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Key indicators

Single-crystal X-ray study
 $T = 296\text{ K}$
 $\text{Mean } \sigma(\text{C-C}) = 0.004\text{ \AA}$
 $R \text{ factor} = 0.043$
 $wR \text{ factor} = 0.114$
Data-to-parameter ratio = 18.0

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

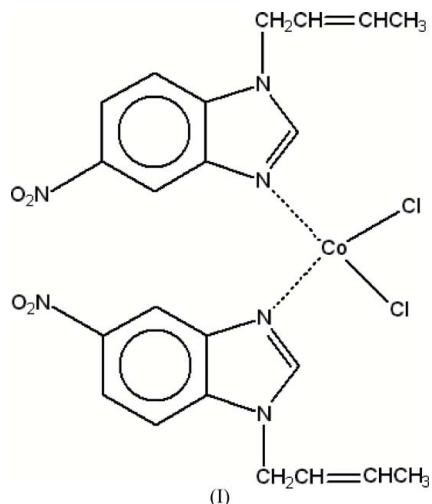
Bis[1-(but-2-enyl)-5-nitro-1*H*-benzimidazole- κN^3]-dichlorocobalt(II)

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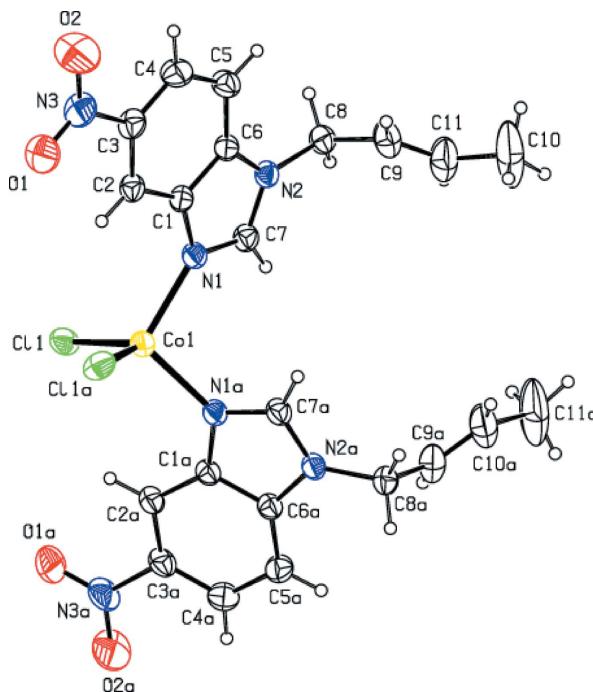
The title compound, $[\text{CoCl}_2(\text{C}_{11}\text{H}_{11}\text{N}_3\text{O}_2)_2]$, was synthesized from 1-(but-2-enyl)-5-nitrobenzimidazole and cobalt dichloride in ethanol. The Co^{II} atom has a distorted tetrahedral geometry, coordinated by two Cl atoms and two N atoms. The molecule is located on a twofold rotation axis, which passes through the Co atom. In the crystal structure, molecules are connected by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions.

Comment

Benzimidazole compounds show a variety of pharmacological activities, such as antifungal, antibacterial, antihelmintic, anti-allergic, antineoplastic, local analgesic, antihistaminic, hypotensive, vasodilator, spasmolytic and anti-ulcer activities (Küçükbay *et al.*, 1995, 1996, 2001; Küçükbay & Durmaz, 1997; Carlsson *et al.*, 2002). In general, heterocyclic compounds and their metal complexes display a wide range of biological activities as antitumor, antibacterial, antifungal and antiviral agents (Arjmand *et al.*, 2005). Metal complexes of biological important ligands are, however, sometimes more effective than the free ligand. Some ruthenium complexes of benzimidazole compounds also show effective catalytic activity for furan synthesis (Küçükbay *et al.*, 1996). The aim of this study was the synthesis and the crystal structure determination of a new benzimidazole cobalt complex and comparison of the results with previous studies (Türktekin *et al.*, 2004; Akkurt *et al.*, 2005).



