Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[2,4-dibromo-6-(1-naphthylimino-methyl)phenolato-κ^2N,O]bis(*N*,*N*′-dimethylformamide-κO)cobalt(II)

Zheng Liu,[a]* Li Xia Jin,[a] Jin Hong Xia,[b] Er Xi Liu[a] and Guang Zhao Li[a]

[a]Department of Materials and Chemical Engineering, Guilin University of Technology, Ministry of Education, Guilin 541004, People's Republic of China, and [b]Institute of Electronic Information Engineering, Guilin University of Electronic Technology, Guilin University of Technology, Ministry of Education, Guilin 541004, People's Republic of China
Correspondence e-mail: lisa4.6@163.com

Received 17 October 2007; accepted 25 October 2007

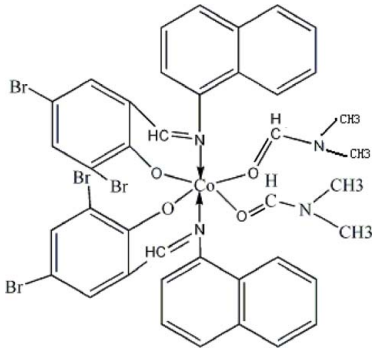
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.057; wR factor = 0.123; data-to-parameter ratio = 15.0.

In the title compound, $[Co(C_{17}H_{10}Br_2NO)_2(C_3H_7NO)_2]$, the cobalt(II) cation is coordinated by two N and two O atoms from two different Schiff base ligands, and two O atoms from dimethylformamide molecules, forming a slightly distorted octahedral geometry. In the crystal structure, C—H···Br hydrogen bonds link the molecules in rows.

Related literature

Schiff bases of isatin have been reported to possess antibacterial, antifungal, antiviral, anti-HIV, antiprotozoal and anthelmintic activities (Erçağ *et al.*, 2006).

For related literature, see: El-Behery & El-Twigry (2007); Mostafa & Haifaa (2007); Musie *et al.* (2003); Patel *et al.* (2006).



Experimental

Crystal data

$[Co(C_{17}H_{10}Br_2NO)_2(C_3H_7NO)_2]$
M_r = 1013.28
Monoclinic, $P2_1/n$
a = 12.2884 (15) Å
b = 17.069 (2) Å
c = 19.373 (2) Å
β = 94.310 (2)°
V = 4052.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.41 mm^{-1}
T = 298 (2) K
0.21 × 0.15 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.458, T_{max} = 0.577
(expected range = 0.428–0.539)
20849 measured reflections
7147 independent reflections
2955 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.123
S = 1.00
7147 reflections
478 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C21A—H28B···Br3A	0.93	2.93	1.870	152

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2437).

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT* (Version 6.45) and *SMART* (Version 5.0). Bruker AXS Inc., Madison, Wisconsin, USA.
El-Behery, M. & El-Twigry, H. (2007). *Spectrochim. Acta Part A*, **66**, 28–36.
Erçağ, A., Yildırım, S. Ö. & Akkurt, M. (2006). *Chin. Chem. Lett.* **17**, 243–246.
Mostafa, E. B. & Haifaa, E. T. (2007). *Spectrochim. Acta Part A*, **66**, 28–36.
Musie, G. T., Li, X. B. & Powell, D. R. (2003). *Inorg. Chim. Acta*, **348**, 69–74.
Patel, R. N., Nripendra Singh, V. L. N. & Gundla, R. N. (2006). *Polyhedron*, **25**, 3312–3318.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

 doi:10.1107/S1600536807053044

supplementary materials

Acta Cryst. (2007). E**63**, m3037 [**doi:10.1107/S1600536807053044**]

Bis[2,4-dibromo-6-(1-naphthyliminomethyl)phenolato-κ^2N,O]bis(*N*,*N*'-dimethylformamide-κO)cobalt(II)

Z. Liu, L. X. Jin, J. H. Xia, E. X. Liu and G. Z. Li

Comment

Schiff bases play an important role in inorganic chemistry as they easily form stable complexes with most transition metal ions (Mostafa & Haifaa, 2007, Musie *et al.*, 2003; Patel *et al.*, 2006). Schiff bases of isatin were reported to possess anti-bacterial, antifungal, antiviral, anti-HIV, antiprotozoal, and anthelmintic activities (Erçağ *et al.*, 2006). We report herein the synthesis and crystal structure of the ternary mixed ligand complex resulting from the condensation of 1-naphthylamine-3,5-bibromo-2-hydroxy- benzaldehyde and $Co(NO_3)_2$.

As shown in Fig. 1, the Co^{II} cation lies on a twofold axis and is coordinated by two N and two O atoms from the Schiff base and two O atoms from *N*,*N*'-dimethyl-formamide, in a slightly distorted octahedral geometry. In the crystal weak, non-classical C—H···Br hydrogen bonds link the molecules in rows (Fig 2).

