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Bis{(*Z*)-*N*′-(2,4-dichlorobenzylidene)-2-hydroxybenzohydrazide-κ^2N',O}bis(pyridine-κN)cobalt(II). Corrigendum

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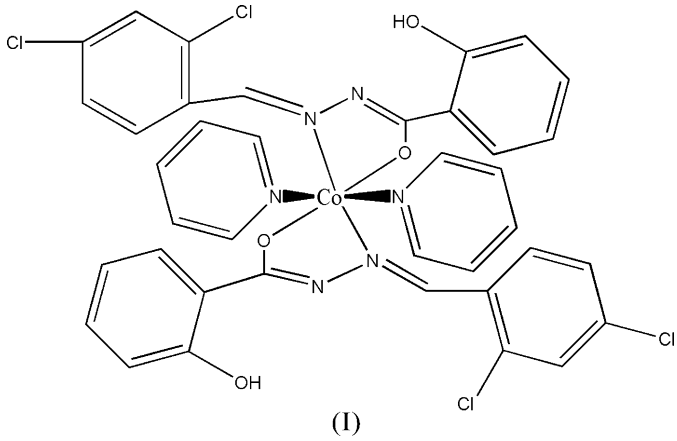
In the original paper by Qiu, Yang, Liu & Zhu [*Acta Cryst.* (2006), E**62**, m1320–m1231], the H atoms attached to N1 and N3 are positioned incorrectly. These have been deleted and the structure rerefined. The correct name of the structure is bis(2,4-dichlorobenzaldehyde 2-hydroxybenzoylhydrazonato-κ^2N,O)bis(pyridine-κN)cobalt(II). The scheme, figure, *Crystal data*, *Refinement* and hydrogen-bond table are corrected.



(I)

Experimental

Crystal data

$[Co(C_{14}H_9Cl_2N_2O_2)_2(C_5H_5N)_2]$
M_r = 833.39
Monoclinic, $P2_1/n$
a = 13.1832 (5) Å
b = 12.2799 (5) Å
c = 23.2108 (10) Å
β = 97.934 (2)°
V = 3721.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 298 (2) K
0.36 × 0.26 × 0.14 mm

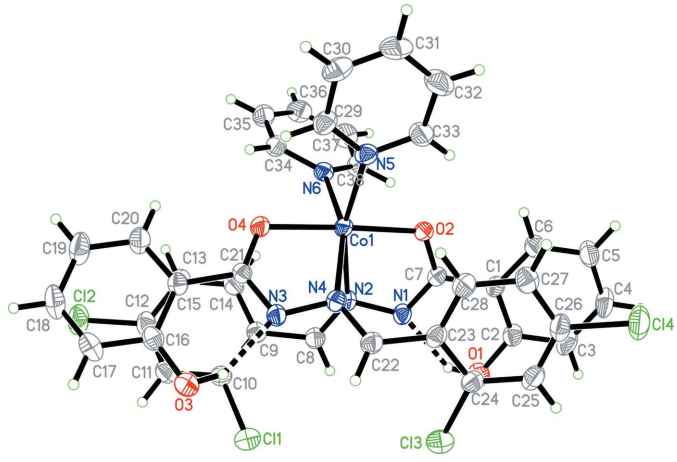


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed lines indicate hydrogen bonds.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.092
Data-to-parameter ratio = 15.8

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

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.092$	
$S = 1.02$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
7675 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
486 parameters	

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.80 (3)	1.87 (3)	2.566 (3)	144 (3)
O3—H16···N3	0.84 (4)	1.83 (4)	2.564 (3)	146 (3)

supporting information

Acta Cryst. (2007). E**63**, e9–e10 [https://doi.org/10.1107/S1600536807006800]

Bis{(*Z*)-*N*′-(2,4-dichlorobenzylidene)-2-hydroxybenzohydrazide-κ^2N',O}bis(pyridine-κN)cobalt(II). Corrigendum

Xiao-Yang Qiu, Sen-Lin Yang, Wei-Sheng Liu and Hai-Liang Zhu

bis(2,4-dichlorobenzaldehyde 2-hydroxybenzoylhydrazonato-κ^2N,O)bis(pyridine-κN)cobalt(II)