The Co atom in the title compound, (I), is coordinated in a distorted tetrahedral manner by two Cl and two N atoms (Fig. 1 and Table 1). Bond lengths and angles around Co are

**Figure 1**

A plot of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. [Symmetry code: (a) $-x, y, \frac{1}{2} - z$.]

comparable with the reported average values in the literature (Türkten et al., 2004; Pan & Xu, 2004; Castro et al., 2002; Allen et al., 1987). The molecule is located on a twofold rotation axis, which passes through the Co atom. The benzimidazole ring system is essentially planar, with a maximum deviation of 0.018 (2) Å for C1.

As seen in Fig. 2, the structure is stabilized by C–H \cdots O hydrogen-bonding interactions (Table 2).

Experimental

1-(But-2-enyl)-5-nitrobenzimidazole was synthesized from 5-nitrobenzimidazole, KOH and but-2-enyl bromide according to the literature procedure of Küçükay et al. (2001). A mixture of 1-(but-2-enyl)-5-nitrobenzimidazole (0.5 g, 23.04 mmol) and cobalt dichloride (0.30 g, 23.04 mmol) in ethanol (20 ml) was heated under reflux for 4 h. All volatiles were removed *in vacuo* (0.02 mm Hg; 1 mm Hg = 133.322 Pa). The crude product was crystallized from an ethanol-propan-2-ol (3:1) mixture upon cooling to 243 K (yield 0.41 g, 63%; m.p. 494–495 K). Analysis calculated for $C_{22}H_{22}Cl_2CoN_6O_4$: C 46.81, H 3.90, N 14.89%; found: C 45.52, H 3.7, N 14.34%.

Crystal data

$[CoCl_2(C_{11}H_{11}N_3O_2)_2]$	$Z = 4$
$M_r = 564.29$	$D_x = 1.463 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 15.9533 (11) \text{ \AA}$	$\mu = 0.92 \text{ mm}^{-1}$
$b = 11.4385 (6) \text{ \AA}$	$T = 296 \text{ K}$
$c = 15.4545 (10) \text{ \AA}$	Prism, violet
$\beta = 114.736 (5)^\circ$	$0.62 \times 0.47 \times 0.38 \text{ mm}$
$V = 2561.4 (3) \text{ \AA}^3$	

Data collection

Stoe IPDS-II diffractometer	21773 measured reflections
ω scans	2882 independent reflections
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	2297 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.069$	
$\theta_{\text{max}} = 27.9^\circ$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 1.122P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.50 \text{ e \AA}^{-3}$
2882 reflections	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$
160 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0010 (4)

Table 1
Selected geometric parameters (Å, °).

Co1–Cl1	2.2680 (8)	N1–C7	1.318 (3)
Co1–N1	2.032 (2)	N2–C6	1.381 (3)
O1–N3	1.204 (4)	N2–C7	1.338 (3)
O2–N3	1.205 (7)	N2–C8	1.473 (3)
N1–C1	1.392 (3)	N3–C3	1.475 (4)
Cl1–Co1–N1	110.76 (6)	O1–N3–C3	119.9 (3)
Cl1–Co1–Cl1 ⁱ	114.43 (3)	O2–N3–C3	117.7 (3)
Cl1–Co1–N1 ⁱ	108.59 (6)	N1–C1–C2	130.3 (2)
N1–Co1–N1 ⁱ	103.14 (8)	N1–C1–C6	108.9 (2)
Co1–N1–C1	128.47 (15)	N3–C3–C2	117.0 (2)
Co1–N1–C7	126.44 (18)	N3–C3–C4	117.9 (3)
C1–N1–C7	104.9 (2)	N2–C6–C1	105.9 (2)
C6–N2–C7	106.77 (19)	N2–C6–C5	131.1 (2)
C6–N2–C8	126.6 (2)	N1–C7–N2	113.6 (2)
C7–N2–C8	126.6 (2)	N2–C8–C9	114.2 (2)
O1–N3–O2	122.4 (3)		