Experimental

1-naphthylamine (0.286 g, 2 mmol) and 3,5-bibromo-2-hydroxy-benzaldehyde (0.560 g, 2 mmol) were mixed in ethanol and and stirred for 30 min at room temperature to yield the Schiff base 2,4-dibromo-6-((naphthalen-1-ylimino) methyl)phenol. A mixture of schiff base (0.201 g, 0.5 mmol), $CoNO_3{\cdot}6H_2O_2$ (0.145 g, 0.5 mmol) and 6 drops of triethylamine in 5 ml e thanol and 5 ml DMF were sealed in a 30 ml Teflon-lined stainless steel vessel, which was heated at 333 K for 7 days under autogenous pressure. On cooling to room temperature blue crystals of the title compound were produced (yield: 53%, based on Co).

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 − 0.96 Å, U_{iso} = 1.2 or 1.5U_{eq} (C).

Figures

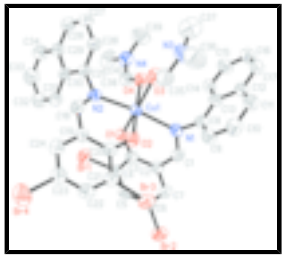


Fig. 1. A view of (I), showing 30% probability displacement ellipsoids.

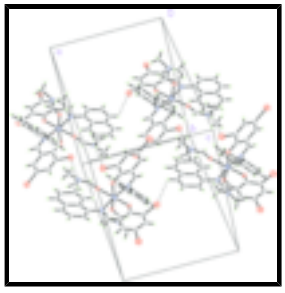


Fig. 2. Crystal packing of (I) with H-bonds drawn as dashed lines.

Bis[2,4-dibromo-6-(1-naphthyliminomethyl)phenolato-κ^2*N*,*O*]\ bis(*N*,*N*'-dimethylformamide-κ*O*)cobalt(II)

Crystal data

$[Co(C_{17}H_{10}Br_2NO)_2(C_3H_7NO)_2]$	F_{000} = 2004
M_r = 1013.28	D_x = 1.661 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3177 reflections
a = 12.2884 (15) Å	θ = 2.6–25.1º
b = 17.069 (2) Å	μ = 4.41 mm^{-1}
c = 19.373 (2) Å	T = 298 (2) K
β = 94.310 (2)º	Block, red
V = 4052.0 (9) Å^3	0.21 × 0.15 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	7147 independent reflections
Radiation source: fine-focus sealed tube	2955 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.090
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −14→14
T_{min} = 0.458, T_{max} = 0.577	k = −20→12
20849 measured reflections	l = −23→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained
$wR(F^2)$ = 0.123	$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001

7147 reflections	$\Delta\rho_{max} = 0.77$ e Å^{-3}
478 parameters	$\Delta\rho_{min} = -0.75$ e Å^{-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 $F^2 > \sigma(F^2)$ 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	0.13607 (7)	0.33654 (5)	0.33329 (5)	0.0563 (3)
Br1	0.12914 (7)	0.62067 (5)	0.30379 (5)	0.0931 (3)
Br2	0.56760 (7)	0.64339 (5)	0.40923 (5)	0.0964 (3)
Br3	0.46208 (6)	0.31966 (5)	0.21106 (5)	0.0806 (3)
Br4	0.22348 (9)	0.36243 (7)	−0.04636 (5)	0.1212 (4)
N1	0.2821 (5)	0.3226 (4)	0.4022 (3)	0.0672 (17)
N2	0.0105 (5)	0.3460 (3)	0.2508 (4)	0.0591 (17)
N3	0.1000 (8)	0.0902 (6)	0.3565 (5)	0.108 (3)
N4	−0.1103 (6)	0.4246 (5)	0.4558 (4)	0.087 (2)
O1	0.1647 (4)	0.4516 (3)	0.3353 (2)	0.0640 (14)
O2	0.2388 (4)	0.3126 (3)	0.2614 (3)	0.0689 (14)
O3	0.0870 (4)	0.2193 (4)	0.3495 (3)	0.0841 (19)
O4	0.0254 (4)	0.3574 (3)	0.4115 (3)	0.0717 (15)
C1	0.3594 (6)	0.3749 (5)	0.4061 (4)	0.069 (2)
H1	0.4280	0.3584	0.4238	0.082*
C2	0.3489 (6)	0.4563 (4)	0.3853 (4)	0.057 (2)
C3	0.2534 (7)	0.4887 (5)	0.3540 (4)	0.058 (2)
C4	0.2571 (6)	0.5715 (5)	0.3426 (4)	0.061 (2)
C5	0.3470 (7)	0.6164 (4)	0.3585 (4)	0.068 (2)
H5	0.3449	0.6701	0.3503	0.081*
C6	0.4417 (6)	0.5815 (5)	0.3871 (4)	0.067 (2)
C7	0.4430 (6)	0.5024 (5)	0.4012 (4)	0.065 (2)
H7	0.5061	0.4792	0.4214	0.078*
C8	0.3173 (7)	0.2432 (5)	0.4243 (5)	0.069 (2)
C9	0.3873 (7)	0.2006 (5)	0.3865 (4)	0.075 (2)
H9	0.4152	0.2230	0.3478	0.090*
C10	0.4171 (7)	0.1233 (6)	0.4058 (5)	0.089 (3)
H10	0.4647	0.0950	0.3802	0.107*

