

## Bis(1*H*-benzimidazole- $\kappa$ N<sup>3</sup>)bis(4-methylbenzoato- $\kappa^2$ O, $O'$ )cobalt(II)

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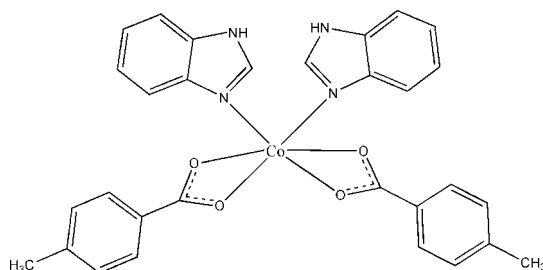
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.050;  $wR$  factor = 0.125; data-to-parameter ratio = 18.1.

In the title mononuclear complex,  $[\text{Co}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{C}_7\text{H}_6\text{N}_2)_2]$ , the Co<sup>II</sup> atom is coordinated by four carboxylate O atoms from two 4-methylbenzoate ligands and two N atoms from two benzimidazole ligands in an octahedral coordination geometry. The molecules are assembled *via* intermolecular N—H...O hydrogen-bonding interactions into a three-dimensional network.

### Related literature

For literature on related structures, see: Song *et al.* (2007).



### Experimental

#### Crystal data

$[\text{Co}(\text{C}_8\text{H}_7\text{O}_2)_2(\text{C}_7\text{H}_6\text{N}_2)_2]$   
 $M_r = 565.48$

Monoclinic,  $P2_1/n$

$a = 13.3209$  (4) Å

$b = 14.5129$  (4) Å

$c = 15.2656$  (4) Å

$\beta = 107.020$  (1)°

$V = 2821.97$  (14) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 0.65$  mm<sup>-1</sup>

$T = 296$  (2) K

$0.35 \times 0.32 \times 0.26$  mm

#### Data collection

Bruker APEXII area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.805$ ,  $T_{\max} = 0.849$

36127 measured reflections

6400 independent reflections

4431 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.125$

$S = 1.05$

6400 reflections

354 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.60$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.33$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O4}^{\text{i}}$	0.86	1.90	2.757 (3)	173
$\text{N4}-\text{H4A}\cdots\text{O2}^{\text{ii}}$	0.86	1.91	2.760 (3)	170

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL-XP (Sheldrick, 2008); software used to prepare material for publication: SHELXTL-XP.

The authors acknowledge Guang Dong Ocean University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2407).

### References

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- Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
- Song, W.-D., Gu, C.-S., Hao, X.-M. & Liu, J.-W. (2007). Acta Cryst. E63, m1023–m1024.

**supplementary materials**

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## Bis(1*H*-benzimidazole- $\kappa$ N<sup>3</sup>)bis(4-methylbenzoato- $\kappa$ <sup>2</sup>O,*O'*)cobalt(II)

W.-D. Song, C.-S. Gu, X.-M. Hao and J.-B. Yan

### Comment

In the structural investigation of 4-methylbenzoate complexes, it has been found that the 4-methylbenzoic acid functions as a multidentate ligand [Song *et al.* (2007)], with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Co complex obtained by the reaction of 4-methylbenzoic acid, benzimidazole and cadmium chloride in alkaline aqueous solution.

As illustrated in Figure 1, the Co<sup>II</sup> atom exists in a disordered octahedral environment, defined by four carboxyl O atoms from two bidentate 4-methylbenzoate ligands and two N atoms from two benzimidazole ligands. Intermolecular N—H $\cdots$ O hydrogen bonding interactions (Table 1) between the benzimidazole molecules and the carboxyl O atoms of 4-methylbenzoate ligands form the structural motif exhibiting non-filled voids. (Fig. 2).

### Experimental

A mixture of cobalt chloride(1 mmol), 4-methylbenzoic acid (1 mmol), benzimidazole(1 mmol), NaOH (1.5 mmol) and H<sub>2</sub>O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h<sup>-1</sup>. The crystals obtained were washed with water and dried in air.