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

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

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
$C7\cdots H7\cdots O2^{ii}$	0.93	2.46	3.255 (5)	143
$C8\cdots H8B\cdots O2^{ii}$	0.97	2.48	3.302 (6)	142

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

All H atoms were positioned geometrically, with C–H = 0.93–0.97 Å, and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

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Bis[1-(but-2-enyl)-5-nitro-1*H*-benzimidazole- κN^3]dichlorocobalt(II)

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Bis[1-(but-2-enyl)-5-nitro-1*H*-benzimidazole- κN^3]dichlorocobalt(II)

Crystal data



$M_r = 564.29$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 15.9533$ (11) Å

$b = 11.4385$ (6) Å

$c = 15.4545$ (10) Å

$\beta = 114.736$ (5)°

$V = 2561.4$ (3) Å³

$Z = 4$

$F(000) = 1156$

$D_x = 1.463$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 33960 reflections

$\theta = 2.3\text{--}28.0^\circ$

$\mu = 0.92$ mm⁻¹

$T = 296$ K

Prism, violet

0.62 × 0.47 × 0.38 mm

Data collection

Stoe IPDS-II

diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4

mm long-fine focus

Plane graphite monochromator

Detector resolution: 6.67 pixels mm⁻¹

ω scans

Absorption correction: integration
(X-RED32; Stoe & Cie, 2002)

$T_{\min} = 0.600$, $T_{\max} = 0.722$

21773 measured reflections

2882 independent reflections

2297 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.069$

$\theta_{\max} = 27.9^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -20 \rightarrow 20$

$k = -15 \rightarrow 15$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.114$

$S = 1.03$

2882 reflections

160 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 1.122P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.50$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ e Å⁻³

Extinction correction: SHELXL97,
 $FC^* = KFC[1 + 0.001XFC^2\Lambda^3/\sin(2\Theta)]^{-1/4}$

Extinction coefficient: 0.0010 (4)

Special details

Experimental. ^1H NMR (DMSO- d_6): δ 1.3 (*d*, CH₃, 6H), 3.9 (*d*, CH₂, 4H), 5.1 (*m*, CH=, 4H), 7.3 (*m*, Ar–H, 6H), 8.8 (*s*, CH, 2H).

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors.

Weighted *R*-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.00000	0.64594 (4)	0.25000	0.0460 (2)
C11	-0.11978 (5)	0.75331 (6)	0.14718 (5)	0.0603 (2)
O1	0.30755 (19)	0.8155 (2)	0.1932 (2)	0.0879 (10)
O2	0.3580 (3)	0.7308 (3)	0.1032 (4)	0.141 (2)
N1	0.04819 (13)	0.53550 (16)	0.17823 (14)	0.0454 (6)
N2	0.05380 (13)	0.38412 (16)	0.09071 (14)	0.0437 (5)
N3	0.30685 (19)	0.7352 (2)	0.1425 (3)	0.0736 (10)
C1	0.12006 (14)	0.55327 (18)	0.15094 (16)	0.0423 (6)
C2	0.18051 (15)	0.64673 (19)	0.16830 (18)	0.0471 (7)
C3	0.24177 (17)	0.6375 (2)	0.1269 (2)	0.0540 (8)
C4	0.24722 (19)	0.5439 (3)	0.0730 (2)	0.0639 (10)
C5	0.18771 (17)	0.4508 (2)	0.0565 (2)	0.0547 (8)
C6	0.12390 (15)	0.45859 (19)	0.09595 (16)	0.0436 (6)
C7	0.01250 (15)	0.43364 (19)	0.14107 (18)	0.0472 (7)
C8	0.02990 (18)	0.2712 (2)	0.04043 (19)	0.0512 (7)
C9	0.0891 (2)	0.1724 (2)	0.0941 (2)	0.0727 (10)
C10	0.0618 (4)	0.0769 (3)	0.1138 (3)	0.0990 (15)
C11	0.1178 (5)	-0.0264 (4)	0.1601 (4)	0.179 (3)
H2	0.17970	0.71070	0.20510	0.0570*
H4	0.29100	0.54370	0.04790	0.0770*
H5	0.19000	0.38640	0.02090	0.0660*
H7	-0.03670	0.39950	0.14910	0.0570*
H8A	0.03440	0.27890	-0.02000	0.0610*
H8B	-0.03380	0.25280	0.02680	0.0610*
H9	0.15250	0.18190	0.11520	0.0870*
H10	-0.00120	0.07080	0.09700	0.1190*
H11A	0.07850	-0.08670	0.16560	0.2680*
H11B	0.16270	-0.00530	0.22250	0.2680*
H11C	0.14870	-0.05430	0.12260	0.2680*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0508 (3)	0.0394 (2)	0.0533 (3)	0.0000	0.0272 (2)	0.0000