C11	0.3740 (7)	0.0896 (5)	0.4641 (5)	0.088 (3)
H11	0.3907	0.0383	0.4771	0.106*
C12	0.3050 (7)	0.1357 (5)	0.5022 (5)	0.072 (2)
C13	0.2740 (6)	0.2138 (5)	0.4797 (5)	0.071 (2)
C14	0.2018 (6)	0.2559 (5)	0.5222 (5)	0.070 (2)
H14	0.1790	0.3062	0.5095	0.084*
C15	0.1672 (7)	0.2232 (6)	0.5794 (5)	0.096 (3)
H15	0.1234	0.2527	0.6067	0.115*
C16	0.1938 (8)	0.1482 (7)	0.5996 (5)	0.101 (3)
H16	0.1651	0.1264	0.6383	0.121*
C17	0.2620 (8)	0.1063 (5)	0.5624 (5)	0.091 (3)
H17	0.2815	0.0561	0.5772	0.109*
C18	0.0265 (6)	0.3441 (4)	0.1871 (5)	0.066 (2)
H18	−0.0356	0.3466	0.1566	0.079*
C19	0.1304 (6)	0.3386 (4)	0.1554 (4)	0.058 (2)
C20	0.2307 (6)	0.3256 (4)	0.1960 (5)	0.060 (2)
C21	0.3282 (6)	0.3260 (4)	0.1587 (4)	0.062 (2)
C22	0.3232 (7)	0.3361 (4)	0.0892 (5)	0.070 (2)
H22	0.3875	0.3360	0.0668	0.084*
C23	0.2257 (8)	0.3464 (5)	0.0510 (4)	0.074 (2)
C24	0.1296 (7)	0.3470 (4)	0.0833 (5)	0.073 (2)
H24	0.0636	0.3531	0.0570	0.087*
C25	−0.1008 (6)	0.3546 (5)	0.2669 (4)	0.064 (2)
C26	−0.1549 (7)	0.2914 (5)	0.2908 (4)	0.079 (2)
H26	−0.1213	0.2426	0.2935	0.095*
C27	−0.2619 (7)	0.3004 (6)	0.3114 (4)	0.085 (3)
H27	−0.2983	0.2574	0.3280	0.101*
C28	−0.3117 (7)	0.3706 (6)	0.3071 (4)	0.081 (3)
H28	−0.3816	0.3756	0.3220	0.098*
C29	−0.2612 (7)	0.4356 (6)	0.2811 (4)	0.073 (2)
C30	−0.1536 (6)	0.4284 (5)	0.2599 (4)	0.065 (2)
C31	−0.1004 (6)	0.4969 (5)	0.2373 (4)	0.073 (2)
H31	−0.0288	0.4938	0.2250	0.088*
C32	−0.1526 (8)	0.5658 (5)	0.2338 (5)	0.096 (3)
H32	−0.1167	0.6104	0.2198	0.115*
C33	−0.2614 (9)	0.5709 (6)	0.2512 (5)	0.107 (3)
H33	−0.2979	0.6185	0.2455	0.129*
C34	−0.3144 (7)	0.5091 (6)	0.2759 (5)	0.092 (3)
H34	−0.3850	0.5147	0.2893	0.111*
C35	0.1276 (9)	0.1659 (7)	0.3330 (5)	0.103 (3)
H35	0.1821	0.1705	0.3025	0.124*
C36	0.1576 (10)	0.0288 (7)	0.3275 (6)	0.148 (4)
H36A	0.1727	−0.0113	0.3617	0.222*
H36B	0.2250	0.0485	0.3124	0.222*
H36C	0.1145	0.0073	0.2887	0.222*
C37	0.0319 (9)	0.0735 (7)	0.4061 (7)	0.147 (5)
H37A	0.0672	0.0381	0.4391	0.220*
H37B	−0.0333	0.0497	0.3853	0.220*
H37C	0.0134	0.1210	0.4291	0.220*

