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Bis(2,4-dioxo-5,5-diphenylimidazolidinido-κN^3)bis(propane-1,3-diamine-$\kappa^2 N,N'$)cobalt(II)

Xilan Hu,[a]* Qing Jiang,[a] Daqi Wang[b] and Haifeng Liu[a]

[a]Huaihai Institute of Technology, Jiangsu 222005, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: huxilan836@sohu.com

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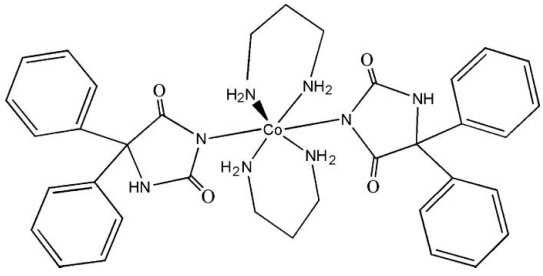
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 14.0.

The complex molecule of the title compound, $[Co(C_{15}H_{11}N_2O_2)_2(C_3H_{10}N_2)_2]$, has crystallographically imposed inversion symmetry. The Co^{II} atom displays a distorted octahedral coordination geometry. In the phenytoin anion, the two phenyl rings form dihedral angles of 62.26 (8) and 57.47 (9)° with the central imidazole ring. Intramolecular N—H···O and C—H···O hydrogen bonds occur. In the crystal, N—H···O and C—H···O hydrogen bonds forming a three-dimensional network.

Related literature

For applications of phenytoin, see: Milne *et al.* (1999); Akitsu *et al.* (1997); Akitsu & Einaga (2005). For related structures, see: Hu *et al.* (2006, 2007, 2009)



Experimental

Crystal data

$[Co(C_{15}H_{11}N_2O_2)_2(C_3H_{10}N_2)_2]$
M_r = 709.71
Monoclinic, $P2_1/n$
a = 10.0368 (12) Å
b = 8.7865 (9) Å
c = 20.684 (2) Å
β = 102.363 (2)°
V = 1781.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 298 K
0.50 × 0.46 × 0.45 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.777, T_{max} = 0.796
8632 measured reflections
3130 independent reflections
2536 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.05
3130 reflections
224 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N2	2.1531 (16)	Co1—N3	2.180 (2)
Co1—N4	2.165 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1	0.90	2.35	3.061 (3)	136
N4—H4B···O2	0.90	2.38	3.095 (3)	137
C5—H5···O2	0.93	2.46	3.089 (3)	125
N1—H1···O1^{i}	0.86	2.02	2.825 (2)	156
N3—H3B···O2^{ii}	0.90	2.34	3.057 (3)	137
N4—H4A···O1^{ii}	0.90	2.27	2.979 (3)	136
C6—H6···O2^{iii}	0.93	2.39	3.293 (3)	165

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2670).

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supporting information

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Bis(2,4-dioxo-5,5-diphenylimidazolidinido-κN^3)bis(propane-1,3-diamine-$\kappa^2 N,N'$)cobalt(II)

Xilan Hu, Qing Jiang, Daqi Wang and Haifeng Liu

S1. Comment

5,5-Diphenylimidazoline-2,4-dione (phenytoin) is a widely used drug in the treatment of epilepsy and an excellent ligand for transition metal complexes (Milne *et al.*, 1999; Akitsu *et al.*, 1997; Akitsu & Einaga, 2005). As a continuation of our research devoted to the design and synthesis of complexes with 5,5-diphenylhydantoinate (Hu *et al.*, 2006, 2007, 2009), we report here the crystal structure of the title compound.

The title compound (Fig. 1) consists of $[Co(pht)_2(pa)_2]$ (Hpht = 5,5-diphenylhydantoin; pa = 1,3-propylendiamine) neutral complex molecules having crystallographically imposed inversion symmetry. The Co atom is coordinated by two nitrogen atoms from two pht anions and four nitrogen atoms from two pa ligands in a distorted octahedral CoN_6 coordination geometry. The Co—N bond distances lie in the range 2.153 (2)–2.180 (2) Å. The imidazole ring (N1/N2/C1–C3) is approximately planar (maximum deviation 0.025 (3) Å for atoms C3) and forms dihedral angles of 62.26 (8) and 57.47 (9)° with the C4–C9 and C10–C15 phenyl rings, respectively. In the crystal structure, intra- and intermolecular N—H···O and C—H···O hydrogen bonds are observed (Table 1), forming a three-dimensional network.