C11	0.0694 (4)	0.0642 (4)	0.0481 (4)	0.0284 (3)	0.0254 (3)	0.0092 (2)
O1	0.0908 (16)	0.0681 (13)	0.112 (2)	-0.0349 (12)	0.0495 (15)	-0.0199 (14)
O2	0.136 (3)	0.114 (2)	0.244 (5)	-0.063 (2)	0.150 (4)	-0.048 (3)
N1	0.0459 (9)	0.0389 (9)	0.0576 (11)	-0.0017 (7)	0.0279 (8)	-0.0003 (8)
N2	0.0443 (9)	0.0368 (8)	0.0513 (10)	-0.0028 (7)	0.0214 (8)	-0.0001 (7)
N3	0.0636 (15)	0.0662 (15)	0.102 (2)	-0.0201 (11)	0.0455 (15)	-0.0009 (14)
C1	0.0403 (10)	0.0386 (10)	0.0491 (12)	0.0017 (8)	0.0199 (9)	0.0050 (8)
C2	0.0449 (11)	0.0411 (10)	0.0558 (13)	-0.0032 (8)	0.0215 (10)	0.0017 (9)
C3	0.0467 (12)	0.0504 (12)	0.0678 (15)	-0.0110 (9)	0.0267 (11)	0.0014 (11)
C4	0.0566 (14)	0.0682 (16)	0.0823 (19)	-0.0068 (12)	0.0444 (14)	-0.0031 (14)
C5	0.0525 (13)	0.0531 (13)	0.0667 (15)	-0.0013 (10)	0.0329 (12)	-0.0061 (11)
C6	0.0428 (10)	0.0397 (10)	0.0491 (12)	0.0012 (8)	0.0201 (9)	0.0033 (8)
C7	0.0444 (11)	0.0418 (10)	0.0590 (14)	-0.0038 (8)	0.0252 (10)	0.0009 (9)
C8	0.0555 (13)	0.0434 (11)	0.0533 (14)	-0.0071 (9)	0.0215 (11)	-0.0061 (9)
C9	0.0820 (19)	0.0470 (14)	0.0711 (19)	0.0020 (13)	0.0142 (15)	-0.0061 (12)
C10	0.134 (3)	0.0503 (17)	0.088 (3)	-0.0097 (18)	0.022 (2)	0.0012 (16)
C11	0.255 (8)	0.050 (2)	0.122 (4)	0.010 (3)	-0.028 (5)	0.007 (2)

Geometric parameters (\AA , $^\circ$)

