25.5^\circ$

$\theta_{\min} = 2.3^\circ$

$h = -21 \rightarrow 21$

$k = -17 \rightarrow 17$

$l = -11 \rightarrow 11$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$$R[F^2 > 2\sigma(F^2)] = 0.041$$

$$wR(F^2) = 0.111$$

$$S = 1.06$$

2253 reflections

180 parameters

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 2.0726P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.49 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

### 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	0.5000	0.76395 (3)	0.7500	0.0542 (2)	
C1	0.63842 (19)	0.7820 (2)	0.9976 (4)	0.0839 (10)	
H1A	0.5975	0.7472	1.0373	0.126*	
H1B	0.6776	0.7906	1.0673	0.126*	
H1C	0.6585	0.7488	0.9191	0.126*	
C2	0.60968 (14)	0.8746 (2)	0.9496 (3)	0.0593 (7)	
C3	0.63991 (16)	0.9577 (2)	1.0038 (3)	0.0678 (8)	
H3	0.6782	0.9552	1.0719	0.081*	
C4	0.61443 (17)	1.0410 (2)	0.9589 (3)	0.0651 (8)	
H4	0.6345	1.0953	0.9966	0.078*	
C5	0.55731 (15)	1.04513 (18)	0.8547 (3)	0.0560 (6)	
C6	0.52910 (13)	0.96006 (17)	0.8040 (2)	0.0471 (6)	
C7	0.52756 (18)	1.1299 (2)	0.8001 (3)	0.0693 (8)	
H7	0.5463	1.1861	0.8338	0.083*	
C8	0.57021 (17)	0.68233 (18)	0.5604 (3)	0.0602 (7)	
C9	0.6070 (2)	0.6373 (2)	0.4415 (3)	0.054 (4)	0.452 (14)
C10	0.68276 (16)	0.6552 (3)	0.4177 (4)	0.066 (3)	0.452 (14)
H10	0.7095	0.6954	0.4766	0.079*	0.452 (14)
C11	0.71880 (15)	0.6135 (3)	0.3065 (4)	0.078 (6)	0.452 (14)
H11	0.7698	0.6255	0.2905	0.094*	0.452 (14)
C12	0.6791 (3)	0.5537 (4)	0.2190 (5)	0.096 (4)	0.452 (14)
H12	0.7034	0.5256	0.1441	0.115*	0.452 (14)
C13	0.6034 (3)	0.5358 (6)	0.2427 (7)	0.111 (4)	0.452 (14)
H13	0.5767	0.4956	0.1838	0.133*	0.452 (14)

## supplementary materials

C14	0.5674 (3)	0.5776 (6)	0.3540 (6)	0.084 (3)	0.452 (14)
H14	0.5164	0.5655	0.3700	0.100*	0.452 (14)
C9'	0.6177 (2)	0.63122 (19)	0.4495 (3)	0.056 (3)	0.548 (14)
C10'	0.68099 (17)	0.6701 (2)	0.3936 (5)	0.064 (3)	0.548 (14)
H10'	0.6970	0.7284	0.4236	0.077*	0.548 (14)
C11'	0.72124 (15)	0.6236 (2)	0.2934 (4)	0.083 (5)	0.548 (14)
H11'	0.7643	0.6505	0.2553	0.100*	0.548 (14)
C12'	0.6981 (3)	0.5377 (2)	0.2495 (5)	0.084 (3)	0.548 (14)
H12'	0.7257	0.5059	0.1823	0.101*	0.548 (14)
C13'	0.6347 (5)	0.4987 (3)	0.3043 (9)	0.090 (3)	0.548 (14)
H13'	0.6185	0.4407	0.2734	0.108*	0.548 (14)
C14'	0.5949 (4)	0.5449 (3)	0.4048 (7)	0.072 (2)	0.548 (14)
H14'	0.5521	0.5177	0.4431	0.087*	0.548 (14)
N1	0.55395 (11)	0.87653 (14)	0.8526 (2)	0.0496 (5)	
O1	0.60107 (14)	0.74637 (15)	0.6274 (3)	0.0847 (5)	
O2	0.50361 (13)	0.65984 (16)	0.5879 (2)	0.0847 (5)	