S2. Experimental

To a solution of 5,5-diphenylhydantoin (1.00 mmol) in methanol (10 ml) was added cobalt(II) acetate tetrahydrate (0.5 mmol) and a solution of 1,3-propylendiamine (1 mmol) in methanol (10 ml). Then the mixture was sealed in a 25 ml stainless steel vessel with Teflon liner and heated to 393 K for 50 h, the fill rate being 80%. After cooling to room temperature, orange single crystals of the title compound suitable for X-ray analysis were obtained.

S3. Refinement

All H atoms were placed at calculated positions, with N—H = 0.86–0.90 Å, C—H = 0.93–0.97Å, and refined as riding, with $U_{iso}(H) = 1.2\ U_{eq}(C, N)$.

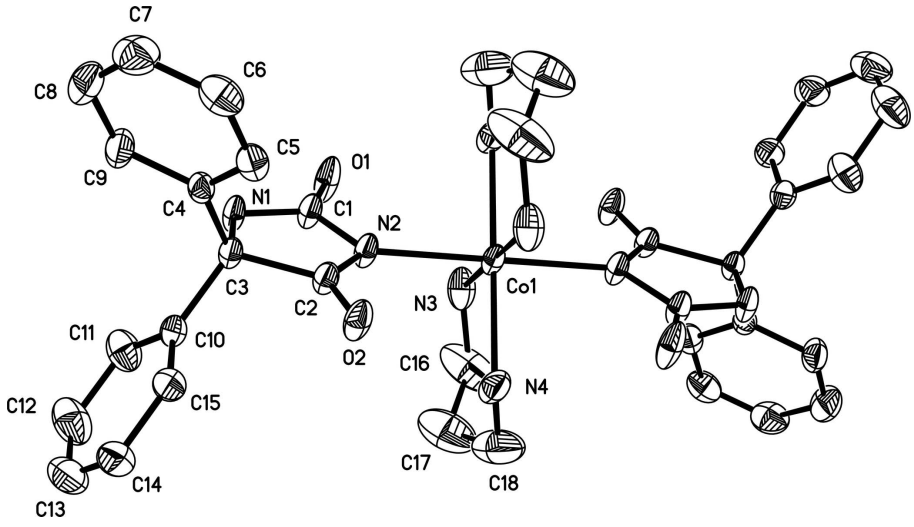

Figure 1

The molecular structure of the title complex showing displacement ellipsoids drawn at the 30% probability level. H-atom are omitted for clarity. Unlabelled atoms are related to the labelled atoms by the symmetry operation 1-x, 1-y, -z.

Bis(2,4-dioxo-5,5-diphenylimidazolidinido-κN^3)bis(propane-1,3- diamine-$\kappa^2 N,N'$)cobalt(II)

Crystal data

$[Co(C_{15}H_{11}N_2O_2)_2(C_3H_{10}N_2)_2]$
$M_r = 709.71$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.0368$ (12) Å
$b = 8.7865$ (9) Å
$c = 20.684$ (2) Å
$\beta = 102.363$ (2)°
$V = 1781.8$ (3) Å^3
$Z = 2$
$F(000) = 746$
$D_x = 1.323$ Mg m^{-3}
Melting point = 534–536 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4059 reflections
$\theta = 2.5$–27.9°
$\mu = 0.53$ mm^{-1}
$T = 298$ K
Block, orange
0.50 × 0.46 × 0.45 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.777$, $T_{max} = 0.796$
8632 measured reflections
3130 independent reflections
2536 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 10$
$l = -19 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 1.05$
3130 reflections
224 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