### Refinement

H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 – 0.97 Å, N—H = 0.86 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ .

### Figures

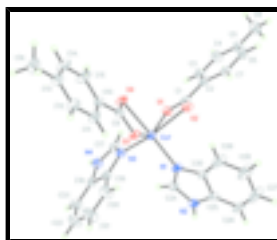


Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids.

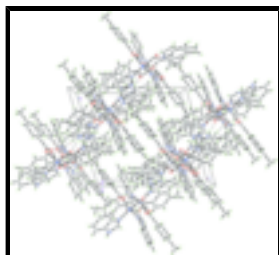


Fig. 2. A packing view of the title compound. The intermolecular hydrogen bonds are shown as dashed lines.

**Bis(1*H*-benzimidazole- $\kappa$ N<sup>3</sup>)bis(4-methylbenzoato- $\kappa^2$ O,*O'*)cobalt(II)**

*Crystal data*

[Co(C<sub>8</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>)<sub>2</sub>]

$M_r = 565.48$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 13.3209$  (4) Å

$b = 14.5129$  (4) Å

$c = 15.2656$  (4) Å

$\beta = 107.020$  (1)°

$V = 2821.97$  (14) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1172$

$D_x = 1.331$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 3500 reflections

$\theta = 1.4$ – $28.0^\circ$

$\mu = 0.65$  mm<sup>-1</sup>

$T = 296$  (2) K

Block, colorless

$0.35 \times 0.32 \times 0.26$  mm

*Data collection*

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

$\varphi$  and  $\omega$  scan

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.805$ ,  $T_{\max} = 0.849$

36127 measured reflections

6400 independent reflections

4431 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\text{max}} = 27.5^\circ$

$\theta_{\text{min}} = 2.0^\circ$

$h = -17 \rightarrow 17$

$k = -18 \rightarrow 18$

$l = -19 \rightarrow 19$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.125$

$S = 1.05$

6400 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 3.4284P]$

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

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

$\Delta\rho_{\text{max}} = 0.60$  e Å<sup>-3</sup>

354 parameters

$$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

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  $F^2 > 2\sigma(F^2)$  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>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8899 (2)	0.68421 (19)	0.14187 (19)	0.0312 (6)
C2	0.9812 (2)	0.69664 (19)	0.10609 (19)	0.0330 (6)
C3	1.0312 (3)	0.7819 (2)	0.1119 (2)	0.0445 (8)
H3	1.0065	0.8321	0.1373	0.053*
C4	1.1174 (3)	0.7916 (2)	0.0798 (3)	0.0531 (9)
H4	1.1504	0.8486	0.0845	0.064*
C5	1.1560 (3)	0.7186 (2)	0.0409 (2)	0.0443 (8)
C6	1.1059 (3)	0.6346 (2)	0.0354 (2)	0.0462 (8)
H6	1.1310	0.5845	0.0102	0.055*
C7	1.0195 (3)	0.6235 (2)	0.0665 (2)	0.0403 (7)
H7	0.9864	0.5665	0.0609	0.048*
C8	1.2497 (3)	0.7308 (3)	0.0059 (3)	0.0640 (11)
H8A	1.2699	0.6722	-0.0126	0.096*
H8B	1.3070	0.7561	0.0536	0.096*
H8C	1.2320	0.7720	-0.0456	0.096*
C9	0.7811 (2)	0.58438 (18)	0.3444 (2)	0.0301 (6)
C10	0.7966 (2)	0.52426 (18)	0.42681 (19)	0.0318 (6)
C11	0.7287 (3)	0.4538 (2)	0.4289 (2)	0.0462 (8)
H11	0.6711	0.4430	0.3781	0.055*
C12	0.7449 (3)	0.3984 (2)	0.5059 (2)	0.0538 (10)
H12	0.6978	0.3511	0.5061	0.065*
C13	0.8299 (3)	0.4123 (2)	0.5826 (2)	0.0414 (7)
C14	0.8973 (3)	0.4815 (3)	0.5790 (2)	0.0566 (10)
H14	0.9557	0.4916	0.6292	0.068*
C15	0.8818 (3)	0.5371 (2)	0.5031 (2)	0.0543 (10)
H15	0.9294	0.5841	0.5033	0.065*
C16	0.8501 (3)	0.3510 (3)	0.6659 (2)	0.0603 (10)
H16A	0.9244	0.3438	0.6930	0.090*
H16B	0.8188	0.2917	0.6481	0.090*
H16C	0.8199	0.3784	0.7096	0.090*