Co1—Cl1	2.2680 (8)	C4—C5	1.378 (4)
Co1—N1	2.032 (2)	C5—C6	1.391 (4)
Co1—Cl1 ⁱ	2.2680 (8)	C8—C9	1.484 (4)
Co1—N1 ⁱ	2.032 (2)	C9—C10	1.260 (5)
O1—N3	1.204 (4)	C10—C11	1.474 (7)
O2—N3	1.205 (7)	C2—H2	0.9300
N1—C1	1.392 (3)	C4—H4	0.9300
N1—C7	1.318 (3)	C5—H5	0.9300
N2—C6	1.381 (3)	C7—H7	0.9300
N2—C7	1.338 (3)	C8—H8A	0.9700
N2—C8	1.473 (3)	C8—H8B	0.9700
N3—C3	1.475 (4)	C9—H9	0.9300
C1—C2	1.389 (3)	C10—H10	0.9300
C1—C6	1.394 (3)	C11—H11A	0.9600
C2—C3	1.378 (4)	C11—H11B	0.9600
C3—C4	1.381 (4)	C11—H11C	0.9600
Co1···H2	3.3000	C7···C7 ⁱ	3.552 (4)
Co1···H2 ⁱ	3.3000	C7···O1 ^{vii}	3.236 (4)
Cl1···N1 ⁱ	3.495 (2)	C8···O2 ^{ix}	3.302 (6)
Cl1···C2 ⁱ	3.587 (3)	C8···C1 ⁱⁱⁱ	3.547 (3)
Cl1···C5 ⁱⁱ	3.591 (3)	C9···O1 ^{vii}	3.416 (4)
Cl1···H5 ⁱⁱⁱ	2.8500	C11···O1 ^x	3.376 (8)
Cl1···H8A ⁱⁱⁱ	2.8500	C2···H11B ^v	2.9300
Cl1···H2 ⁱ	2.8600	C3···H11B ^v	2.7300
O1···C11 ^{iv}	3.376 (8)	C4···H11B ^v	2.9300
O1···C6 ^v	3.393 (4)	C5···H8A	2.9700
O1···C7 ^v	3.236 (4)	C8···H5	3.0000

O1···N2 ^v	3.237 (3)	H2···Co1	3.3000
O1···C9 ^v	3.416 (4)	H2···O1	2.4400
O2···C7 ^{vi}	3.255 (5)	H2···Cl1 ⁱ	2.8600
O2···C8 ^{vi}	3.302 (6)	H4···O2	2.3900
O1···H2	2.4400	H5···C8	3.0000
O1···H11C ^{iv}	2.7400	H5···Cl1 ⁱⁱⁱ	2.8500
O2···H4	2.3900	H7···H8B	2.5400
O2···H7 ^{vi}	2.4600	H7···O2 ^{ix}	2.4600
O2···H8B ^{vi}	2.4800	H8A···C5	2.9700
N1···N2	2.222 (3)	H8A···Cl1 ⁱⁱⁱ	2.8500
N1···Cl1 ⁱ	3.495 (2)	H8B···H7	2.5400
N1···N1 ⁱ	3.184 (3)	H8B···H10	2.3000
N2···N1	2.222 (3)	H8B···O2 ^{ix}	2.4800
N2···O1 ^{vii}	3.237 (3)	H10···H8B	2.3000
C1···C8 ⁱⁱⁱ	3.547 (3)	H11B···C2 ^{vii}	2.9300
C2···Cl1 ⁱ	3.587 (3)	H11B···C3 ^{vii}	2.7300
C5···Cl1 ^{viii}	3.591 (3)	H11B···C4 ^{vii}	2.9300
C6···O1 ^{vii}	3.393 (4)	H11C···O1 ^x	2.7400
C7···O2 ^{ix}	3.255 (5)		
Cl1—Co1—N1	110.76 (6)	N1—C7—N2	113.6 (2)
Cl1—Co1—Cl1 ⁱ	114.43 (3)	N2—C8—C9	114.2 (2)
Cl1—Co1—N1 ⁱ	108.59 (6)	C8—C9—C10	126.3 (4)
Cl1 ⁱ —Co1—N1	108.59 (6)	C9—C10—C11	127.7 (6)
N1—Co1—N1 ⁱ	103.14 (8)	C1—C2—H2	123.00
Cl1 ⁱ —Co1—N1 ⁱ	110.76 (6)	C3—C2—H2	123.00
Co1—N1—C1	128.47 (15)	C3—C4—H4	120.00
Co1—N1—C7	126.44 (18)	C5—C4—H4	120.00
C1—N1—C7	104.9 (2)	C4—C5—H5	122.00
C6—N2—C7	106.77 (19)	C6—C5—H5	122.00
C6—N2—C8	126.6 (2)	N1—C7—H7	123.00
C7—N2—C8	126.6 (2)	N2—C7—H7	123.00
O1—N3—O2	122.4 (3)	N2—C8—H8A	109.00
O1—N3—C3	119.9 (3)	N2—C8—H8B	109.00
O2—N3—C3	117.7 (3)	C9—C8—H8A	109.00
N1—C1—C2	130.3 (2)	C9—C8—H8B	109.00
N1—C1—C6	108.9 (2)	H8A—C8—H8B	108.00
C2—C1—C6	120.8 (2)	C8—C9—H9	117.00
C1—C2—C3	114.9 (2)	C10—C9—H9	117.00
N3—C3—C2	117.0 (2)	C9—C10—H10	116.00
N3—C3—C4	117.9 (3)	C11—C10—H10	116.00
C2—C3—C4	125.1 (3)	C10—C11—H11A	109.00
C3—C4—C5	119.9 (3)	C10—C11—H11B	109.00
C4—C5—C6	116.3 (2)	C10—C11—H11C	110.00
N2—C6—C1	105.9 (2)	H11A—C11—H11B	109.00
N2—C6—C5	131.1 (2)	H11A—C11—H11C	110.00
C1—C6—C5	123.0 (2)	H11B—C11—H11C	110.00

