Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

The 2:1 adduct of 8-hydroxyquinoline *N*-oxide and diaquabis(8-hydroxyquinoline *N*-oxide)dithiocyanatocobalt(II)

Shi-Guo Zhang,[a] Hai-Yan Xu[b] and Jing-Min Shi[b]*

[a]Department of Chemistry and Chemical Engineering, Institute of Materials Chemistry, Binzhou University, Binzhou 256603, People's Republic of China, and [b]Department of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China
Correspondence e-mail: shijingmin@beelink.com

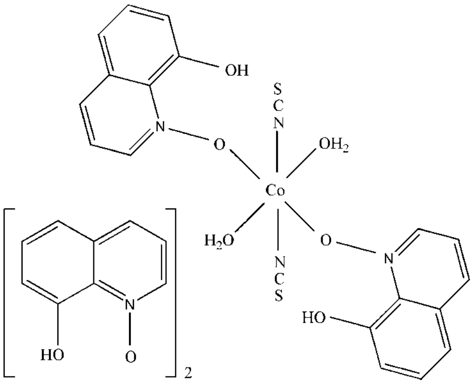
Received 25 June 2007; accepted 4 July 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.122; data-to-parameter ratio = 15.6.

In the crystal structure of the title adduct, $[Co(NCS)_2(C_9H_7NO_2)_2(H_2O)_2]\cdot 2C_9H_7NO_2$, the uncoordinated 8-hydroxyquinoline molecules and complex molecules are connected by intermolecular O—H···O and C—H···S hydrogen bonds. In the complex molecule, the Co^{II} atom lies on a crystallographic inversion centre and has a slightly distorted octahedral coordination geometry. In addition, weak π–π stacking interactions between the uncoordinated and coordinated ring systems, with ring–centroid separations of 3.7554 (18) Å, consolidate the crystal structure.

Related literature

For related crystal structures, see: Desiderato *et al.* (1971); Shi *et al.* (2006).



Experimental

Crystal data

$[Co(NCS)_2(C_9H_7NO_2)_2(H_2O)_2].2C_9H_7NO_2$
M_r = 855.75
Monoclinic, $P2_1/n$
a = 8.6381 (13) Å
b = 17.133 (3) Å
c = 12.6809 (19) Å
β = 93.967 (2)°
V = 1872.2 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 298 (2) K
0.46 × 0.38 × 0.21 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) T_{min} = 0.758, T_{max} = 0.878
10783 measured reflections
4049 independent reflections
2959 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.122
S = 0.99
4049 reflections
259 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H7···O5^{i}	0.84	2.02	2.849 (2)	168
O1—H6···O4^{ii}	0.85	1.97	2.786 (3)	162
C5—H5···S1^{iii}	0.93	2.77	3.695 (4)	173
C12—H12···S1^{iv}	0.93	2.85	3.768 (4)	170
O3—H1···O2	0.82	1.81	2.527 (2)	145
O3—H1···N2	0.82	2.46	2.878 (2)	113
O5—H2···O4	0.82	1.72	2.460 (3)	150
O5—H2···N3	0.82	2.34	2.796 (3)	116

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

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

The authors thank the Natural Science Foundation of Shandong Province of China (grant No. Y2005B25).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2445).

References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5.06a). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiderato, R., Terry, J. C., Freemann, G. R. & Levy, H. A. (1971). *Acta Cryst.* B**27**, 2443–2447.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Shi, J. M., Sun, Y. M., Zhang, X., Yi, L. & Cheng, P. (2006). *J. Phys. Chem. A*, **110**, 7677–7681.

doi:10.1107/S1600536807032722

supplementary materials

Acta Cryst. (2007). E**63**, m2083 [**doi:10.1107/S1600536807032722**]

The 2:1 adduct of 8-hydroxyquinoline *N*-oxide and diaquabis(8-hydroxyquinoline *N*-oxide)dithiocyanatocobalt(II)

S.-G. Zhang, H.-Y. Xu and J.-M. Shi

Comment

The thiocyanate anion is a versatile ligand and a large number of complexes have been synthisized with it as a termianl or as a bridging ligand (*e.g.* Shi *et al.*, 2006). Our interest in complexes containing the thiocyanate ligand resulted in us obtaining the title adduct. Here we report its cystal structure. The crystal structure of 8-hydroxyquinoline N-oxide has previously been reported (Desiderato *et al.*, 1971).