## supplementary materials

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C17	0.6908 (2)	0.87357 (19)	0.2698 (2)	0.0348 (7)
H17	0.7554	0.8953	0.2669	0.042*
C18	0.5341 (2)	0.8715 (2)	0.2899 (2)	0.0372 (7)
C19	0.5603 (2)	0.7845 (2)	0.2655 (2)	0.0356 (7)
C20	0.4904 (3)	0.7117 (2)	0.2553 (3)	0.0589 (10)
H20	0.5074	0.6532	0.2392	0.071*
C21	0.3955 (4)	0.7290 (3)	0.2696 (4)	0.0806 (15)
H21	0.3471	0.6813	0.2628	0.097*
C22	0.3697 (3)	0.8165 (3)	0.2944 (3)	0.0742 (13)
H22	0.3048	0.8256	0.3044	0.089*
C23	0.4375 (3)	0.8892 (3)	0.3041 (3)	0.0550 (10)
H23	0.4198	0.9478	0.3196	0.066*
C24	0.5534 (3)	0.7473 (2)	0.0435 (2)	0.0411 (8)
H24	0.5471	0.7972	0.0797	0.049*
C25	0.5272 (2)	0.6580 (2)	-0.0758 (2)	0.0368 (7)
C26	0.4969 (3)	0.6177 (2)	-0.1616 (2)	0.0509 (9)
H26	0.4460	0.6443	-0.2103	0.061*
C27	0.5453 (4)	0.5368 (3)	-0.1715 (3)	0.0814 (16)
H27	0.5275	0.5077	-0.2282	0.098*
C28	0.6212 (4)	0.4971 (3)	-0.0973 (3)	0.0939 (19)
H28	0.6522	0.4419	-0.1061	0.113*
C29	0.6513 (3)	0.5373 (2)	-0.0118 (3)	0.0689 (13)
H29	0.7010	0.5099	0.0371	0.083*
C30	0.6042 (2)	0.6207 (2)	-0.0017 (2)	0.0381 (7)
Co1	0.73145 (3)	0.68195 (2)	0.20032 (3)	0.02980 (12)
N1	0.61978 (19)	0.67861 (16)	0.07391 (16)	0.0346 (6)
N2	0.4965 (2)	0.73853 (18)	-0.04404 (17)	0.0387 (6)
H2	0.4494	0.7762	-0.0747	0.046*
N3	0.65969 (19)	0.78738 (15)	0.25232 (16)	0.0326 (5)
N4	0.6196 (2)	0.92647 (16)	0.29238 (17)	0.0377 (6)
H4A	0.6260	0.9841	0.3059	0.045*
O1	0.85066 (16)	0.75360 (13)	0.17053 (14)	0.0347 (5)
O2	0.85031 (16)	0.60520 (13)	0.14347 (14)	0.0359 (5)
O3	0.70607 (16)	0.56763 (13)	0.27254 (13)	0.0340 (5)
O4	0.84150 (16)	0.65163 (13)	0.34567 (13)	0.0368 (5)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0313 (15)	0.0250 (13)	0.0310 (14)	0.0020 (12)	-0.0005 (12)	0.0031 (12)
C2	0.0346 (16)	0.0307 (15)	0.0292 (14)	0.0034 (12)	0.0023 (12)	0.0058 (12)
C3	0.050 (2)	0.0316 (16)	0.055 (2)	-0.0030 (15)	0.0202 (17)	-0.0036 (15)
C4	0.054 (2)	0.0427 (19)	0.064 (2)	-0.0119 (17)	0.0201 (19)	0.0022 (17)
C5	0.0439 (19)	0.0492 (19)	0.0397 (18)	0.0022 (16)	0.0121 (15)	0.0085 (15)
C6	0.053 (2)	0.0419 (18)	0.046 (2)	0.0054 (16)	0.0173 (17)	0.0019 (15)
C7	0.0444 (19)	0.0323 (16)	0.0425 (18)	-0.0010 (14)	0.0103 (15)	0.0012 (14)
C8	0.064 (3)	0.071 (3)	0.066 (3)	-0.006 (2)	0.032 (2)	0.007 (2)
C9	0.0304 (15)	0.0238 (13)	0.0333 (15)	-0.0010 (12)	0.0050 (12)	-0.0068 (12)