$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 1.1953P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0318 (15)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.0000	0.03637 (17)
N1	0.92944 (16)	0.6118 (2)	0.05822 (9)	0.0418 (5)
H1	1.0091	0.6117	0.0491	0.050*
N2	0.70243 (16)	0.5782 (2)	0.04395 (9)	0.0412 (5)
N3	0.5249 (2)	0.5748 (3)	−0.09720 (10)	0.0615 (6)
H3A	0.6148	0.5873	−0.0949	0.074*
H3B	0.4972	0.4981	−0.1258	0.074*
N4	0.4168 (2)	0.7172 (3)	0.02120 (11)	0.0583 (6)
H4A	0.3484	0.6978	0.0419	0.070*
H4B	0.4822	0.7657	0.0505	0.070*
O1	0.81717 (15)	0.4817 (2)	−0.03302 (8)	0.0642 (6)
O2	0.66668 (15)	0.6952 (2)	0.13808 (8)	0.0539 (5)
C1	0.8178 (2)	0.5516 (3)	0.01896 (11)	0.0435 (6)
C2	0.7420 (2)	0.6519 (3)	0.10189 (11)	0.0392 (5)
C3	0.89906 (19)	0.6768 (3)	0.11802 (10)	0.0350 (5)
C4	0.9728 (2)	0.5888 (3)	0.17903 (11)	0.0370 (5)
C5	0.9063 (3)	0.5142 (3)	0.22210 (12)	0.0478 (6)
H5	0.8117	0.5177	0.2147	0.057*
C6	0.9794 (3)	0.4346 (3)	0.27608 (14)	0.0630 (7)
H6	0.9333	0.3851	0.3045	0.076*
C7	1.1180 (4)	0.4283 (4)	0.28789 (15)	0.0725 (9)
H7	1.1664	0.3750	0.3242	0.087*
C8	1.1861 (3)	0.5014 (4)	0.24573 (17)	0.0729 (9)
H8	1.2808	0.4970	0.2534	0.087*
C9	1.1138 (2)	0.5813 (3)	0.19190 (13)	0.0555 (7)
H9	1.1607	0.6309	0.1639	0.067*
C10	0.9329 (2)	0.8457 (3)	0.12697 (11)	0.0405 (5)
C11	1.0033 (3)	0.9222 (3)	0.08683 (14)	0.0627 (7)
H11	1.0304	0.8712	0.0524	0.075*
C12	1.0341 (4)	1.0768 (4)	0.09782 (17)	0.0823 (10)
H12	1.0823	1.1282	0.0708	0.099*