Figure 1 shows a symmetry complete complex molecule and a symmetry unique 8-hydroxyquinoline molecule. Atom Co1 is in a slightly distorted octahedral CoN_2O_4 coordination geometry. In the crystal structure both the uncoordinated and coordinated 8-hydroxyquinoline molecules contain intramolecular O—H···O and O—H···N hydrogen bonds. Intermolecular O—H···O and C—H···S hydrogen bonds are observed between uncoordinated 8-hydroxyquinoline molecules and complex molecules (Fig. 2). In addition, there is a weak π-π stacking interaction between adjacent C11—C16 and N2/C6—C10 rings, with $Cg1\cdots Cg2$ = 3.7554 (18) Å and $Cg1\cdots Cg2_{\rm perp}$ = 3.471 Å [$Cg1\cdots Cg2$ is the distance between the two ring centroids, and $Cg1\cdots Cg2_{\rm perp}$ is the perpendicular distance of the two rings]. The dihedral anagle of the planes of the two rings is 14.6°. The overall result of the hydrogen bonding and π···π stacking interactions leads to the formation of a super-molecular three-dimensional structure.

Experimental

15 ml H_2O solution containing $Co(ClO_4)_2\cdot 6H_2O$ (0.1578 g, 0.431 mmol) and NaSCN (0.0702 g, 0.866 mmol) was added into 20 ml 8-hydroxyquinoline N-oxide (0.1321 g, 0.820 mmol) ethanol solution, and stirred for a few minutes. The red single crystals were obtained after the mixed solution had been allowed to stand at room temperature for four weeks. The strong and sharp IR peaks at 1399 cm^{-1} may be attributed to the stretching vibrations of the C=C and C=N bonds, whereas peak at 2088 cm^{-1} is assigned to the stretching vibration of thiocyanate group.

Refinement

H atoms of water molecule were located in a difference Fourier map and refined as riding in their as-found positions, with O—H = 0.841–0.846 Å, $U_{\rm iso}$(H) = 1.5 $U_{\rm eq}$(O). Other H atoms were placed in calculated positions, and refined as riding, with C—H = 0.93 Å, $U_{\rm iso}$(H) = $1.2_{\rm eq}$(C); O—H = 0.82 Å, $U_{\rm iso}$(H) = 1.5 $U_{\rm eq}$(O) for hydroxyl groups.

Figures

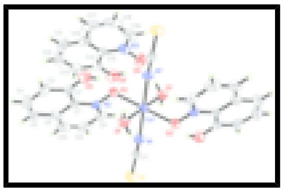


Fig. 1. The molecular structure showing the atom numbering scheme and thermal ellipsoids drawn at the 30% probability level. [Symmetry code: (i) −*x* + 1, −*y*, −*z* + 1]. Only a symmetry unique uncoordinated 8-hydroxyquinoline molecule is shown.

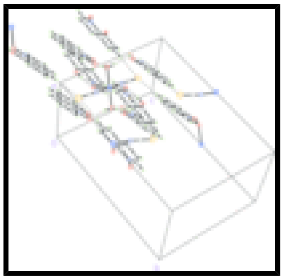


Fig. 2. Part of the crystal structure showing hydrogen bonds as dahed lines.

8-hydroxyquinoline *N*-oxide–diaquabis(8-hydroxyquinoline N-oxide-κ*O*^{1})bis(thiocyanato-κ*N*)cobalt(II) (2/1)

Crystal data

$[Co(NCS)_2(C_9H_7NO_2)_2(H_2O)_2].2C_9H_7NO_2$

M_r = 855.75

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

a = 8.6381 (13) Å

b = 17.133 (3) Å

c = 12.6809 (19) Å

β = 93.967 (2)°

V = 1872.2 (5) Å^3

Z = 2

F_{000} = 882

D_x = 1.518 Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 3119 reflections