C10	0.0366 (17)	0.0252 (14)	0.0302 (15)	0.0003 (12)	0.0047 (13)	-0.0019 (12)
C11	0.048 (2)	0.0497 (19)	0.0348 (17)	-0.0165 (16)	0.0026 (15)	-0.0002 (15)
C12	0.063 (2)	0.053 (2)	0.0426 (19)	-0.0238 (18)	0.0107 (18)	0.0033 (17)
C13	0.0453 (19)	0.0419 (17)	0.0364 (17)	0.0000 (15)	0.0112 (15)	0.0043 (14)
C14	0.059 (2)	0.055 (2)	0.0392 (19)	-0.0156 (19)	-0.0111 (17)	0.0093 (17)
C15	0.054 (2)	0.047 (2)	0.045 (2)	-0.0251 (17)	-0.0123 (17)	0.0124 (16)
C16	0.075 (3)	0.064 (2)	0.041 (2)	-0.006 (2)	0.0161 (19)	0.0134 (18)
C17	0.0373 (17)	0.0269 (14)	0.0374 (16)	-0.0011 (13)	0.0066 (14)	0.0012 (12)
C18	0.0403 (18)	0.0321 (16)	0.0371 (17)	0.0006 (13)	0.0080 (14)	-0.0054 (13)
C19	0.0363 (17)	0.0309 (15)	0.0372 (16)	-0.0009 (13)	0.0070 (14)	-0.0039 (13)
C20	0.060 (2)	0.0373 (18)	0.085 (3)	-0.0164 (17)	0.030 (2)	-0.0177 (19)
C21	0.062 (3)	0.062 (3)	0.132 (4)	-0.028 (2)	0.050 (3)	-0.028 (3)
C22	0.054 (3)	0.074 (3)	0.106 (4)	-0.012 (2)	0.041 (3)	-0.025 (3)
C23	0.047 (2)	0.050 (2)	0.067 (2)	0.0048 (17)	0.0159 (19)	-0.0165 (18)
C24	0.0419 (19)	0.0420 (17)	0.0359 (17)	0.0160 (15)	0.0057 (14)	0.0024 (14)
C25	0.0305 (16)	0.0295 (15)	0.0418 (17)	-0.0006 (12)	-0.0029 (14)	0.0042 (13)
C26	0.054 (2)	0.0337 (17)	0.0445 (19)	0.0019 (16)	-0.0171 (16)	0.0004 (15)
C27	0.110 (4)	0.041 (2)	0.057 (2)	0.020 (2)	-0.032 (2)	-0.0226 (19)
C28	0.120 (4)	0.043 (2)	0.073 (3)	0.042 (2)	-0.042 (3)	-0.027 (2)
C29	0.079 (3)	0.0350 (18)	0.060 (2)	0.0212 (19)	-0.031 (2)	-0.0129 (17)
C30	0.0364 (17)	0.0276 (14)	0.0386 (17)	-0.0007 (13)	-0.0071 (14)	-0.0009 (13)
Co1	0.0307 (2)	0.02232 (18)	0.0311 (2)	0.00253 (17)	0.00082 (16)	-0.00087 (16)
N1	0.0317 (13)	0.0303 (12)	0.0337 (13)	0.0065 (11)	-0.0030 (11)	0.0002 (11)
N2	0.0334 (15)	0.0429 (15)	0.0342 (14)	0.0135 (12)	0.0008 (11)	0.0033 (12)
N3	0.0365 (14)	0.0233 (11)	0.0354 (13)	-0.0015 (10)	0.0065 (11)	-0.0023 (10)
N4	0.0419 (15)	0.0210 (12)	0.0471 (16)	0.0001 (11)	0.0083 (12)	-0.0047 (11)
O1	0.0374 (12)	0.0251 (10)	0.0383 (11)	0.0017 (9)	0.0062 (9)	0.0001 (9)
O2	0.0367 (12)	0.0245 (10)	0.0426 (12)	0.0000 (9)	0.0054 (10)	0.0026 (9)
O3	0.0352 (12)	0.0277 (10)	0.0308 (11)	-0.0015 (9)	-0.0033 (9)	-0.0016 (8)
O4	0.0385 (12)	0.0314 (10)	0.0323 (11)	-0.0073 (9)	-0.0027 (9)	0.0016 (9)