Crystal data

$[Ni(C_{14}H_9Cl_2N_2O_2)_2(C_5H_5N)_2]$
$M_r = 833.39$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 13.1832$ (5) Å
$b = 12.2799$ (5) Å
$c = 23.2108$ (10) Å
$\beta = 97.934$ (2)°
$V = 3721.6$ (3) Å^3
$Z = 4$
$F(000) = 1700$
$D_x = 1.487$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6285 reflections
$\theta = 4.2$–26°
$\mu = 0.80$ mm^{-1}
$T = 298$ K
Block, red
0.36 × 0.26 × 0.14 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.778$, $T_{max} = 0.889$
21284 measured reflections
7675 independent reflections
5595 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.8°$
$h = -16\rightarrow16$
$k = -15\rightarrow15$
$l = -29\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.092$
$S = 1.02$
7675 reflections
486 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 1.5838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.15574 (17)	0.11735 (19)	0.12753 (10)	0.0378 (6)
C2	1.22602 (19)	0.1207 (2)	0.17894 (11)	0.0470 (7)
C3	1.3216 (2)	0.0729 (3)	0.17980 (13)	0.0601 (8)
H3A	1.3692	0.0776	0.2132	0.072*
C4	1.3469 (2)	0.0190 (3)	0.13222 (14)	0.0663 (9)
H4	1.4108	−0.0140	0.1339	0.080*
C5	1.2782 (2)	0.0132 (3)	0.08185 (13)	0.0635 (8)
H5	1.2951	−0.0237	0.0495	0.076*
C6	1.1844 (2)	0.0627 (2)	0.07994 (12)	0.0499 (7)
H6	1.1387	0.0596	0.0457	0.060*
C7	1.05404 (17)	0.17037 (18)	0.12285 (11)	0.0355 (6)
C8	0.90674 (19)	0.3037 (2)	0.20930 (11)	0.0451 (6)
H8	0.9582	0.3118	0.2407	0.054*
C9	0.80515 (19)	0.3460 (2)	0.21520 (10)	0.0423 (6)
C10	0.7922 (2)	0.4400 (2)	0.24674 (11)	0.0467 (6)
C11	0.6970 (2)	0.4766 (2)	0.25651 (12)	0.0541 (7)
H11	0.6904	0.5401	0.2775	0.065*
C12	0.6124 (2)	0.4172 (3)	0.23463 (12)	0.0547 (7)
C13	0.6206 (2)	0.3239 (2)	0.20292 (13)	0.0565 (7)
H13	0.5625	0.2845	0.1883	0.068*
C14	0.7169 (2)	0.2894 (2)	0.19313 (11)	0.0490 (7)
H14	0.7226	0.2268	0.1712	0.059*
C15	0.68982 (18)	0.53726 (19)	0.09960 (11)	0.0390 (6)
C16	0.7077 (2)	0.6370 (2)	0.12921 (11)	0.0440 (6)
C17	0.6250 (2)	0.6985 (2)	0.14198 (13)	0.0593 (8)
H17	0.6368	0.7630	0.1628	0.071*
C18	0.5266 (2)	0.6652 (3)	0.12437 (15)	0.0702 (9)
H18	0.4721	0.7078	0.1328	0.084*
C19	0.5075 (2)	0.5687 (3)	0.09409 (16)	0.0701 (9)
H19	0.4406	0.5465	0.0818	0.084*
C20	0.5886 (2)	0.5059 (2)	0.08241 (13)	0.0545 (7)
H20	0.5756	0.4406	0.0625	0.065*
C21	0.77413 (18)	0.46514 (18)	0.08709 (10)	0.0351 (5)
C22	1.03437 (19)	0.4669 (2)	0.10234 (11)	0.0446 (6)
H22	1.0435	0.5292	0.1252	0.054*