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0625 (3)	0.0494 (3)	0.0509 (3)	0.000	0.0041 (2)	0.000
C1	0.076 (2)	0.098 (3)	0.077 (2)	0.0292 (18)	-0.0178 (17)	0.0002 (18)
C2	0.0486 (14)	0.0791 (19)	0.0502 (15)	0.0093 (13)	0.0026 (11)	-0.0044 (13)
C3	0.0521 (16)	0.098 (2)	0.0530 (16)	-0.0035 (15)	-0.0033 (12)	-0.0160 (15)
C4	0.0679 (18)	0.075 (2)	0.0522 (16)	-0.0159 (15)	0.0081 (13)	-0.0161 (14)
C5	0.0638 (16)	0.0613 (16)	0.0433 (13)	-0.0074 (12)	0.0138 (12)	-0.0070 (11)
C6	0.0506 (14)	0.0547 (14)	0.0363 (12)	0.0007 (11)	0.0101 (10)	-0.0017 (10)
C7	0.099 (2)	0.0540 (16)	0.0549 (17)	-0.0078 (14)	0.0167 (14)	-0.0058 (12)
C8	0.0749 (18)	0.0479 (15)	0.0579 (16)	-0.0033 (13)	0.0010 (14)	0.0031 (12)
C9	0.059 (5)	0.049 (7)	0.055 (7)	0.002 (5)	0.015 (5)	0.007 (5)
C10	0.066 (8)	0.075 (6)	0.056 (5)	-0.008 (5)	-0.008 (5)	-0.001 (4)
C11	0.051 (9)	0.105 (12)	0.079 (10)	0.001 (8)	0.001 (7)	0.006 (10)
C12	0.096 (7)	0.120 (9)	0.072 (6)	0.012 (6)	0.010 (5)	-0.035 (5)
C13	0.103 (7)	0.129 (9)	0.103 (7)	-0.024 (7)	0.017 (6)	-0.059 (7)
C14	0.074 (5)	0.089 (6)	0.088 (6)	-0.014 (5)	0.013 (5)	-0.034 (5)
C9'	0.062 (5)	0.058 (6)	0.047 (6)	-0.003 (4)	-0.004 (4)	-0.006 (4)
C10'	0.062 (6)	0.059 (4)	0.073 (4)	0.000 (4)	0.004 (4)	0.009 (4)
C11'	0.071 (9)	0.099 (9)	0.080 (9)	0.007 (7)	0.028 (7)	0.012 (8)
C12'	0.076 (4)	0.110 (6)	0.067 (4)	0.015 (5)	0.016 (4)	-0.010 (5)
C13'	0.097 (6)	0.086 (5)	0.086 (5)	-0.018 (4)	0.010 (4)	-0.039 (4)
C14'	0.068 (4)	0.073 (4)	0.077 (4)	-0.020 (3)	0.016 (4)	-0.014 (3)
N1	0.0488 (12)	0.0589 (13)	0.0412 (11)	0.0050 (9)	0.0029 (9)	-0.0033 (9)
O1	0.0876 (11)	0.0800 (11)	0.0870 (11)	-0.0088 (8)	0.0221 (9)	-0.0209 (8)
O2	0.0876 (11)	0.0800 (11)	0.0870 (11)	-0.0088 (8)	0.0221 (9)	-0.0209 (8)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Co1—N1	2.114 (2)	C8—C9	1.465 (4)
--------	-----------	-------	-----------