*Geometric parameters (Å, °)*

C1—O2	1.265 (3)	C17—H17	0.9300
C1—O1	1.270 (3)	C18—N4	1.382 (4)
C1—C2	1.482 (4)	C18—C19	1.390 (4)
C2—C7	1.391 (4)	C18—C23	1.390 (5)
C2—C3	1.395 (4)	C19—C20	1.387 (4)
C3—C4	1.381 (5)	C19—N3	1.397 (4)
C3—H3	0.9300	C20—C21	1.367 (5)
C4—C5	1.385 (5)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.397 (6)
C5—C6	1.381 (5)	C21—H21	0.9300
C5—C8	1.505 (5)	C22—C23	1.369 (5)
C6—C7	1.376 (4)	C22—H22	0.9300
C6—H6	0.9300	C23—H23	0.9300
C7—H7	0.9300	C24—N1	1.323 (4)
C8—H8A	0.9600	C24—N2	1.335 (4)
C8—H8B	0.9600	C24—H24	0.9300

## supplementary materials

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C8—H8C	0.9600	C25—N2	1.372 (4)
C9—O4	1.262 (3)	C25—C26	1.383 (4)
C9—O3	1.273 (3)	C25—C30	1.395 (4)
C9—C10	1.494 (4)	C26—C27	1.369 (5)
C10—C11	1.373 (4)	C26—H26	0.9300
C10—C15	1.380 (4)	C27—C28	1.402 (5)
C11—C12	1.389 (5)	C27—H27	0.9300
C11—H11	0.9300	C28—C29	1.378 (5)
C12—C13	1.384 (5)	C28—H28	0.9300
C12—H12	0.9300	C29—C30	1.391 (4)
C13—C14	1.359 (5)	C29—H29	0.9300
C13—C16	1.511 (4)	C30—N1	1.394 (4)
C14—C15	1.377 (5)	Co1—O1	2.057 (2)
C14—H14	0.9300	Co1—N1	2.064 (2)
C15—H15	0.9300	Co1—O3	2.074 (2)
C16—H16A	0.9600	Co1—N3	2.081 (2)
C16—H16B	0.9600	Co1—O2	2.303 (2)
C16—H16C	0.9600	Co1—O4	2.316 (2)
C17—N3	1.320 (4)	N2—H2	0.8600
C17—N4	1.341 (4)	N4—H4A	0.8600
O2—C1—O1	119.7 (3)	C21—C20—H20	121.2
O2—C1—C2	120.6 (3)	C19—C20—H20	121.2
O1—C1—C2	119.7 (2)	C20—C21—C22	121.5 (4)
C7—C2—C3	118.3 (3)	C20—C21—H21	119.2
C7—C2—C1	120.8 (3)	C22—C21—H21	119.2
C3—C2—C1	120.8 (3)	C23—C22—C21	121.6 (4)
C4—C3—C2	120.0 (3)	C23—C22—H22	119.2
C4—C3—H3	120.0	C21—C22—H22	119.2
C2—C3—H3	120.0	C22—C23—C18	116.9 (3)
C3—C4—C5	121.7 (3)	C22—C23—H23	121.6
C3—C4—H4	119.2	C18—C23—H23	121.6
C5—C4—H4	119.2	N1—C24—N2	113.9 (3)
C6—C5—C4	117.9 (3)	N1—C24—H24	123.0
C6—C5—C8	121.3 (3)	N2—C24—H24	123.0
C4—C5—C8	120.8 (3)	N2—C25—C26	131.3 (3)
C7—C6—C5	121.4 (3)	N2—C25—C30	105.6 (3)
C7—C6—H6	119.3	C26—C25—C30	123.1 (3)
C5—C6—H6	119.3	C27—C26—C25	116.8 (3)