Cl1—Co1—N1—C1	93.72 (19)	O1—N3—C3—C2	3.4 (5)
Cl1 ⁱ —Co1—N1—C1	-32.7 (2)	O2—N3—C3—C2	-176.7 (4)
N1 ⁱ —Co1—N1—C1	-150.28 (19)	O2—N3—C3—C4	3.8 (5)
Cl1—Co1—N1—C7	-80.8 (2)	O1—N3—C3—C4	-176.1 (3)
Cl1 ⁱ —Co1—N1—C7	152.80 (19)	N1—C1—C2—C3	-177.5 (2)
N1 ⁱ —Co1—N1—C7	35.3 (2)	C6—C1—C2—C3	0.5 (3)
Co1—N1—C1—C2	3.3 (4)	C2—C1—C6—C5	0.7 (4)
C7—N1—C1—C2	178.7 (3)	N1—C1—C6—N2	-0.1 (3)
Co1—N1—C1—C6	-174.81 (16)	C2—C1—C6—N2	-178.4 (2)
C7—N1—C1—C6	0.6 (3)	N1—C1—C6—C5	179.1 (2)
C1—N1—C7—N2	-1.0 (3)	C1—C2—C3—N3	179.4 (3)
Co1—N1—C7—N2	174.57 (16)	C1—C2—C3—C4	-1.2 (4)
C6—N2—C7—N1	0.9 (3)	C2—C3—C4—C5	0.7 (5)
C7—N2—C6—C1	-0.5 (3)	N3—C3—C4—C5	-179.9 (3)
C7—N2—C6—C5	-179.5 (3)	C3—C4—C5—C6	0.5 (4)
C8—N2—C6—C5	1.2 (4)	C4—C5—C6—N2	177.6 (3)
C8—N2—C6—C1	-179.8 (2)	C4—C5—C6—C1	-1.2 (4)
C6—N2—C8—C9	80.8 (3)	N2—C8—C9—C10	125.8 (4)
C7—N2—C8—C9	-98.4 (3)	C8—C9—C10—C11	174.7 (4)
C8—N2—C7—N1	-179.8 (2)		

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $x-1/2, y+1/2, z$; (iii) $-x, -y+1, -z$; (iv) $x, y+1, z$; (v) $-x+1/2, y+1/2, -z+1/2$; (vi) $x+1/2, y+1/2, z$; (vii) $-x+1/2, y-1/2, -z+1/2$; (viii) $x+1/2, y-1/2, z$; (ix) $x-1/2, y-1/2, z$; (x) $x, y-1, z$.

Hydrogen-bond geometry (\AA , °)

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C7—H7 ^{ix} —O2 ^{ix}	0.93	2.46	3.255 (5)	143
C8—H8B ^{ix} —O2 ^{ix}	0.97	2.48	3.302 (6)	142

Symmetry code: (ix) $x-1/2, y-1/2, z$.