Co1—N1 <sup>i</sup>	2.114 (2)	C8—C9'	1.544 (4)
Co1—O1	2.159 (2)	C9—C10	1.3816 (16)
Co1—O1 <sup>i</sup>	2.159 (2)	C9—C14	1.3816 (16)
Co1—O2 <sup>i</sup>	2.154 (2)	C10—C11	1.3815 (16)
Co1—O2	2.154 (2)	C10—H10	0.9300
Co1—C8 <sup>i</sup>	2.498 (3)	C11—C12	1.3816 (16)
C1—C2	1.497 (4)	C11—H11	0.9300
C1—H1A	0.9600	C12—C13	1.3816 (16)
C1—H1B	0.9600	C12—H12	0.9300
C1—H1C	0.9600	C13—C14	1.3816 (16)
C2—N1	1.339 (3)	C13—H13	0.9300
C2—C3	1.406 (4)	C14—H14	0.9300
C3—C4	1.349 (4)	C9'—C10'	1.3643 (16)
C3—H3	0.9300	C9'—C14'	1.3726 (16)
C4—C5	1.406 (4)	C10'—C11'	1.3726 (16)
C4—H4	0.9300	C10'—H10'	0.9300
C5—C6	1.406 (3)	C11'—C12'	1.3660 (16)
C5—C7	1.425 (4)	C11'—H11'	0.9300
C6—N1	1.360 (3)	C12'—C13'	1.3619 (15)
C6—C6 <sup>i</sup>	1.444 (5)	C12'—H12'	0.9300
C7—C7 <sup>i</sup>	1.353 (6)	C13'—C14'	1.3685 (16)
C7—H7	0.9300	C13'—H13'	0.9300
C8—O1	1.243 (3)	C14'—H14'	0.9300
C8—O2	1.249 (3)		
N1—Co1—N1 <sup>i</sup>	79.73 (11)	O1—C8—C9	122.0 (3)
N1—Co1—O2 <sup>i</sup>	102.73 (9)	O2—C8—C9	118.4 (3)
N1 <sup>i</sup> —Co1—O2 <sup>i</sup>	148.05 (8)	O1—C8—C9'	117.9 (3)
N1—Co1—O2	148.05 (8)	O2—C8—C9'	122.7 (3)
N1 <sup>i</sup> —Co1—O2	102.73 (9)	C10—C9—C14	120.0
O2 <sup>i</sup> —Co1—O2	91.74 (13)	C10—C9—C8	118.9 (2)
N1—Co1—O1	88.33 (8)	C14—C9—C8	121.1 (2)
N1 <sup>i</sup> —Co1—O1	102.08 (9)	C11—C10—C9	120.0
O2 <sup>i</sup> —Co1—O1	109.81 (9)	C11—C10—H10	120.0
O2—Co1—O1	59.85 (8)	C9—C10—H10	120.0
N1—Co1—O1 <sup>i</sup>	102.08 (9)	C10—C11—C12	120.0
N1 <sup>i</sup> —Co1—O1 <sup>i</sup>	88.33 (8)	C10—C11—H11	120.0
O2 <sup>i</sup> —Co1—O1 <sup>i</sup>	59.85 (8)	C12—C11—H11	120.0
O2—Co1—O1 <sup>i</sup>	109.81 (9)	C11—C12—C13	120.0
O1—Co1—O1 <sup>i</sup>	166.53 (12)	C11—C12—H12	120.0
N1—Co1—C8 <sup>i</sup>	104.54 (8)	C13—C12—H12	120.0
N1 <sup>i</sup> —Co1—C8 <sup>i</sup>	118.14 (8)	C12—C13—C14	120.0
O2 <sup>i</sup> —Co1—C8 <sup>i</sup>	30.01 (8)	C12—C13—H13	120.0
O2—Co1—C8 <sup>i</sup>	102.14 (9)	C14—C13—H13	120.0
O1—Co1—C8 <sup>i</sup>	139.20 (10)	C9—C14—C13	120.0