C23	1.12506 (18)	0.41165 (19)	0.08684 (11)	0.0414 (6)
C24	1.21444 (19)	0.4029 (2)	0.12690 (12)	0.0469 (6)
C25	1.3026 (2)	0.3577 (2)	0.11159 (13)	0.0537 (7)
H25	1.3616	0.3525	0.1385	0.064*
C26	1.3016 (2)	0.3206 (2)	0.05573 (14)	0.0528 (7)
C27	1.2152 (2)	0.3261 (2)	0.01503 (13)	0.0516 (7)
H27	1.2158	0.2998	−0.0225	0.062*
C28	1.1275 (2)	0.3719 (2)	0.03130 (12)	0.0468 (6)
H28	1.0687	0.3760	0.0042	0.056*
C29	0.7867 (2)	0.3100 (2)	−0.06182 (12)	0.0522 (7)
H29	0.7391	0.3505	−0.0448	0.063*
C30	0.7740 (2)	0.3005 (3)	−0.12136 (13)	0.0640 (9)
H30	0.7186	0.3338	−0.1437	0.077*
C31	0.8426 (3)	0.2422 (3)	−0.14754 (13)	0.0691 (9)
H31	0.8349	0.2344	−0.1878	0.083*
C32	0.9237 (3)	0.1952 (3)	−0.11271 (13)	0.0749 (10)
H32	0.9728	0.1557	−0.1291	0.090*
C33	0.9314 (2)	0.2073 (2)	−0.05322 (12)	0.0599 (8)
H33	0.9861	0.1744	−0.0301	0.072*
C34	0.66922 (19)	0.1427 (2)	0.05502 (11)	0.0478 (7)
H34	0.6426	0.2112	0.0446	0.057*
C35	0.6021 (2)	0.0575 (2)	0.05737 (13)	0.0564 (7)
H35	0.5318	0.0686	0.0489	0.068*
C36	0.6398 (2)	−0.0433 (2)	0.07224 (13)	0.0604 (8)
H36	0.5958	−0.1021	0.0738	0.072*
C37	0.7435 (2)	−0.0569 (2)	0.08490 (13)	0.0616 (8)
H37	0.7710	−0.1249	0.0954	0.074*
C38	0.8065 (2)	0.0320 (2)	0.08182 (12)	0.0516 (7)
H38	0.8769	0.0221	0.0905	0.062*
Cl1	0.89932 (6)	0.51535 (7)	0.27491 (4)	0.0763 (3)
Cl2	0.49246 (6)	0.46033 (9)	0.24863 (4)	0.0851 (3)
Cl3	1.21388 (6)	0.44738 (7)	0.19762 (3)	0.0738 (2)
Cl4	1.41345 (6)	0.26759 (7)	0.03511 (5)	0.0838 (3)
Co1	0.87434 (2)	0.26990 (3)	0.067207 (14)	0.03589 (10)
H1	1.149 (2)	0.196 (3)	0.2236 (14)	0.079 (12)*
H16	0.846 (3)	0.634 (3)	0.1355 (16)	0.100 (14)*
N1	1.02840 (15)	0.21304 (16)	0.17093 (9)	0.0406 (5)
N2	0.92933 (14)	0.25629 (15)	0.16358 (9)	0.0374 (5)
N3	0.86780 (15)	0.50435 (16)	0.10100 (9)	0.0396 (5)
N4	0.94306 (14)	0.43349 (15)	0.08595 (8)	0.0370 (5)
N5	0.86424 (16)	0.26376 (17)	−0.02715 (9)	0.0439 (5)
N6	0.77133 (15)	0.13159 (16)	0.06701 (9)	0.0408 (5)
O1	1.20508 (17)	0.1707 (2)	0.22773 (9)	0.0692 (7)
O2	0.99765 (12)	0.17201 (13)	0.07302 (7)	0.0397 (4)
O3	0.80262 (17)	0.67721 (17)	0.14589 (9)	0.0606 (6)
O4	0.75276 (12)	0.37119 (13)	0.06474 (7)	0.0419 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0347 (13)	0.0391 (13)	0.0397 (15)	0.0035 (11)	0.0050 (11)	0.0079 (11)
C2	0.0418 (15)	0.0583 (17)	0.0398 (16)	0.0097 (13)	0.0021 (12)	0.0072 (13)
C3	0.0376 (15)	0.087 (2)	0.0523 (19)	0.0130 (15)	−0.0051 (13)	0.0138 (16)
C4	0.0415 (16)	0.093 (2)	0.066 (2)	0.0248 (16)	0.0130 (15)	0.0192 (18)
C5	0.0543 (18)	0.086 (2)	0.0520 (19)	0.0229 (17)	0.0140 (14)	−0.0014 (16)
C6	0.0465 (16)	0.0593 (17)	0.0430 (16)	0.0125 (14)	0.0028 (12)	0.0008 (13)
C7	0.0348 (13)	0.0315 (12)	0.0389 (15)	0.0007 (10)	0.0011 (11)	0.0053 (10)
C8	0.0460 (15)	0.0539 (16)	0.0350 (15)	0.0073 (13)	0.0039 (12)	0.0026 (12)