θ = 2.4–24.1°

μ = 0.64 mm^{-1}

T = 298 (2) K

Block, red

0.46 × 0.38 × 0.21 mm

Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 298(2) K

φ and ω scans

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

T_{min} = 0.758, T_{max} = 0.878

10783 measured reflections

4049 independent reflections

2959 reflections with $I > 2\sigma(I)$

R_{int} = 0.026

θ_{max} = 27.0°

θ_{min} = 2.0°

$h = -10 \rightarrow 11$

$k = -20 \rightarrow 21$

$l = -11 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.0781P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} = 0.002$
4049 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
259 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 > 2sigma(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}
O1	0.30709 (16)	0.07591 (9)	0.46163 (12)	0.0570 (4)
H6	0.2606	0.0565	0.4069	0.085*
H7	0.2497	0.0762	0.5126	0.085*
Co1	0.5000	0.0000	0.5000	0.04581 (15)
O2	0.63297 (17)	0.09338 (8)	0.56295 (12)	0.0520 (4)
N2	0.69243 (19)	0.15070 (10)	0.50537 (13)	0.0479 (4)
O5	1.0743 (2)	0.07773 (12)	0.61024 (16)	0.0881 (6)
H2	1.0359	0.0360	0.6264	0.132*
C7	0.6420 (2)	0.22599 (13)	0.51917 (16)	0.0497 (5)
C15	0.9009 (2)	0.11953 (14)	0.73717 (18)	0.0545 (5)
O3	0.4624 (2)	0.19045 (10)	0.65009 (14)	0.0710 (5)
H1	0.4987	0.1473	0.6384	0.107*
N1	0.5638 (2)	0.01197 (11)	0.34865 (16)	0.0576 (5)
N3	0.8489 (2)	0.04347 (14)	0.75126 (17)	0.0678 (6)
C8	0.8003 (3)	0.13268 (18)	0.4404 (2)	0.0678 (7)
H8	0.8319	0.0811	0.4343	0.081*
C1	0.6113 (3)	0.02121 (12)	0.26736 (18)	0.0494 (5)