C38	−0.0267 (7)	0.4174 (5)	0.4162 (4)	0.076 (2)
H38	−0.0072	0.4607	0.3907	0.091*
C39	−0.1474 (8)	0.3588 (7)	0.4917 (5)	0.130 (4)
H39A	−0.1188	0.3118	0.4727	0.195*
H39B	−0.2257	0.3572	0.4870	0.195*
H39C	−0.1229	0.3627	0.5398	0.195*
C40	−0.1711 (7)	0.4979 (6)	0.4565 (5)	0.118 (4)
H40A	−0.1250	0.5404	0.4446	0.177*
H40B	−0.1951	0.5065	0.5019	0.177*
H40C	−0.2334	0.4951	0.4236	0.177*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0579 (6)	0.0443 (6)	0.0663 (7)	−0.0026 (5)	0.0021 (5)	0.0004 (5)
Br1	0.0924 (7)	0.0550 (6)	0.1277 (8)	0.0024 (5)	−0.0203 (6)	0.0118 (5)
Br2	0.0829 (6)	0.0771 (6)	0.1281 (9)	−0.0278 (5)	−0.0003 (6)	−0.0108 (6)
Br3	0.0589 (5)	0.0855 (7)	0.0980 (7)	−0.0019 (4)	0.0084 (5)	−0.0063 (5)
Br4	0.1367 (9)	0.1577 (10)	0.0710 (7)	0.0335 (8)	0.0197 (6)	−0.0053 (7)
N1	0.074 (5)	0.050 (4)	0.077 (5)	−0.002 (4)	0.004 (4)	0.005 (4)
N2	0.051 (4)	0.053 (4)	0.074 (5)	0.003 (3)	0.009 (4)	−0.001 (4)
N3	0.122 (8)	0.070 (7)	0.131 (9)	−0.004 (6)	−0.007 (6)	0.021 (6)
N4	0.082 (6)	0.097 (7)	0.082 (6)	0.006 (5)	0.012 (5)	−0.009 (5)
O1	0.063 (3)	0.049 (3)	0.079 (4)	−0.004 (3)	0.000 (3)	0.002 (3)
O2	0.061 (3)	0.076 (4)	0.070 (4)	0.010 (3)	0.004 (3)	−0.002 (3)
O3	0.079 (4)	0.063 (4)	0.108 (5)	0.014 (3)	−0.008 (3)	−0.011 (4)
O4	0.072 (4)	0.069 (4)	0.074 (4)	0.008 (3)	0.007 (3)	0.001 (3)
C1	0.067 (5)	0.061 (6)	0.076 (6)	0.001 (5)	−0.007 (4)	0.002 (5)
C2	0.062 (5)	0.047 (5)	0.060 (5)	−0.001 (4)	0.006 (4)	−0.003 (4)
C3	0.065 (6)	0.050 (5)	0.059 (5)	−0.004 (5)	0.010 (5)	−0.001 (4)
C4	0.064 (5)	0.054 (5)	0.065 (6)	−0.004 (4)	0.002 (4)	0.005 (4)
C5	0.077 (6)	0.050 (5)	0.076 (6)	−0.013 (5)	0.007 (5)	0.003 (4)
C6	0.072 (6)	0.057 (6)	0.072 (6)	−0.016 (4)	0.004 (5)	−0.010 (4)
C7	0.063 (5)	0.061 (6)	0.073 (6)	−0.001 (4)	0.005 (4)	−0.013 (4)
C8	0.070 (6)	0.065 (6)	0.072 (7)	−0.009 (5)	0.000 (5)	0.003 (5)
C9	0.079 (6)	0.067 (7)	0.080 (7)	0.006 (5)	0.014 (5)	0.000 (5)
C10	0.092 (7)	0.082 (8)	0.093 (8)	0.014 (6)	0.005 (6)	−0.014 (6)
C11	0.091 (7)	0.076 (7)	0.097 (8)	−0.010 (6)	−0.003 (6)	0.009 (6)
C12	0.072 (6)	0.070 (7)	0.073 (7)	−0.008 (5)	0.002 (5)	0.008 (6)
C13	0.070 (6)	0.071 (7)	0.071 (7)	−0.014 (5)	0.004 (5)	0.008 (5)
C14	0.074 (6)	0.064 (6)	0.072 (6)	0.000 (5)	0.005 (5)	0.014 (5)
C15	0.101 (7)	0.093 (8)	0.097 (9)	−0.004 (6)	0.023 (6)	0.011 (6)
C16	0.102 (8)	0.109 (9)	0.094 (8)	−0.001 (7)	0.020 (6)	0.023 (7)
C17	0.092 (7)	0.087 (7)	0.091 (8)	−0.007 (6)	−0.006 (6)	0.022 (6)
C18	0.062 (6)	0.052 (5)	0.083 (7)	0.007 (4)	−0.002 (5)	−0.005 (5)
C19	0.064 (6)	0.052 (5)	0.058 (6)	0.001 (4)	0.002 (5)	−0.005 (4)
C20	0.065 (6)	0.051 (5)	0.063 (6)	0.006 (4)	0.009 (5)	−0.004 (4)
C21	0.075 (6)	0.052 (5)	0.061 (6)	0.006 (4)	0.013 (5)	−0.008 (4)

C22	0.075 (6)	0.068 (6)	0.071 (7)	0.007 (5)	0.024 (5)	−0.011 (5)
C23	0.086 (6)	0.072 (6)	0.065 (6)	0.011 (5)	0.008 (6)	−0.009 (4)
C24	0.075 (6)	0.073 (6)	0.070 (7)	0.007 (5)	0.002 (5)	−0.007 (5)
C25	0.056 (5)	0.057 (6)	0.078 (6)	−0.001 (5)	−0.002 (4)	0.004 (4)
C26	0.061 (6)	0.071 (6)	0.106 (7)	−0.001 (5)	0.007 (5)	0.007 (5)
C27	0.067 (6)	0.086 (8)	0.101 (7)	−0.026 (5)	0.012 (5)	0.013 (6)
C28	0.065 (6)	0.091 (8)	0.089 (7)	−0.010 (6)	0.007 (5)	−0.002 (6)
C29	0.066 (6)	0.076 (7)	0.078 (6)	0.009 (5)	0.007 (5)	−0.002 (5)
C30	0.053 (5)	0.067 (6)	0.075 (6)	0.002 (5)	0.006 (4)	−0.001 (5)
C31	0.064 (5)	0.065 (6)	0.092 (7)	0.012 (5)	0.010 (5)	0.010 (5)
C32	0.085 (7)	0.073 (7)	0.132 (9)	0.016 (6)	0.019 (6)	0.017 (6)
C33	0.101 (8)	0.086 (8)	0.137 (9)	0.037 (7)	0.018 (7)	0.015 (7)
C34	0.077 (7)	0.093 (8)	0.110 (8)	0.018 (6)	0.022 (6)	0.003 (6)
C35	0.105 (8)	0.097 (10)	0.108 (9)	−0.002 (7)	0.002 (6)	−0.001 (8)
C36	0.178 (12)	0.112 (10)	0.155 (12)	−0.020 (9)	0.018 (9)	−0.004 (8)
C37	0.142 (11)	0.142 (11)	0.157 (13)	−0.002 (9)	0.018 (9)	−0.041 (9)
C38	0.072 (6)	0.079 (7)	0.078 (7)	0.004 (5)	0.010 (5)	−0.006 (5)
C39	0.132 (9)	0.144 (10)	0.120 (9)	−0.002 (8)	0.053 (7)	0.016 (8)
C40	0.106 (8)	0.136 (10)	0.113 (8)	0.035 (7)	0.006 (6)	−0.041 (7)