C9	0.0464 (15)	0.0499 (15)	0.0310 (14)	0.0077 (12)	0.0069 (11)	0.0035 (11)
C10	0.0470 (15)	0.0560 (17)	0.0360 (15)	0.0020 (13)	0.0017 (11)	−0.0024 (12)
C11	0.0589 (18)	0.0598 (18)	0.0440 (17)	0.0124 (15)	0.0085 (13)	−0.0091 (13)
C12	0.0488 (17)	0.069 (2)	0.0481 (18)	0.0133 (15)	0.0147 (13)	0.0027 (15)
C13	0.0462 (16)	0.0639 (19)	0.060 (2)	−0.0035 (14)	0.0093 (14)	0.0003 (15)
C14	0.0531 (17)	0.0478 (16)	0.0469 (17)	0.0038 (13)	0.0101 (13)	−0.0051 (12)
C15	0.0404 (14)	0.0334 (13)	0.0442 (15)	0.0017 (11)	0.0096 (11)	0.0044 (11)
C16	0.0493 (16)	0.0386 (14)	0.0454 (16)	0.0037 (12)	0.0107 (12)	0.0028 (12)
C17	0.071 (2)	0.0452 (16)	0.066 (2)	0.0084 (15)	0.0253 (16)	−0.0031 (14)
C18	0.058 (2)	0.056 (2)	0.104 (3)	0.0163 (16)	0.0368 (18)	0.0052 (18)
C19	0.0408 (16)	0.057 (2)	0.116 (3)	0.0041 (15)	0.0217 (17)	0.0066 (19)
C20	0.0427 (15)	0.0419 (15)	0.080 (2)	0.0006 (13)	0.0122 (14)	0.0005 (14)
C21	0.0375 (13)	0.0322 (13)	0.0354 (14)	0.0029 (11)	0.0039 (10)	0.0028 (10)
C22	0.0401 (14)	0.0399 (14)	0.0534 (17)	−0.0035 (12)	0.0051 (12)	−0.0027 (12)
C23	0.0340 (13)	0.0370 (14)	0.0531 (17)	−0.0039 (11)	0.0055 (11)	0.0034 (12)
C24	0.0388 (14)	0.0467 (15)	0.0542 (17)	−0.0033 (12)	0.0026 (12)	−0.0035 (13)
C25	0.0360 (14)	0.0523 (17)	0.070 (2)	0.0006 (13)	−0.0018 (13)	0.0011 (15)
C26	0.0390 (15)	0.0434 (15)	0.079 (2)	0.0000 (12)	0.0196 (14)	0.0012 (15)
C27	0.0527 (17)	0.0523 (17)	0.0527 (18)	−0.0029 (14)	0.0176 (14)	0.0039 (13)
C28	0.0418 (15)	0.0506 (16)	0.0477 (17)	−0.0024 (12)	0.0049 (12)	0.0060 (13)
C29	0.0456 (16)	0.0614 (18)	0.0474 (18)	0.0039 (13)	−0.0011 (13)	0.0063 (13)
C30	0.0603 (19)	0.078 (2)	0.048 (2)	−0.0065 (17)	−0.0109 (15)	0.0132 (16)
C31	0.083 (2)	0.086 (2)	0.0353 (17)	−0.009 (2)	−0.0024 (16)	0.0006 (16)
C32	0.094 (3)	0.087 (2)	0.0434 (19)	0.019 (2)	0.0076 (17)	−0.0079 (16)
C33	0.0655 (19)	0.067 (2)	0.0441 (18)	0.0195 (16)	−0.0020 (14)	−0.0029 (14)
C34	0.0437 (15)	0.0396 (15)	0.0585 (18)	0.0008 (12)	0.0016 (12)	−0.0046 (12)
C35	0.0484 (16)	0.0516 (17)	0.069 (2)	−0.0060 (14)	0.0081 (14)	−0.0086 (14)
C36	0.067 (2)	0.0477 (17)	0.067 (2)	−0.0162 (15)	0.0113 (16)	−0.0042 (14)
C37	0.075 (2)	0.0356 (15)	0.074 (2)	0.0010 (15)	0.0081 (16)	0.0064 (14)
C38	0.0497 (16)	0.0417 (15)	0.0614 (19)	0.0032 (13)	0.0010 (13)	−0.0003 (13)
Cl1	0.0597 (5)	0.0816 (6)	0.0836 (6)	−0.0050 (4)	−0.0037 (4)	−0.0258 (5)
Cl2	0.0551 (5)	0.1155 (8)	0.0891 (7)	0.0219 (5)	0.0260 (4)	−0.0083 (5)
Cl3	0.0667 (5)	0.0908 (6)	0.0597 (5)	0.0029 (4)	−0.0064 (4)	−0.0201 (4)
Cl4	0.0486 (4)	0.0769 (6)	0.1316 (8)	0.0043 (4)	0.0327 (5)	−0.0163 (5)
Co1	0.03361 (18)	0.03478 (17)	0.0377 (2)	0.00443 (14)	−0.00086 (13)	−0.00057 (14)
N1	0.0366 (11)	0.0490 (12)	0.0357 (12)	0.0095 (10)	0.0031 (9)	0.0034 (10)
N2	0.0348 (11)	0.0379 (11)	0.0398 (12)	0.0047 (9)	0.0065 (9)	0.0036 (9)