## supplementary materials

O1 <sup>i</sup> —Co1—C8 <sup>i</sup>	29.84 (8)	C9—C14—H14	120.0
C2—C1—H1A	109.5	C13—C14—H14	120.0
C2—C1—H1B	109.5	C10 <sup>'</sup> —C9 <sup>'</sup> —C14 <sup>'</sup>	119.2
H1A—C1—H1B	109.5	C10 <sup>'</sup> —C9 <sup>'</sup> —C8	121.72 (19)
C2—C1—H1C	109.5	C14 <sup>'</sup> —C9 <sup>'</sup> —C8	119.06 (19)
H1A—C1—H1C	109.5	C9 <sup>'</sup> —C10 <sup>'</sup> —C11 <sup>'</sup>	120.3
H1B—C1—H1C	109.5	C9 <sup>'</sup> —C10 <sup>'</sup> —H10 <sup>'</sup>	119.8
N1—C2—C3	120.4 (3)	C11 <sup>'</sup> —C10 <sup>'</sup> —H10 <sup>'</sup>	119.8
N1—C2—C1	118.1 (3)	C12 <sup>'</sup> —C11 <sup>'</sup> —C10 <sup>'</sup>	120.0
C3—C2—C1	121.4 (3)	C12 <sup>'</sup> —C11 <sup>'</sup> —H11 <sup>'</sup>	120.0
C4—C3—C2	121.2 (3)	C10 <sup>'</sup> —C11 <sup>'</sup> —H11 <sup>'</sup>	120.0
C4—C3—H3	119.4	C13 <sup>'</sup> —C12 <sup>'</sup> —C11 <sup>'</sup>	120.0
C2—C3—H3	119.4	C13 <sup>'</sup> —C12 <sup>'</sup> —H12 <sup>'</sup>	120.0
C3—C4—C5	119.6 (3)	C11 <sup>'</sup> —C12 <sup>'</sup> —H12 <sup>'</sup>	120.0
C3—C4—H4	120.2	C12 <sup>'</sup> —C13 <sup>'</sup> —C14 <sup>'</sup>	119.9
C5—C4—H4	120.2	C12 <sup>'</sup> —C13 <sup>'</sup> —H13 <sup>'</sup>	120.0
C4—C5—C6	116.9 (3)	C14 <sup>'</sup> —C13 <sup>'</sup> —H13 <sup>'</sup>	120.0
C4—C5—C7	123.4 (3)	C13 <sup>'</sup> —C14 <sup>'</sup> —C9 <sup>'</sup>	120.5
C6—C5—C7	119.7 (2)	C13 <sup>'</sup> —C14 <sup>'</sup> —H14 <sup>'</sup>	119.8
N1—C6—C5	123.0 (2)	C9 <sup>'</sup> —C14 <sup>'</sup> —H14 <sup>'</sup>	119.8
N1—C6—C6 <sup>i</sup>	117.74 (13)	C2—N1—C6	118.9 (2)
C5—C6—C6 <sup>i</sup>	119.30 (15)	C2—N1—Co1	128.61 (18)
C7 <sup>i</sup> —C7—C5	120.99 (16)	C6—N1—Co1	112.39 (15)
C7 <sup>i</sup> —C7—H7	119.5	C8—O1—Co1	90.36 (19)
C5—C7—H7	119.5	C8—O2—Co1	90.41 (17)
O1—C8—O2	119.4 (3)		
N1—C2—C3—C4	-0.8 (4)	C3—C2—N1—C6	2.3 (4)
C1—C2—C3—C4	179.2 (3)	C1—C2—N1—C6	-177.6 (2)
C2—C3—C4—C5	-0.8 (4)	C3—C2—N1—Co1	178.41 (18)
C3—C4—C5—C6	0.8 (4)	C1—C2—N1—Co1	-1.5 (4)
C3—C4—C5—C7	-179.4 (3)	C5—C6—N1—C2	-2.4 (3)
C4—C5—C6—N1	0.9 (4)	C6 <sup>i</sup> —C6—N1—C2	177.8 (2)
C7—C5—C6—N1	-179.0 (2)	C5—C6—N1—Co1	-179.10 (18)
C4—C5—C6—C6 <sup>i</sup>	-179.4 (2)	C6 <sup>i</sup> —C6—N1—Co1	1.2 (3)
C7—C5—C6—C6 <sup>i</sup>	0.8 (4)	N1 <sup>i</sup> —Co1—N1—C2	-176.7 (3)
C4—C5—C7—C7 <sup>i</sup>	-179.9 (3)	O2 <sup>i</sup> —Co1—N1—C2	35.9 (2)
C6—C5—C7—C7 <sup>i</sup>	0.0 (5)	O2—Co1—N1—C2	-79.0 (3)
O1—C8—C9—C10	11.2 (5)	O1—Co1—N1—C2	-74.1 (2)
O2—C8—C9—C10	-174.2 (4)	O1 <sup>i</sup> —Co1—N1—C2	97.3 (2)
C9 <sup>'</sup> —C8—C9—C10	-49.13 (12)	C8 <sup>i</sup> —Co1—N1—C2	66.7 (2)
O1—C8—C9—C14	-169.0 (5)	N1 <sup>i</sup> —Co1—N1—C6	-0.41 (11)
O2—C8—C9—C14	5.7 (5)	O2 <sup>i</sup> —Co1—N1—C6	-147.88 (16)
C9 <sup>'</sup> —C8—C9—C14	130.70 (19)	O2—Co1—N1—C6	97.2 (2)
C14—C9—C10—C11	0.0	O1—Co1—N1—C6	102.19 (17)
C8—C9—C10—C11	179.8 (3)	O1 <sup>i</sup> —Co1—N1—C6	-86.45 (17)