Geometric parameters (Å, °)

Co1—O2	1.992 (5)	C15—C16	1.371 (11)
Co1—O1	1.996 (5)	C15—H15	0.9300
Co1—O3	2.120 (6)	C16—C17	1.350 (11)
Co1—O4	2.140 (5)	C16—H16	0.9300
Co1—N2	2.143 (6)	C17—H17	0.9300
Co1—N1	2.168 (6)	C18—C19	1.461 (10)
Br1—C4	1.887 (7)	C18—H18	0.9300
Br2—C6	1.896 (7)	C19—C24	1.405 (9)
Br3—C21	1.870 (8)	C19—C20	1.429 (10)
Br4—C23	1.904 (8)	C20—C21	1.444 (9)
N1—C1	1.301 (8)	C21—C22	1.354 (9)
N1—C8	1.474 (9)	C22—C23	1.371 (10)
N2—C18	1.264 (8)	C22—H22	0.9300
N2—C25	1.433 (8)	C23—C24	1.377 (10)
N3—C37	1.351 (11)	C24—H24	0.9300
N3—C36	1.405 (11)	C25—C26	1.365 (9)
N3—C35	1.420 (12)	C25—C30	1.419 (9)
N4—C38	1.333 (9)	C26—C27	1.411 (10)
N4—C39	1.415 (10)	C26—H26	0.9300
N4—C40	1.457 (10)	C27—C28	1.345 (10)
O1—C3	1.288 (8)	C27—H27	0.9300
O2—C20	1.282 (8)	C28—C29	1.384 (10)
O3—C35	1.098 (10)	C28—H28	0.9300
O4—C38	1.215 (8)	C29—C34	1.415 (11)
C1—C2	1.451 (9)	C29—C30	1.420 (9)
C1—H1	0.9300	C30—C31	1.425 (10)
C2—C3	1.394 (9)	C31—C32	1.338 (10)

C2—C7	1.413 (9)	C31—H31	0.9300
C3—C4	1.433 (9)	C32—C33	1.406 (11)
C4—C5	1.361 (9)	C32—H32	0.9300
C5—C6	1.386 (9)	C33—C34	1.346 (11)
C5—H5	0.9300	C33—H33	0.9300
C6—C7	1.377 (9)	C34—H34	0.9300
C7—H7	0.9300	C35—H35	0.9300
C8—C13	1.333 (10)	C36—H36A	0.9600
C8—C9	1.378 (10)	C36—H36B	0.9600
C9—C10	1.412 (10)	C36—H36C	0.9600
C9—H9	0.9300	C37—H37A	0.9600
C10—C11	1.407 (10)	C37—H37B	0.9600
C10—H10	0.9300	C37—H37C	0.9600
C11—C12	1.407 (10)	C38—H38	0.9300
C11—H11	0.9300	C39—H39A	0.9600
C12—C17	1.408 (11)	C39—H39B	0.9600
C12—C13	1.444 (11)	C39—H39C	0.9600
C13—C14	1.445 (10)	C40—H40A	0.9600
C14—C15	1.338 (10)	C40—H40B	0.9600
C14—H14	0.9300	C40—H40C	0.9600
O2—Co1—O1	95.51 (19)	N2—C18—C19	128.1 (8)
O2—Co1—O3	96.4 (2)	N2—C18—H18	116.0
O1—Co1—O3	167.9 (2)	C19—C18—H18	116.0
O2—Co1—O4	177.7 (2)	C24—C19—C20	120.4 (7)
O1—Co1—O4	86.7 (2)	C24—C19—C18	118.0 (8)
O3—Co1—O4	81.3 (2)	C20—C19—C18	121.6 (7)
O2—Co1—N2	87.3 (2)	O2—C20—C19	124.8 (7)
O1—Co1—N2	93.2 (2)	O2—C20—C21	119.3 (7)
O3—Co1—N2	89.1 (2)	C19—C20—C21	115.9 (7)
O4—Co1—N2	93.2 (2)	C22—C21—C20	121.4 (7)
O2—Co1—N1	82.5 (2)	C22—C21—Br3	121.2 (6)
O1—Co1—N1	87.7 (2)	C20—C21—Br3	117.2 (6)
O3—Co1—N1	92.1 (2)	C21—C22—C23	121.7 (7)
O4—Co1—N1	97.1 (2)	C21—C22—H22	119.1
N2—Co1—N1	169.8 (2)	C23—C22—H22	119.1
C1—N1—C8	114.6 (6)	C22—C23—C24	120.0 (8)
C1—N1—Co1	121.7 (5)	C22—C23—Br4	120.0 (7)
C8—N1—Co1	119.4 (5)	C24—C23—Br4	120.0 (7)
C18—N2—C25	115.9 (7)	C23—C24—C19	120.5 (8)
C18—N2—Co1	124.8 (5)	C23—C24—H24	119.7
C25—N2—Co1	119.4 (5)	C19—C24—H24	119.7
C37—N3—C36	119.0 (10)	C26—C25—C30	120.2 (7)
C37—N3—C35	126.5 (11)	C26—C25—N2	119.4 (7)
C36—N3—C35	114.3 (11)	C30—C25—N2	120.4 (7)
C38—N4—C39	120.0 (8)	C25—C26—C27	119.9 (8)
C38—N4—C40	120.2 (9)	C25—C26—H26	120.1
C39—N4—C40	119.5 (8)	C27—C26—H26	120.1
C3—O1—Co1	129.3 (5)	C28—C27—C26	120.6 (8)
C20—O2—Co1	130.5 (5)	C28—C27—H27	119.7