C13	0.9935 (3)	1.1521 (4)	0.14804 (17)	0.0768 (10)
H13	1.0125	1.2553	0.1545	0.092*
C14	0.9256 (3)	1.0773 (3)	0.18856 (16)	0.0663 (8)
H14	0.8990	1.1289	0.2230	0.080*
C15	0.8962 (2)	0.9249 (3)	0.17859 (13)	0.0514 (6)
H15	0.8508	0.8741	0.2069	0.062*
C16	0.4548 (6)	0.7161 (5)	−0.12703 (18)	0.1266 (19)
H16A	0.3618	0.6906	−0.1486	0.152*
H16B	0.5005	0.7526	−0.1609	0.152*
C17	0.4511 (6)	0.8423 (5)	−0.0788 (2)	0.1254 (17)
H17A	0.5435	0.8589	−0.0540	0.150*
H17B	0.4228	0.9343	−0.1039	0.150*
C18	0.3650 (5)	0.8236 (4)	−0.0320 (2)	0.1069 (15)
H18A	0.2760	0.7890	−0.0555	0.128*
H18B	0.3529	0.9220	−0.0128	0.128*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0217 (2)	0.0489 (3)	0.0374 (3)	0.00008 (18)	0.00402 (16)	−0.0121 (2)
N1	0.0222 (9)	0.0644 (13)	0.0398 (10)	−0.0066 (8)	0.0089 (7)	−0.0201 (9)
N2	0.0228 (9)	0.0589 (13)	0.0419 (10)	−0.0021 (8)	0.0073 (7)	−0.0200 (9)
N3	0.0480 (12)	0.0901 (18)	0.0444 (12)	−0.0201 (12)	0.0055 (9)	−0.0083 (12)
N4	0.0365 (11)	0.0634 (15)	0.0690 (15)	0.0073 (10)	−0.0021 (10)	−0.0241 (12)
O1	0.0278 (8)	0.1144 (17)	0.0514 (10)	−0.0071 (9)	0.0108 (7)	−0.0475 (11)
O2	0.0294 (8)	0.0796 (13)	0.0547 (10)	−0.0015 (8)	0.0131 (7)	−0.0340 (9)
C1	0.0249 (10)	0.0628 (16)	0.0426 (13)	−0.0021 (10)	0.0068 (9)	−0.0168 (11)
C2	0.0266 (10)	0.0497 (14)	0.0410 (12)	−0.0001 (10)	0.0068 (9)	−0.0134 (11)
C3	0.0243 (10)	0.0445 (13)	0.0361 (11)	−0.0024 (9)	0.0062 (8)	−0.0114 (10)
C4	0.0320 (11)	0.0368 (13)	0.0410 (12)	−0.0042 (9)	0.0056 (9)	−0.0123 (10)
C5	0.0460 (13)	0.0482 (15)	0.0509 (14)	−0.0082 (11)	0.0143 (11)	−0.0066 (12)
C6	0.084 (2)	0.0521 (17)	0.0553 (17)	−0.0086 (15)	0.0196 (15)	0.0014 (14)
C7	0.086 (2)	0.062 (2)	0.0620 (19)	0.0063 (17)	−0.0028 (16)	0.0124 (16)
C8	0.0444 (15)	0.083 (2)	0.081 (2)	0.0034 (15)	−0.0087 (14)	0.0110 (18)
C9	0.0341 (12)	0.0646 (18)	0.0640 (17)	−0.0067 (12)	0.0022 (11)	0.0078 (14)
C10	0.0319 (11)	0.0443 (14)	0.0405 (12)	−0.0013 (10)	−0.0032 (9)	−0.0016 (10)
C11	0.0733 (18)	0.0644 (19)	0.0480 (15)	−0.0186 (15)	0.0075 (13)	−0.0012 (14)
C12	0.097 (3)	0.071 (2)	0.071 (2)	−0.029 (2)	0.0016 (18)	0.0202 (18)
C13	0.089 (2)	0.0456 (17)	0.081 (2)	−0.0035 (16)	−0.0157 (18)	−0.0020 (17)
C14	0.0643 (18)	0.0494 (18)	0.079 (2)	0.0019 (14)	0.0018 (15)	−0.0148 (16)
C15	0.0469 (14)	0.0455 (15)	0.0602 (16)	−0.0001 (12)	0.0077 (12)	−0.0128 (13)
C16	0.230 (6)	0.074 (3)	0.057 (2)	−0.036 (3)	−0.013 (3)	0.012 (2)
C17	0.201 (6)	0.072 (3)	0.096 (3)	−0.007 (3)	0.015 (3)	0.013 (3)
C18	0.120 (3)	0.070 (2)	0.105 (3)	0.030 (2)	−0.032 (3)	−0.018 (2)

Geometric parameters (Å, º)