N3	0.0358 (11)	0.0360 (11)	0.0470 (13)	0.0036 (9)	0.0059 (9)	−0.0022 (9)
N4	0.0356 (11)	0.0356 (11)	0.0396 (12)	0.0022 (9)	0.0044 (9)	0.0048 (9)
N5	0.0451 (12)	0.0442 (12)	0.0402 (12)	0.0020 (10)	−0.0024 (10)	0.0011 (10)
N6	0.0422 (12)	0.0366 (11)	0.0426 (13)	0.0010 (9)	0.0023 (9)	−0.0036 (9)
O1	0.0576 (14)	0.1012 (18)	0.0439 (13)	0.0299 (13)	−0.0107 (10)	−0.0091 (11)
O2	0.0374 (9)	0.0447 (10)	0.0352 (10)	0.0081 (8)	−0.0016 (7)	−0.0016 (7)
O3	0.0556 (13)	0.0482 (12)	0.0759 (15)	0.0019 (11)	0.0018 (11)	−0.0170 (10)
O4	0.0350 (9)	0.0357 (9)	0.0534 (11)	0.0024 (7)	0.0005 (8)	−0.0052 (8)

Geometric parameters (Å, º)

C1—C6	1.388 (3)	C22—H22	0.9300
C1—C2	1.407 (3)	C23—C28	1.383 (3)
C1—C7	1.481 (3)	C23—C24	1.401 (3)
C2—O1	1.350 (3)	C24—C25	1.378 (4)
C2—C3	1.388 (4)	C24—Cl3	1.731 (3)
C3—C4	1.368 (4)	C25—C26	1.373 (4)
C3—H3A	0.9300	C25—H25	0.9300
C4—C5	1.379 (4)	C26—C27	1.377 (4)
C4—H4	0.9300	C26—Cl4	1.738 (3)
C5—C6	1.373 (4)	C27—C28	1.384 (4)
C5—H5	0.9300	C27—H27	0.9300
C6—H6	0.9300	C28—H28	0.9300
C7—O2	1.286 (3)	C29—N5	1.337 (3)
C7—N1	1.319 (3)	C29—C30	1.374 (4)
C8—N2	1.281 (3)	C29—H29	0.9300
C8—C9	1.460 (3)	C30—C31	1.361 (4)
C8—H8	0.9300	C30—H30	0.9300
C9—C10	1.391 (4)	C31—C32	1.375 (4)
C9—C14	1.391 (3)	C31—H31	0.9300
C10—C11	1.381 (4)	C32—C33	1.379 (4)
C10—Cl1	1.738 (3)	C32—H32	0.9300
C11—C12	1.370 (4)	C33—N5	1.334 (3)
C11—H11	0.9300	C33—H33	0.9300
C12—C13	1.374 (4)	C34—N6	1.343 (3)
C12—Cl2	1.740 (3)	C34—C35	1.377 (4)
C13—C14	1.386 (4)	C34—H34	0.9300
C13—H13	0.9300	C35—C36	1.360 (4)
C14—H14	0.9300	C35—H35	0.9300
C15—C20	1.393 (3)	C36—C37	1.368 (4)
C15—C16	1.409 (3)	C36—H36	0.9300
C15—C21	1.481 (3)	C37—C38	1.379 (4)
C16—O3	1.351 (3)	C37—H37	0.9300
C16—C17	1.392 (4)	C38—N6	1.336 (3)
C17—C18	1.368 (4)	C38—H38	0.9300
C17—H17	0.9300	Co1—O2	2.0112 (15)
C18—C19	1.384 (4)	Co1—O4	2.0234 (16)
C18—H18	0.9300	Co1—N6	2.174 (2)

C19—C20	1.376 (4)	Co1—N5	2.177 (2)
C19—H19	0.9300	Co1—N4	2.2219 (19)
C20—H20	0.9300	Co1—N2	2.260 (2)
C21—O4	1.280 (3)	N1—N2	1.398 (3)
C21—N3	1.323 (3)	N3—N4	1.400 (3)
C22—N4	1.279 (3)	O1—H1	0.80 (3)
C22—C23	1.462 (3)	O3—H16	0.84 (4)