C6—C7—C2	120.7 (3)	C27—C26—H26	121.6
C6—C7—H7	119.6	C25—C26—H26	121.6
C2—C7—H7	119.6	C26—C27—C28	121.0 (3)
C5—C8—H8A	109.5	C26—C27—H27	119.5
C5—C8—H8B	109.5	C28—C27—H27	119.5
H8A—C8—H8B	109.5	C29—C28—C27	122.2 (4)
C5—C8—H8C	109.5	C29—C28—H28	118.9
H8A—C8—H8C	109.5	C27—C28—H28	118.9
H8B—C8—H8C	109.5	C28—C29—C30	117.2 (3)
O4—C9—O3	119.8 (3)	C28—C29—H29	121.4
O4—C9—C10	120.6 (3)	C30—C29—H29	121.4



O3—C9—C10	119.7 (2)	C29—C30—C25	119.8 (3)
C11—C10—C15	117.8 (3)	C29—C30—N1	130.8 (3)
C11—C10—C9	121.6 (3)	C25—C30—N1	109.4 (3)
C15—C10—C9	120.6 (3)	O1—Co1—N1	101.36 (9)
C10—C11—C12	120.7 (3)	O1—Co1—O3	141.11 (8)
C10—C11—H11	119.6	N1—Co1—O3	107.06 (9)
C12—C11—H11	119.6	O1—Co1—N3	100.55 (9)
C13—C12—C11	121.2 (3)	N1—Co1—N3	95.05 (10)
C13—C12—H12	119.4	O3—Co1—N3	102.76 (9)
C11—C12—H12	119.4	O1—Co1—O2	60.06 (7)
C14—C13—C12	117.4 (3)	N1—Co1—O2	91.33 (9)
C14—C13—C16	120.8 (3)	O3—Co1—O2	92.89 (7)
C12—C13—C16	121.7 (3)	N3—Co1—O2	160.49 (8)
C13—C14—C15	121.9 (3)	O1—Co1—O4	89.70 (8)
C13—C14—H14	119.0	N1—Co1—O4	166.53 (9)
C15—C14—H14	119.0	O3—Co1—O4	59.64 (7)
C14—C15—C10	121.0 (3)	N3—Co1—O4	90.39 (9)
C14—C15—H15	119.5	O2—Co1—O4	87.53 (7)
C10—C15—H15	119.5	C24—N1—C30	104.0 (2)
C13—C16—H16A	109.5	C24—N1—Co1	122.4 (2)
C13—C16—H16B	109.5	C30—N1—Co1	132.88 (19)
H16A—C16—H16B	109.5	C24—N2—C25	107.1 (2)
C13—C16—H16C	109.5	C24—N2—H2	126.5
H16A—C16—H16C	109.5	C25—N2—H2	126.5
H16B—C16—H16C	109.5	C17—N3—C19	104.7 (2)
N3—C17—N4	113.0 (3)	C17—N3—Co1	128.5 (2)
N3—C17—H17	123.5	C19—N3—Co1	126.41 (19)
N4—C17—H17	123.5	C17—N4—C18	107.6 (2)
N4—C18—C19	105.2 (3)	C17—N4—H4A	126.2
N4—C18—C23	133.0 (3)	C18—N4—H4A	126.2
C19—C18—C23	121.8 (3)	C1—O1—Co1	95.61 (17)
C18—C19—C20	120.6 (3)	C1—O2—Co1	84.59 (16)
C18—C19—N3	109.5 (3)	C9—O3—Co1	95.55 (17)
C20—C19—N3	129.8 (3)	C9—O4—Co1	84.87 (16)
C21—C20—C19	117.6 (3)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2\cdots O4^i$	0.86	1.90	2.757 (3)	173
$N4-H4A\cdots O2^{ii}$	0.86	1.91	2.760 (3)	170