C16	0.8379 (3)	0.18037 (19)	0.7958 (2)	0.0733 (8)
C9	0.8669 (3)	0.1907 (3)	0.3808 (2)	0.0929 (11)
H9	0.9425	0.1781	0.3348	0.111*
C6	0.7082 (3)	0.28558 (17)	0.4597 (2)	0.0728 (8)
C2	0.5277 (3)	0.24412 (14)	0.59013 (18)	0.0566 (6)
C14	1.0138 (3)	0.13580 (16)	0.66616 (19)	0.0606 (6)
C4	0.5457 (5)	0.37788 (19)	0.5420 (3)	0.1031 (12)
H4	0.5125	0.4290	0.5506	0.124*
O4	0.9025 (2)	−0.01479 (11)	0.69366 (18)	0.0851 (6)
C3	0.4817 (3)	0.31982 (17)	0.5988 (2)	0.0793 (8)
H3	0.4053	0.3322	0.6443	0.095*
C13	1.0592 (3)	0.2099 (2)	0.6527 (3)	0.0868 (9)
H13	1.1338	0.2209	0.6053	0.104*
C18	0.6822 (4)	0.0881 (3)	0.8789 (3)	0.1141 (15)
H18	0.6098	0.0767	0.9276	0.137*
C19	0.7415 (3)	0.0290 (2)	0.8207 (3)	0.0929 (10)
H19	0.7069	−0.0219	0.8294	0.111*
C10	0.8200 (4)	0.2656 (3)	0.3908 (2)	0.0954 (11)
H10	0.8634	0.3043	0.3508	0.114*
C12	0.9966 (5)	0.2699 (2)	0.7082 (4)	0.1114 (13)
H12	1.0298	0.3208	0.6972	0.134*
C11	0.8899 (5)	0.2572 (2)	0.7773 (3)	0.1041 (12)
H11	0.8494	0.2989	0.8134	0.125*
C5	0.6557 (5)	0.36344 (18)	0.4736 (3)	0.0981 (11)
H5	0.6968	0.4041	0.4359	0.118*
C17	0.7273 (4)	0.1617 (3)	0.8661 (3)	0.1088 (14)
H17	0.6840	0.2012	0.9049	0.131*
S1	0.67766 (10)	0.03564 (5)	0.15248 (6)	0.0848 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0554 (9)	0.0602 (9)	0.0560 (9)	0.0069 (7)	0.0085 (7)	−0.0016 (7)
Co1	0.0487 (2)	0.0473 (2)	0.0425 (2)	0.00069 (17)	0.01068 (17)	0.00210 (17)
O2	0.0607 (9)	0.0485 (8)	0.0474 (8)	−0.0054 (7)	0.0081 (7)	0.0023 (7)
N2	0.0430 (9)	0.0597 (11)	0.0413 (9)	−0.0064 (8)	0.0058 (7)	−0.0031 (8)
O5	0.0686 (11)	0.1132 (15)	0.0857 (14)	0.0141 (11)	0.0285 (10)	−0.0130 (12)
C7	0.0521 (12)	0.0533 (12)	0.0427 (11)	−0.0106 (10)	−0.0037 (9)	0.0011 (10)
C15	0.0407 (11)	0.0715 (15)	0.0501 (13)	0.0027 (10)	−0.0042 (9)	−0.0024 (11)
O3	0.0749 (11)	0.0797 (12)	0.0614 (11)	0.0046 (9)	0.0259 (9)	−0.0049 (9)
N1	0.0611 (12)	0.0670 (12)	0.0460 (10)	−0.0026 (9)	0.0128 (9)	0.0020 (9)
N3	0.0524 (11)	0.0882 (16)	0.0613 (13)	0.0012 (11)	−0.0069 (10)	0.0103 (12)
C8	0.0476 (13)	0.0967 (19)	0.0603 (15)	−0.0067 (12)	0.0124 (11)	−0.0184 (14)
C1	0.0536 (12)	0.0451 (11)	0.0505 (13)	0.0002 (9)	0.0097 (10)	−0.0021 (9)
C16	0.0552 (14)	0.102 (2)	0.0603 (16)	0.0173 (14)	−0.0110 (12)	−0.0229 (15)
C9	0.0602 (17)	0.162 (3)	0.0589 (18)	−0.041 (2)	0.0204 (14)	−0.014 (2)
C6	0.0731 (17)	0.0812 (18)	0.0616 (16)	−0.0341 (14)	−0.0132 (14)	0.0175 (14)
C2	0.0580 (13)	0.0606 (14)	0.0500 (13)	0.0034 (11)	−0.0061 (11)	−0.0113 (11)

C14	0.0453 (12)	0.0802 (17)	0.0562 (14)	0.0019 (12)	0.0026 (10)	0.0001 (12)
C4	0.122 (3)	0.0600 (18)	0.121 (3)	0.002 (2)	−0.039 (3)	−0.007 (2)
O4	0.0760 (13)	0.0685 (12)	0.1083 (17)	0.0125 (9)	−0.0125 (12)	−0.0076 (11)
C3	0.0859 (19)	0.0710 (18)	0.078 (2)	0.0145 (15)	−0.0143 (16)	−0.0179 (15)
C13	0.0696 (18)	0.105 (2)	0.085 (2)	−0.0220 (17)	−0.0049 (16)	0.0168 (19)
C18	0.063 (2)	0.229 (5)	0.0507 (18)	0.002 (3)	0.0101 (15)	0.012 (3)
C19	0.0594 (16)	0.140 (3)	0.077 (2)	−0.0225 (18)	−0.0114 (16)	0.042 (2)
C10	0.083 (2)	0.138 (3)	0.0649 (19)	−0.063 (2)	0.0007 (16)	0.023 (2)
C12	0.107 (3)	0.078 (2)	0.142 (4)	−0.015 (2)	−0.043 (3)	−0.005 (2)
C11	0.097 (2)	0.091 (3)	0.118 (3)	0.024 (2)	−0.038 (2)	−0.044 (2)
C5	0.120 (3)	0.0609 (18)	0.107 (3)	−0.0371 (19)	−0.035 (2)	0.0288 (17)
C17	0.0613 (19)	0.203 (4)	0.062 (2)	0.029 (2)	0.0004 (15)	−0.039 (3)
S1	0.1174 (6)	0.0820 (5)	0.0604 (4)	−0.0090 (4)	0.0450 (4)	−0.0001 (4)