C6—C1—C2	118.0 (2)	C24—C25—H25	120.7
C6—C1—C7	119.8 (2)	C25—C26—C27	122.1 (3)
C2—C1—C7	122.2 (2)	C25—C26—Cl4	119.1 (2)
O1—C2—C3	118.1 (2)	C27—C26—Cl4	118.8 (2)
O1—C2—C1	122.6 (2)	C26—C27—C28	118.4 (3)
C3—C2—C1	119.3 (3)	C26—C27—H27	120.8
C4—C3—C2	121.0 (3)	C28—C27—H27	120.8
C4—C3—H3A	119.5	C23—C28—C27	121.7 (2)
C2—C3—H3A	119.5	C23—C28—H28	119.2
C3—C4—C5	120.3 (3)	C27—C28—H28	119.2
C3—C4—H4	119.9	N5—C29—C30	123.1 (3)
C5—C4—H4	119.9	N5—C29—H29	118.4
C6—C5—C4	119.2 (3)	C30—C29—H29	118.4
C6—C5—H5	120.4	C31—C30—C29	119.8 (3)
C4—C5—H5	120.4	C31—C30—H30	120.1
C5—C6—C1	122.1 (2)	C29—C30—H30	120.1
C5—C6—H6	119.0	C30—C31—C32	118.0 (3)
C1—C6—H6	119.0	C30—C31—H31	121.0
O2—C7—N1	124.8 (2)	C32—C31—H31	121.0
O2—C7—C1	118.6 (2)	C31—C32—C33	119.1 (3)
N1—C7—C1	116.6 (2)	C31—C32—H32	120.4
N2—C8—C9	124.1 (2)	C33—C32—H32	120.4
N2—C8—H8	118.0	N5—C33—C32	123.3 (3)
C9—C8—H8	118.0	N5—C33—H33	118.3
C10—C9—C14	116.8 (2)	C32—C33—H33	118.3
C10—C9—C8	121.7 (2)	N6—C34—C35	123.1 (2)
C14—C9—C8	121.3 (2)	N6—C34—H34	118.5
C11—C10—C9	122.5 (2)	C35—C34—H34	118.5
C11—C10—Cl1	118.4 (2)	C36—C35—C34	119.1 (3)
C9—C10—Cl1	119.2 (2)	C36—C35—H35	120.4
C12—C11—C10	118.5 (3)	C34—C35—H35	120.4
C12—C11—H11	120.7	C35—C36—C37	119.0 (3)
C10—C11—H11	120.7	C35—C36—H36	120.5
C11—C12—C13	121.5 (3)	C37—C36—H36	120.5
C11—C12—Cl2	118.9 (2)	C36—C37—C38	118.9 (3)
C13—C12—Cl2	119.6 (2)	C36—C37—H37	120.5
C12—C13—C14	118.9 (3)	C38—C37—H37	120.5
C12—C13—H13	120.5	N6—C38—C37	123.2 (3)
C14—C13—H13	120.5	N6—C38—H38	118.4
C13—C14—C9	121.7 (3)	C37—C38—H38	118.4

C13—C14—H14	119.1	O2—Co1—O4	177.51 (6)
C9—C14—H14	119.1	O2—Co1—N6	91.84 (7)
C20—C15—C16	118.0 (2)	O4—Co1—N6	89.31 (7)
C20—C15—C21	119.6 (2)	O2—Co1—N5	89.05 (7)
C16—C15—C21	122.4 (2)	O4—Co1—N5	93.13 (7)
O3—C16—C17	117.6 (2)	N6—Co1—N5	91.11 (8)
O3—C16—C15	122.9 (2)	O2—Co1—N4	102.90 (7)
C17—C16—C15	119.5 (3)	O4—Co1—N4	75.51 (7)
C18—C17—C16	120.9 (3)	N6—Co1—N4	160.80 (8)
C18—C17—H17	119.5	N5—Co1—N4	101.24 (7)
C16—C17—H17	119.5	O2—Co1—N2	75.15 (7)
C17—C18—C19	120.4 (3)	O4—Co1—N2	102.59 (7)
C17—C18—H18	119.8	N6—Co1—N2	93.40 (7)
C19—C18—H18	119.8	N5—Co1—N2	163.68 (7)
C20—C19—C18	119.3 (3)	N4—Co1—N2	78.85 (7)
C20—C19—H19	120.4	C7—N1—N2	113.07 (18)
C18—C19—H19	120.4	C8—N2—N1	113.06 (19)
C19—C20—C15	121.9 (3)	C8—N2—Co1	134.96 (16)
C19—C20—H20	119.1	N1—N2—Co1	108.38 (14)
C15—C20—H20	119.1	C21—N3—N4	112.49 (19)
O4—C21—N3	124.9 (2)	C22—N4—N3	113.4 (2)
O4—C21—C15	119.3 (2)	C22—N4—Co1	133.59 (17)
N3—C21—C15	115.8 (2)	N3—N4—Co1	109.09 (13)
N4—C22—C23	123.1 (2)	C33—N5—C29	116.6 (2)
N4—C22—H22	118.4	C33—N5—Co1	121.49 (17)
C23—C22—H22	118.4	C29—N5—Co1	121.76 (19)
C28—C23—C24	117.8 (2)	C38—N6—C34	116.7 (2)
C28—C23—C22	121.2 (2)	C38—N6—Co1	121.33 (17)
C24—C23—C22	120.9 (2)	C34—N6—Co1	121.91 (17)
C25—C24—C23	121.5 (3)	C2—O1—H1	112 (2)
C25—C24—Cl3	119.1 (2)	C7—O2—Co1	115.55 (15)
C23—C24—Cl3	119.5 (2)	C16—O3—H16	109 (3)
C26—C25—C24	118.6 (2)	C21—O4—Co1	114.42 (14)
C26—C25—H25	120.7		