C9—C10—C11—C12	0.0	C8 <sup>i</sup> —Co1—N1—C6	-117.03 (16)
C10—C11—C12—C13	0.0	O2—C8—O1—Co1	0.7 (3)
C11—C12—C13—C14	0.0	C9—C8—O1—Co1	175.3 (3)
C10—C9—C14—C13	0.0	C9'—C8—O1—Co1	-177.0 (2)
C8—C9—C14—C13	-179.8 (3)	N1—Co1—O1—C8	-177.35 (18)
C12—C13—C14—C9	0.0	N1 <sup>i</sup> —Co1—O1—C8	-98.22 (18)
O1—C8—C9'—C10'	-20.3 (5)	O2 <sup>i</sup> —Co1—O1—C8	79.71 (19)
O2—C8—C9'—C10'	162.1 (4)	O2—Co1—O1—C8	-0.39 (17)
C9—C8—C9'—C10'	103.27 (16)	O1 <sup>i</sup> —Co1—O1—C8	41.69 (17)
O1—C8—C9'—C14'	160.6 (4)	C8 <sup>i</sup> —Co1—O1—C8	72.1 (3)
O2—C8—C9'—C14'	-17.0 (5)	O1—C8—O2—Co1	-0.7 (3)
C9—C8—C9'—C14'	-75.85 (18)	C9—C8—O2—Co1	-175.5 (3)
C14'—C9'—C10'—C11'	0.3	C9'—C8—O2—Co1	176.9 (3)
C8—C9'—C10'—C11'	-178.9 (3)	N1—Co1—O2—C8	6.1 (3)
C9'—C10'—C11'—C12'	-0.3	N1 <sup>i</sup> —Co1—O2—C8	97.09 (18)
C10'—C11'—C12'—C13'	0.6	O2 <sup>i</sup> —Co1—O2—C8	-111.61 (19)
C11'—C12'—C13'—C14'	-1.0	O1—Co1—O2—C8	0.38 (17)
C12'—C13'—C14'—C9'	1.0	O1 <sup>i</sup> —Co1—O2—C8	-170.06 (17)
C10'—C9'—C14'—C13'	-0.6	C8 <sup>i</sup> —Co1—O2—C8	-140.01 (16)
C8—C9'—C14'—C13'	178.5 (3)		

Symmetry codes: (i)  $-x+1, y, -z+3/2$ .

Fig. 1

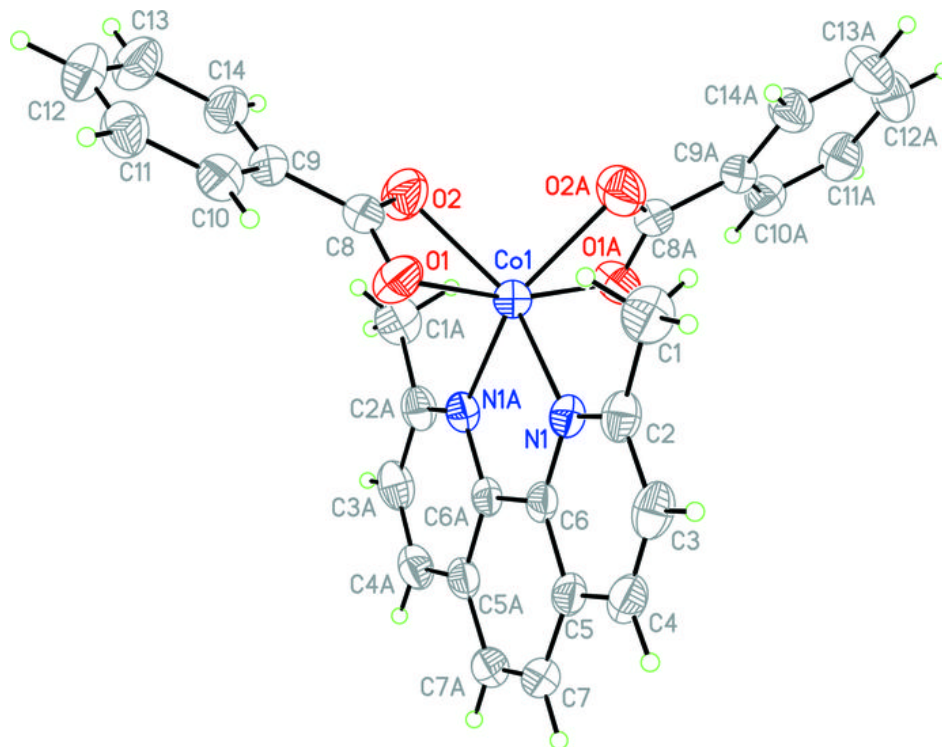


Fig. 2