C35—O3—Co1	126.8 (8)	C26—C27—H27	119.7
C38—O4—Co1	124.0 (6)	C27—C28—C29	121.4 (8)
N1—C1—C2	126.4 (7)	C27—C28—H28	119.3
N1—C1—H1	116.8	C29—C28—H28	119.3
C2—C1—H1	116.8	C28—C29—C34	121.3 (9)
C3—C2—C7	121.6 (7)	C28—C29—C30	119.3 (8)
C3—C2—C1	123.7 (7)	C34—C29—C30	119.4 (9)
C7—C2—C1	114.7 (8)	C25—C30—C29	118.5 (8)
O1—C3—C2	126.5 (7)	C25—C30—C31	122.8 (7)
O1—C3—C4	118.5 (7)	C29—C30—C31	118.5 (8)
C2—C3—C4	115.0 (7)	C32—C31—C30	120.5 (8)
C5—C4—C3	123.7 (7)	C32—C31—H31	119.7
C5—C4—Br1	118.6 (6)	C30—C31—H31	119.7
C3—C4—Br1	117.7 (6)	C31—C32—C33	120.2 (9)
C4—C5—C6	119.4 (7)	C31—C32—H32	119.9
C4—C5—H5	120.3	C33—C32—H32	119.9
C6—C5—H5	120.3	C34—C33—C32	122.0 (9)
C7—C6—C5	119.9 (7)	C34—C33—H33	119.0
C7—C6—Br2	120.3 (7)	C32—C33—H33	119.0
C5—C6—Br2	119.8 (6)	C33—C34—C29	119.2 (9)
C6—C7—C2	120.3 (7)	C33—C34—H34	120.4
C6—C7—H7	119.9	C29—C34—H34	120.4
C2—C7—H7	119.9	O3—C35—N3	122.5 (12)
C13—C8—C9	122.1 (9)	O3—C35—H35	118.7
C13—C8—N1	116.9 (8)	N3—C35—H35	118.7
C9—C8—N1	120.8 (8)	N3—C36—H36A	109.5
C8—C9—C10	120.8 (8)	N3—C36—H36B	109.5
C8—C9—H9	119.6	H36A—C36—H36B	109.5
C10—C9—H9	119.6	N3—C36—H36C	109.5
C11—C10—C9	119.3 (8)	H36A—C36—H36C	109.5
C11—C10—H10	120.4	H36B—C36—H36C	109.5
C9—C10—H10	120.4	N3—C37—H37A	109.5
C12—C11—C10	118.1 (9)	N3—C37—H37B	109.5
C12—C11—H11	121.0	H37A—C37—H37B	109.5
C10—C11—H11	121.0	N3—C37—H37C	109.5
C11—C12—C17	120.9 (9)	H37A—C37—H37C	109.5
C11—C12—C13	120.9 (9)	H37B—C37—H37C	109.5
C17—C12—C13	118.2 (9)	O4—C38—N4	123.7 (9)
C8—C13—C12	118.6 (9)	O4—C38—H38	118.2
C8—C13—C14	124.8 (9)	N4—C38—H38	118.2
C12—C13—C14	116.5 (8)	N4—C39—H39A	109.5
C15—C14—C13	120.7 (8)	N4—C39—H39B	109.5
C15—C14—H14	119.6	H39A—C39—H39B	109.5
C13—C14—H14	119.6	N4—C39—H39C	109.5
C14—C15—C16	122.8 (9)	H39A—C39—H39C	109.5
C14—C15—H15	118.6	H39B—C39—H39C	109.5
C16—C15—H15	118.6	N4—C40—H40A	109.5
C17—C16—C15	119.1 (10)	N4—C40—H40B	109.5
C17—C16—H16	120.4	H40A—C40—H40B	109.5