C6—C1—C2—O1	−179.3 (3)	C9—C8—N2—Co1	31.0 (4)
C7—C1—C2—O1	1.2 (4)	C7—N1—N2—C8	−175.9 (2)
C6—C1—C2—C3	1.9 (4)	C7—N1—N2—Co1	−14.0 (2)
C7—C1—C2—C3	−177.6 (2)	O2—Co1—N2—C8	171.0 (2)
O1—C2—C3—C4	178.6 (3)	O4—Co1—N2—C8	−8.0 (2)
C1—C2—C3—C4	−2.6 (4)	N6—Co1—N2—C8	−98.0 (2)
C2—C3—C4—C5	1.4 (5)	N5—Co1—N2—C8	156.2 (3)
C3—C4—C5—C6	0.4 (5)	N4—Co1—N2—C8	64.3 (2)
C4—C5—C6—C1	−1.0 (5)	O2—Co1—N2—N1	14.76 (13)
C2—C1—C6—C5	−0.2 (4)	O4—Co1—N2—N1	−164.18 (13)
C7—C1—C6—C5	179.3 (3)	N6—Co1—N2—N1	105.77 (14)
C6—C1—C7—O2	−5.6 (3)	N5—Co1—N2—N1	0.0 (3)
C2—C1—C7—O2	174.0 (2)	N4—Co1—N2—N1	−91.96 (14)