Co1—N2^{i}	2.1531 (16)	C6—C7	1.361 (4)
Co1—N2	2.1531 (16)	C6—H6	0.9300
Co1—N4^{i}	2.165 (2)	C7—C8	1.377 (4)
Co1—N4	2.165 (2)	C7—H7	0.9300
Co1—N3^{i}	2.180 (2)	C8—C9	1.384 (4)
Co1—N3	2.180 (2)	C8—H8	0.9300
N1—C1	1.343 (3)	C9—H9	0.9300
N1—C3	1.453 (3)	C10—C11	1.375 (3)
N1—H1	0.8600	C10—C15	1.389 (3)
N2—C2	1.345 (3)	C11—C12	1.401 (5)
N2—C1	1.385 (3)	C11—H11	0.9300
N3—C16	1.494 (5)	C12—C13	1.366 (5)
N3—H3A	0.9000	C12—H12	0.9300
N3—H3B	0.9000	C13—C14	1.358 (4)
N4—C18	1.452 (4)	C13—H13	0.9300
N4—H4A	0.9000	C14—C15	1.378 (4)
N4—H4B	0.9000	C14—H14	0.9300
O1—C1	1.237 (3)	C15—H15	0.9300
O2—C2	1.232 (2)	C16—C17	1.498 (6)
C2—C3	1.555 (3)	C16—H16A	0.9700
C3—C10	1.525 (3)	C16—H16B	0.9700
C3—C4	1.529 (3)	C17—C18	1.438 (6)
C4—C9	1.384 (3)	C17—H17A	0.9700
C4—C5	1.387 (3)	C17—H17B	0.9700
C5—C6	1.387 (4)	C18—H18A	0.9700
C5—H5	0.9300	C18—H18B	0.9700
N2^{i}—Co1—N2	180.00 (10)	C4—C5—H5	119.6
N2^{i}—Co1—N4^{i}	90.18 (7)	C7—C6—C5	120.6 (3)
N2—Co1—N4^{i}	89.82 (7)	C7—C6—H6	119.7
N2^{i}—Co1—N4	89.82 (7)	C5—C6—H6	119.7
N2—Co1—N4	90.18 (7)	C6—C7—C8	119.6 (3)
N4^{i}—Co1—N4	180.00 (12)	C6—C7—H7	120.2
N2^{i}—Co1—N3^{i}	90.51 (7)	C8—C7—H7	120.2
N2—Co1—N3^{i}	89.49 (7)	C7—C8—C9	120.0 (3)
N4^{i}—Co1—N3^{i}	92.65 (10)	C7—C8—H8	120.0
N4—Co1—N3^{i}	87.35 (10)	C9—C8—H8	120.0
N2^{i}—Co1—N3	89.49 (7)	C4—C9—C8	121.2 (3)
N2—Co1—N3	90.51 (7)	C4—C9—H9	119.4
N4^{i}—Co1—N3	87.35 (10)	C8—C9—H9	119.4
N4—Co1—N3	92.65 (10)	C11—C10—C15	118.3 (2)
N3^{i}—Co1—N3	180.00 (13)	C11—C10—C3	122.2 (2)
C1—N1—C3	111.68 (16)	C15—C10—C3	119.5 (2)
C1—N1—H1	124.2	C10—C11—C12	120.0 (3)
C3—N1—H1	124.2	C10—C11—H11	120.0
C2—N2—C1	107.61 (17)	C12—C11—H11	120.0

C2—N2—Co1	126.99 (13)	C13—C12—C11	120.2 (3)
C1—N2—Co1	125.27 (14)	C13—C12—H12	119.9
C16—N3—Co1	119.6 (2)	C11—C12—H12	119.9
C16—N3—H3A	107.4	C14—C13—C12	120.4 (3)
Co1—N3—H3A	107.4	C14—C13—H13	119.8
C16—N3—H3B	107.4	C12—C13—H13	119.8
Co1—N3—H3B	107.4	C13—C14—C15	119.9 (3)
H3A—N3—H3B	106.9	C13—C14—H14	120.1
C18—N4—Co1	120.3 (2)	C15—C14—H14	120.1
C18—N4—H4A	107.2	C14—C15—C10	121.2 (3)
Co1—N4—H4A	107.2	C14—C15—H15	119.4
C18—N4—H4B	107.2	C10—C15—H15	119.4
Co1—N4—H4B	107.2	N3—C16—C17	114.6 (3)
H4A—N4—H4B	106.9	N3—C16—H16A	108.6
O1—C1—N1	124.70 (19)	C17—C16—H16A	108.6
O1—C1—N2	123.96 (19)	N3—C16—H16B	108.6
N1—C1—N2	111.35 (19)	C17—C16—H16B	108.6
O2—C2—N2	125.96 (19)	H16A—C16—H16B	107.6
O2—C2—C3	123.48 (19)	C18—C17—C16	117.9 (4)
N2—C2—C3	110.56 (17)	C18—C17—H17A	107.8
N1—C3—C10	113.85 (19)	C16—C17—H17A	107.8
N1—C3—C4	110.53 (17)	C18—C17—H17B	107.8
C10—C3—C4	109.62 (17)	C16—C17—H17B	107.8
N1—C3—C2	98.61 (15)	H17A—C17—H17B	107.2
C10—C3—C2	110.65 (17)	C17—C18—N4	114.5 (4)
C4—C3—C2	113.27 (18)	C17—C18—H18A	108.6
C9—C4—C5	117.8 (2)	N4—C18—H18A	108.6
C9—C4—C3	118.5 (2)	C17—C18—H18B	108.6
C5—C4—C3	123.67 (19)	N4—C18—H18B	108.6
C6—C5—C4	120.7 (2)	H18A—C18—H18B	107.6
C6—C5—H5	119.6		