C15—C16—H16	120.4	N4—C40—H40C	109.5
C16—C17—C12	122.6 (9)	H40A—C40—H40C	109.5
C16—C17—H17	118.7	H40B—C40—H40C	109.5
C12—C17—H17	118.7		
O2—Co1—N1—C1	72.8 (6)	C10—C11—C12—C17	−177.9 (7)
O1—Co1—N1—C1	−23.0 (6)	C10—C11—C12—C13	3.6 (12)
O3—Co1—N1—C1	169.1 (6)	C9—C8—C13—C12	2.4 (12)
O4—Co1—N1—C1	−109.4 (6)	N1—C8—C13—C12	178.9 (6)
N2—Co1—N1—C1	72.4 (15)	C9—C8—C13—C14	178.9 (7)
O2—Co1—N1—C8	−82.7 (6)	N1—C8—C13—C14	−4.6 (11)
O1—Co1—N1—C8	−178.5 (6)	C11—C12—C13—C8	−3.9 (11)
O3—Co1—N1—C8	13.6 (6)	C17—C12—C13—C8	177.6 (7)
O4—Co1—N1—C8	95.1 (6)	C11—C12—C13—C14	179.3 (7)
N2—Co1—N1—C8	−83.1 (14)	C17—C12—C13—C14	0.8 (10)
O2—Co1—N2—C18	−7.3 (6)	C8—C13—C14—C15	−176.0 (8)
O1—Co1—N2—C18	88.1 (6)	C12—C13—C14—C15	0.6 (11)
O3—Co1—N2—C18	−103.8 (6)	C13—C14—C15—C16	−2.8 (14)
O4—Co1—N2—C18	174.9 (6)	C14—C15—C16—C17	3.5 (15)
N1—Co1—N2—C18	−6.9 (17)	C15—C16—C17—C12	−2.0 (14)
O2—Co1—N2—C25	172.2 (5)	C11—C12—C17—C16	−178.6 (9)
O1—Co1—N2—C25	−92.5 (5)	C13—C12—C17—C16	−0.1 (12)
O3—Co1—N2—C25	75.7 (5)	C25—N2—C18—C19	177.8 (7)
O4—Co1—N2—C25	−5.6 (5)	Co1—N2—C18—C19	−2.7 (11)
N1—Co1—N2—C25	172.6 (12)	N2—C18—C19—C24	−172.4 (7)
O2—Co1—O1—C3	−64.5 (6)	N2—C18—C19—C20	7.2 (11)
O3—Co1—O1—C3	106.9 (11)	Co1—O2—C20—C19	−21.0 (10)
O4—Co1—O1—C3	114.9 (6)	Co1—O2—C20—C21	160.2 (5)
N2—Co1—O1—C3	−152.1 (6)	C24—C19—C20—O2	−175.6 (7)
N1—Co1—O1—C3	17.7 (6)	C18—C19—C20—O2	4.8 (11)
O1—Co1—O2—C20	−73.7 (6)	C24—C19—C20—C21	3.1 (9)
O3—Co1—O2—C20	108.1 (6)	C18—C19—C20—C21	−176.5 (6)
O4—Co1—O2—C20	120 (5)	O2—C20—C21—C22	177.1 (7)
N2—Co1—O2—C20	19.3 (6)	C19—C20—C21—C22	−1.7 (10)
N1—Co1—O2—C20	−160.6 (6)	O2—C20—C21—Br3	−7.4 (9)
O2—Co1—O3—C35	15.3 (9)	C19—C20—C21—Br3	173.7 (5)
O1—Co1—O3—C35	−156.1 (10)	C20—C21—C22—C23	0.0 (11)
O4—Co1—O3—C35	−164.2 (9)	Br3—C21—C22—C23	−175.2 (6)
N2—Co1—O3—C35	102.4 (9)	C21—C22—C23—C24	0.2 (12)
N1—Co1—O3—C35	−67.4 (9)	C21—C22—C23—Br4	178.8 (6)
O2—Co1—O4—C38	−162 (5)	C22—C23—C24—C19	1.2 (12)
O1—Co1—O4—C38	31.4 (6)	Br4—C23—C24—C19	−177.3 (5)
O3—Co1—O4—C38	−150.3 (6)	C20—C19—C24—C23	−3.0 (11)
N2—Co1—O4—C38	−61.7 (6)	C18—C19—C24—C23	176.6 (7)
N1—Co1—O4—C38	118.7 (6)	C18—N2—C25—C26	105.7 (8)
C8—N1—C1—C2	177.4 (7)	Co1—N2—C25—C26	−73.8 (8)
Co1—N1—C1—C2	20.8 (10)	C18—N2—C25—C30	−76.0 (9)
N1—C1—C2—C3	−4.1 (12)	Co1—N2—C25—C30	104.5 (7)
N1—C1—C2—C7	174.1 (7)	C30—C25—C26—C27	−2.7 (12)
Co1—O1—C3—C2	−8.2 (11)	N2—C25—C26—C27	175.6 (7)