C6—C1—C7—N1	174.6 (2)	O4—C21—N3—N4	3.0 (3)
C2—C1—C7—N1	−5.9 (3)	C15—C21—N3—N4	−177.76 (19)
N2—C8—C9—C10	−145.2 (3)	C23—C22—N4—N3	−174.2 (2)
N2—C8—C9—C14	39.7 (4)	C23—C22—N4—Co1	31.2 (4)
C14—C9—C10—C11	0.4 (4)	C21—N3—N4—C22	−175.8 (2)
C8—C9—C10—C11	−174.9 (2)	C21—N3—N4—Co1	−15.0 (2)
C14—C9—C10—Cl1	−179.36 (19)	O2—Co1—N4—C22	−6.5 (2)
C8—C9—C10—Cl1	5.3 (3)	O4—Co1—N4—C22	171.5 (2)
C9—C10—C11—C12	0.6 (4)	N6—Co1—N4—C22	132.8 (3)
Cl1—C10—C11—C12	−179.7 (2)	N5—Co1—N4—C22	−98.1 (2)
C10—C11—C12—C13	−0.8 (4)	N2—Co1—N4—C22	65.2 (2)
C10—C11—C12—Cl2	178.0 (2)	O2—Co1—N4—N3	−161.98 (13)
C11—C12—C13—C14	0.2 (4)	O4—Co1—N4—N3	16.06 (13)
Cl2—C12—C13—C14	−178.7 (2)	N6—Co1—N4—N3	−22.7 (3)
C12—C13—C14—C9	0.8 (4)	N5—Co1—N4—N3	106.41 (14)
C10—C9—C14—C13	−1.1 (4)	N2—Co1—N4—N3	−90.23 (14)
C8—C9—C14—C13	174.3 (2)	C32—C33—N5—C29	−0.1 (4)
C20—C15—C16—O3	−177.4 (2)	C32—C33—N5—Co1	175.4 (2)
C21—C15—C16—O3	3.4 (4)	C30—C29—N5—C33	0.7 (4)
C20—C15—C16—C17	2.2 (4)	C30—C29—N5—Co1	−174.9 (2)
C21—C15—C16—C17	−177.0 (2)	O2—Co1—N5—C33	−0.6 (2)
O3—C16—C17—C18	177.3 (3)	O4—Co1—N5—C33	178.2 (2)
C15—C16—C17—C18	−2.4 (4)	N6—Co1—N5—C33	−92.4 (2)
C16—C17—C18—C19	0.9 (5)	N4—Co1—N5—C33	102.4 (2)
C17—C18—C19—C20	0.7 (5)	N2—Co1—N5—C33	13.7 (4)
C18—C19—C20—C15	−0.8 (5)	O2—Co1—N5—C29	174.7 (2)
C16—C15—C20—C19	−0.7 (4)	O4—Co1—N5—C29	−6.5 (2)
C21—C15—C20—C19	178.5 (3)	N6—Co1—N5—C29	82.9 (2)
C20—C15—C21—O4	−5.4 (4)	N4—Co1—N5—C29	−82.3 (2)
C16—C15—C21—O4	173.7 (2)	N2—Co1—N5—C29	−171.0 (2)
C20—C15—C21—N3	175.3 (2)	C37—C38—N6—C34	0.2 (4)
C16—C15—C21—N3	−5.6 (3)	C37—C38—N6—Co1	176.9 (2)
N4—C22—C23—C28	42.1 (4)	C35—C34—N6—C38	−0.1 (4)
N4—C22—C23—C24	−141.6 (3)	C35—C34—N6—Co1	−176.7 (2)
C28—C23—C24—C25	0.9 (4)	O2—Co1—N6—C38	13.6 (2)
C22—C23—C24—C25	−175.5 (2)	O4—Co1—N6—C38	−164.2 (2)
C28—C23—C24—Cl3	−177.86 (19)	N5—Co1—N6—C38	102.7 (2)
C22—C23—C24—Cl3	5.7 (3)	N4—Co1—N6—C38	−126.9 (2)
C23—C24—C25—C26	−0.2 (4)	N2—Co1—N6—C38	−61.6 (2)
Cl3—C24—C25—C26	178.6 (2)	O2—Co1—N6—C34	−169.89 (19)
C24—C25—C26—C27	−0.7 (4)	O4—Co1—N6—C34	12.31 (19)
C24—C25—C26—Cl4	177.9 (2)	N5—Co1—N6—C34	−80.8 (2)
C25—C26—C27—C28	0.8 (4)	N4—Co1—N6—C34	49.6 (3)
Cl4—C26—C27—C28	−177.8 (2)	N2—Co1—N6—C34	114.89 (19)
C24—C23—C28—C27	−0.9 (4)	N1—C7—O2—Co1	11.2 (3)
C22—C23—C28—C27	175.5 (2)	C1—C7—O2—Co1	−168.56 (16)
C26—C27—C28—C23	0.1 (4)	O4—Co1—O2—C7	10.9 (17)
N5—C29—C30—C31	−0.4 (5)	N6—Co1—O2—C7	−106.70 (17)

C29—C30—C31—C32	−0.5 (5)	N5—Co1—O2—C7	162.22 (17)
C30—C31—C32—C33	1.0 (5)	N4—Co1—O2—C7	60.90 (17)
C31—C32—C33—N5	−0.7 (5)	N2—Co1—O2—C7	−13.68 (16)
N6—C34—C35—C36	−0.3 (4)	N3—C21—O4—Co1	12.5 (3)
C34—C35—C36—C37	0.5 (4)	C15—C21—O4—Co1	−166.72 (16)
C35—C36—C37—C38	−0.4 (5)	O2—Co1—O4—C21	35.5 (17)
C36—C37—C38—N6	0.1 (5)	N6—Co1—O4—C21	153.12 (17)
O2—C7—N1—N2	3.4 (3)	N5—Co1—O4—C21	−115.80 (17)
C1—C7—N1—N2	−176.80 (19)	N4—Co1—O4—C21	−14.99 (16)
C9—C8—N2—N1	−173.6 (2)	N2—Co1—O4—C21	59.80 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.80 (3)	1.87 (3)	2.566 (3)	144 (3)
O3—H16···N3	0.84 (4)	1.83 (4)	2.564 (3)	146 (3)