Geometric parameters (Å, °)

O1—Co1	2.1431 (14)	C1—S1	1.621 (2)
O1—H6	0.8463	C16—C17	1.389 (5)
O1—H7	0.8407	C16—C11	1.416 (5)
Co1—N1^{i}	2.044 (2)	C9—C10	1.354 (5)
Co1—N1	2.044 (2)	C9—H9	0.9300
Co1—O2	2.0951 (14)	C6—C10	1.390 (4)
Co1—O2^{i}	2.0951 (14)	C6—C5	1.424 (4)
Co1—O1^{i}	2.1431 (14)	C2—C3	1.363 (3)
O2—N2	1.346 (2)	C14—C13	1.344 (4)
N2—C8	1.322 (3)	C4—C5	1.353 (5)
N2—C7	1.376 (3)	C4—C3	1.367 (4)
O5—C14	1.348 (3)	C4—H4	0.9300
O5—H2	0.8200	C3—H3	0.9300
C7—C6	1.413 (3)	C13—C12	1.377 (5)
C7—C2	1.416 (3)	C13—H13	0.9300
C15—N3	1.394 (3)	C18—C17	1.333 (5)
C15—C14	1.401 (3)	C18—C19	1.373 (5)
C15—C16	1.411 (3)	C18—H18	0.9300
O3—C2	1.342 (3)	C19—H19	0.9300
O3—H1	0.8200	C10—H10	0.9300
N1—C1	1.146 (3)	C12—C11	1.333 (5)
N3—O4	1.338 (3)	C12—H12	0.9300
N3—C19	1.345 (4)	C11—H11	0.9300
C8—C9	1.397 (4)	C5—H5	0.9300
C8—H8	0.9300	C17—H17	0.9300
Co1—O1—H6	105.4	C10—C9—H9	120.5
Co1—O1—H7	108.6	C8—C9—H9	120.5
H6—O1—H7	111.2	C10—C6—C7	118.8 (3)
N1^{i}—Co1—N1	180.0	C10—C6—C5	123.4 (3)
N1^{i}—Co1—O2	83.99 (7)	C7—C6—C5	117.8 (3)
N1—Co1—O2	96.01 (7)	O3—C2—C3	118.0 (2)
N1^{i}—Co1—O2^{i}	96.01 (7)	O3—C2—C7	123.3 (2)

N1—Co1—O2^{i}	83.99 (7)	C3—C2—C7	118.7 (2)
O2—Co1—O2^{i}	180.00 (5)	C13—C14—O5	120.3 (3)
N1^{i}—Co1—O1	91.03 (7)	C13—C14—C15	119.5 (3)
N1—Co1—O1	88.97 (7)	O5—C14—C15	120.3 (2)
O2—Co1—O1	91.16 (6)	C5—C4—C3	122.2 (3)
O2^{i}—Co1—O1	88.84 (6)	C5—C4—H4	118.9
N1^{i}—Co1—O1^{i}	88.97 (7)	C3—C4—H4	118.9
N1—Co1—O1^{i}	91.03 (7)	C2—C3—C4	121.2 (3)
O2—Co1—O1^{i}	88.84 (6)	C2—C3—H3	119.4
O2^{i}—Co1—O1^{i}	91.16 (6)	C4—C3—H3	119.4
O1—Co1—O1^{i}	180.00 (8)	C14—C13—C12	120.8 (3)
N2—O2—Co1	124.75 (12)	C14—C13—H13	119.6
C8—N2—O2	118.6 (2)	C12—C13—H13	119.6
C8—N2—C7	122.7 (2)	C17—C18—C19	120.7 (3)
O2—N2—C7	118.60 (16)	C17—C18—H18	119.7
C14—O5—H2	109.5	C19—C18—H18	119.7
N2—C7—C6	117.8 (2)	N3—C19—C18	121.0 (3)
N2—C7—C2	121.80 (19)	N3—C19—H19	119.5
C6—C7—C2	120.4 (2)	C18—C19—H19	119.5
N3—C15—C14	120.9 (2)	C9—C10—C6	121.2 (3)
N3—C15—C16	118.9 (2)	C9—C10—H10	119.4
C14—C15—C16	120.2 (2)	C6—C10—H10	119.4
C2—O3—H1	109.5	C11—C12—C13	121.8 (4)
C1—N1—Co1	174.2 (2)	C11—C12—H12	119.1
O4—N3—C19	120.0 (3)	C13—C12—H12	119.1
O4—N3—C15	120.0 (2)	C12—C11—C16	120.2 (3)
C19—N3—C15	120.0 (3)	C12—C11—H11	119.9
N2—C8—C9	120.4 (3)	C16—C11—H11	119.9
N2—C8—H8	119.8	C4—C5—C6	119.6 (3)
C9—C8—H8	119.8	C4—C5—H5	120.2
N1—C1—S1	179.1 (2)	C6—C5—H5	120.2
C17—C16—C15	118.4 (3)	C18—C17—C16	121.0 (4)
C17—C16—C11	124.1 (3)	C18—C17—H17	119.5
C15—C16—C11	117.5 (3)	C16—C17—H17	119.5
C10—C9—C8	119.1 (3)		