N4^{i}—Co1—N2—C2	−133.8 (2)	N2—C2—C3—C4	−114.1 (2)
N4—Co1—N2—C2	46.2 (2)	N1—C3—C4—C9	59.8 (3)
N3^{i}—Co1—N2—C2	−41.2 (2)	C10—C3—C4—C9	−66.5 (3)
N3—Co1—N2—C2	138.8 (2)	C2—C3—C4—C9	169.3 (2)
N4^{i}—Co1—N2—C1	41.5 (2)	N1—C3—C4—C5	−119.5 (2)
N4—Co1—N2—C1	−138.5 (2)	C10—C3—C4—C5	114.2 (2)
N3^{i}—Co1—N2—C1	134.1 (2)	C2—C3—C4—C5	−9.9 (3)
N3—Co1—N2—C1	−45.9 (2)	C9—C4—C5—C6	−0.2 (4)
N2^{i}—Co1—N3—C16	75.1 (2)	C3—C4—C5—C6	179.1 (2)
N2—Co1—N3—C16	−104.9 (2)	C4—C5—C6—C7	0.1 (4)
N4^{i}—Co1—N3—C16	165.3 (2)	C5—C6—C7—C8	−0.2 (5)
N4—Co1—N3—C16	−14.7 (2)	C6—C7—C8—C9	0.3 (5)
N2^{i}—Co1—N4—C18	−72.1 (3)	C5—C4—C9—C8	0.4 (4)
N2—Co1—N4—C18	107.9 (3)	C3—C4—C9—C8	−179.0 (3)
N3^{i}—Co1—N4—C18	−162.7 (3)	C7—C8—C9—C4	−0.5 (5)
N3—Co1—N4—C18	17.3 (3)	N1—C3—C10—C11	−8.7 (3)

C3—N1—C1—O1	−175.7 (3)	C4—C3—C10—C11	115.7 (2)
C3—N1—C1—N2	4.5 (3)	C2—C3—C10—C11	−118.6 (2)
C2—N2—C1—O1	177.8 (3)	N1—C3—C10—C15	173.60 (19)
Co1—N2—C1—O1	1.7 (4)	C4—C3—C10—C15	−62.0 (3)
C2—N2—C1—N1	−2.4 (3)	C2—C3—C10—C15	63.6 (3)
Co1—N2—C1—N1	−178.51 (16)	C15—C10—C11—C12	−1.1 (4)
C1—N2—C2—O2	179.5 (3)	C3—C10—C11—C12	−178.9 (2)
Co1—N2—C2—O2	−4.5 (4)	C10—C11—C12—C13	−0.5 (5)
C1—N2—C2—C3	−0.4 (3)	C11—C12—C13—C14	1.4 (5)
Co1—N2—C2—C3	175.61 (15)	C12—C13—C14—C15	−0.7 (5)
C1—N1—C3—C10	−121.4 (2)	C13—C14—C15—C10	−1.0 (4)
C1—N1—C3—C4	114.7 (2)	C11—C10—C15—C14	1.8 (4)
C1—N1—C3—C2	−4.2 (2)	C3—C10—C15—C14	179.6 (2)
O2—C2—C3—N1	−177.2 (2)	Co1—N3—C16—C17	38.1 (5)
N2—C2—C3—N1	2.7 (2)	N3—C16—C17—C18	−70.4 (6)
O2—C2—C3—C10	−57.6 (3)	C16—C17—C18—N4	74.0 (5)
N2—C2—C3—C10	122.3 (2)	Co1—N4—C18—C17	−44.7 (4)
O2—C2—C3—C4	66.0 (3)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1	0.90	2.35	3.061 (3)	136
N4—H4*B*···O2	0.90	2.38	3.095 (3)	137
C5—H5···O2	0.93	2.46	3.089 (3)	125
N1—H1···O1^{ii}	0.86	2.02	2.825 (2)	156
N3—H3*B*···O2^{i}	0.90	2.34	3.057 (3)	137
N4—H4*A*···O1^{i}	0.90	2.27	2.979 (3)	136
C6—H6···O2^{iii}	0.93	2.39	3.293 (3)	165

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+3/2, *y*−1/2, −*z*+1/2.