Co1—O1—C3—C4	172.3 (5)	C25—C26—C27—C28	0.5 (13)
C7—C2—C3—O1	177.6 (6)	C26—C27—C28—C29	1.5 (13)
C1—C2—C3—O1	−4.4 (12)	C27—C28—C29—C34	179.2 (8)
C7—C2—C3—C4	−2.8 (10)	C27—C28—C29—C30	−1.4 (12)
C1—C2—C3—C4	175.2 (6)	C26—C25—C30—C29	2.8 (11)
O1—C3—C4—C5	−178.3 (7)	N2—C25—C30—C29	−175.5 (7)
C2—C3—C4—C5	2.1 (10)	C26—C25—C30—C31	177.9 (7)
O1—C3—C4—Br1	2.1 (9)	N2—C25—C30—C31	−0.4 (12)
C2—C3—C4—Br1	−177.5 (5)	C28—C29—C30—C25	−0.7 (11)
C3—C4—C5—C6	0.3 (11)	C34—C29—C30—C25	178.7 (7)
Br1—C4—C5—C6	179.9 (5)	C28—C29—C30—C31	−176.1 (7)
C4—C5—C6—C7	−2.2 (11)	C34—C29—C30—C31	3.3 (12)
C4—C5—C6—Br2	179.8 (5)	C25—C30—C31—C32	−177.7 (8)
C5—C6—C7—C2	1.4 (11)	C29—C30—C31—C32	−2.5 (12)
Br2—C6—C7—C2	179.5 (5)	C30—C31—C32—C33	−1.2 (14)
C3—C2—C7—C6	1.2 (11)	C31—C32—C33—C34	4.3 (15)
C1—C2—C7—C6	−177.0 (7)	C32—C33—C34—C29	−3.4 (15)
C1—N1—C8—C13	116.2 (8)	C28—C29—C34—C33	179.0 (9)
Co1—N1—C8—C13	−86.6 (8)	C30—C29—C34—C33	−0.4 (13)
C1—N1—C8—C9	−67.2 (9)	Co1—O3—C35—N3	168.7 (6)
Co1—N1—C8—C9	90.0 (8)	C37—N3—C35—O3	−7.6 (17)
C13—C8—C9—C10	−0.7 (12)	C36—N3—C35—O3	177.5 (11)
N1—C8—C9—C10	−177.1 (7)	Co1—O4—C38—N4	166.4 (6)
C8—C9—C10—C11	0.4 (12)	C39—N4—C38—O4	−4.2 (13)
C9—C10—C11—C12	−1.9 (12)	C40—N4—C38—O4	−177.7 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21a—H28b···Br3a	0.930	2.932	1.870	151.6

Fig. 1

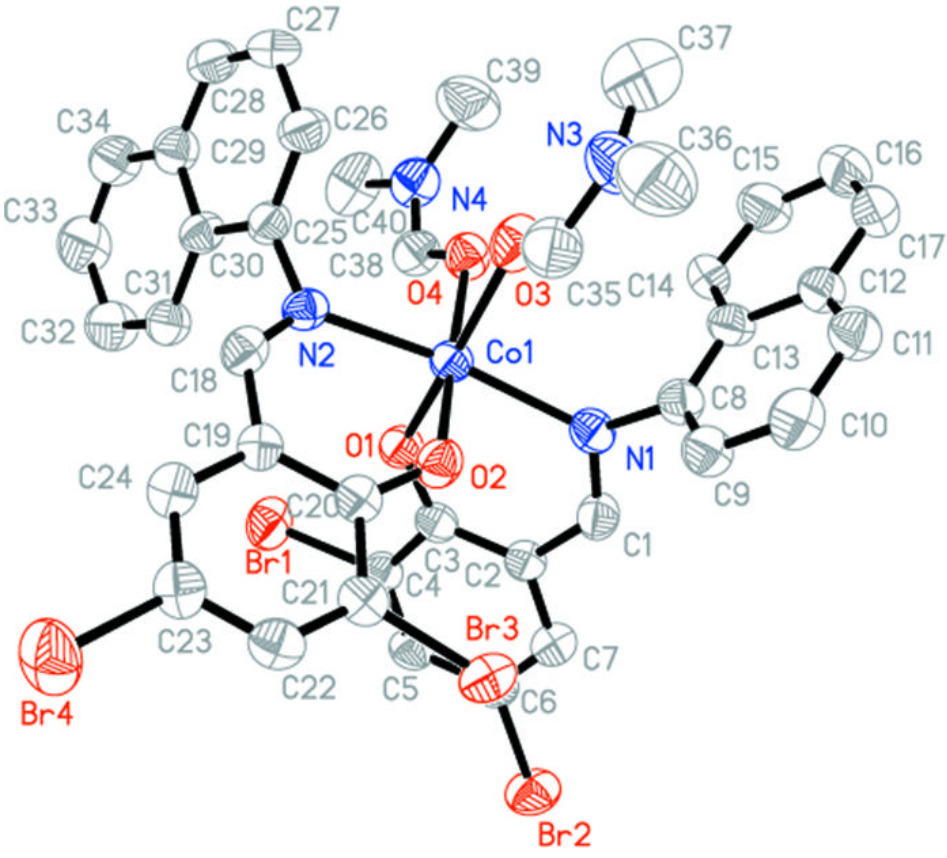

C27
C37
C39
C28
C34
C26
N3
C36
C29
C15
C16
C33
N4
C40
C25
C17
C38
C30
O4
O3
C35
C14
C12
C31
C32
N2
Co1
C13
C11
C18
C8
C19
O1
N1
C10
C24
O2
C9
C20
C1
Br1
C3
C2
C21
C4
Br3
C23
C7
C22
C5
C6
Br4
Br2

Fig. 2