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

Fig. 1

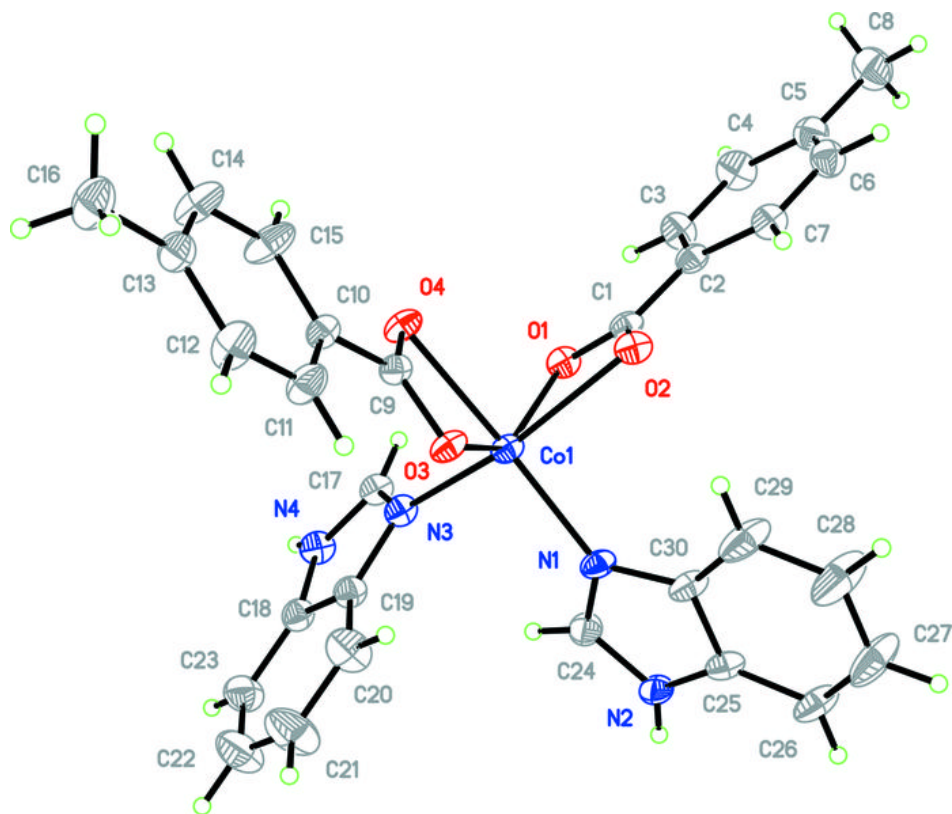


Fig. 2