N1^{i}—Co1—O2—N2	−162.65 (15)	N2—C7—C2—C3	−179.1 (2)
N1—Co1—O2—N2	17.35 (15)	C6—C7—C2—C3	0.8 (3)
O1—Co1—O2—N2	−71.73 (14)	N3—C15—C14—C13	178.6 (2)
O1^{i}—Co1—O2—N2	108.27 (14)	C16—C15—C14—C13	−1.4 (4)
Co1—O2—N2—C8	−65.6 (2)	N3—C15—C14—O5	−0.1 (3)
Co1—O2—N2—C7	116.45 (17)	C16—C15—C14—O5	179.9 (2)
C8—N2—C7—C6	0.8 (3)	O3—C2—C3—C4	178.5 (3)
O2—N2—C7—C6	178.66 (18)	C7—C2—C3—C4	−1.2 (4)
C8—N2—C7—C2	−179.2 (2)	C5—C4—C3—C2	0.9 (5)
O2—N2—C7—C2	−1.4 (3)	O5—C14—C13—C12	179.0 (3)
C14—C15—N3—O4	−2.6 (3)	C15—C14—C13—C12	0.3 (4)

C16—C15—N3—O4	177.5 (2)	O4—N3—C19—C18	−178.5 (3)
C14—C15—N3—C19	179.3 (2)	C15—N3—C19—C18	−0.4 (4)
C16—C15—N3—C19	−0.7 (3)	C17—C18—C19—N3	1.5 (5)
O2—N2—C8—C9	−178.8 (2)	C8—C9—C10—C6	0.6 (5)
C7—N2—C8—C9	−1.0 (4)	C7—C6—C10—C9	−0.7 (4)
N3—C15—C16—C17	0.6 (4)	C5—C6—C10—C9	179.6 (3)
C14—C15—C16—C17	−179.4 (2)	C14—C13—C12—C11	0.3 (5)
N3—C15—C16—C11	−178.2 (2)	C13—C12—C11—C16	0.2 (5)
C14—C15—C16—C11	1.9 (4)	C17—C16—C11—C12	−180.0 (3)
N2—C8—C9—C10	0.2 (4)	C15—C16—C11—C12	−1.3 (4)
N2—C7—C6—C10	0.0 (3)	C3—C4—C5—C6	−0.2 (5)
C2—C7—C6—C10	−179.9 (2)	C10—C6—C5—C4	179.6 (3)
N2—C7—C6—C5	179.8 (2)	C7—C6—C5—C4	−0.1 (4)
C2—C7—C6—C5	−0.2 (4)	C19—C18—C17—C16	−1.6 (6)
N2—C7—C2—O3	1.2 (3)	C15—C16—C17—C18	0.6 (5)
C6—C7—C2—O3	−178.8 (2)	C11—C16—C17—C18	179.2 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H7···O5$^{\text{ii}}$	0.84	2.02	2.849 (2)	168
O1—H6···O4$^{\text{i}}$	0.85	1.97	2.786 (3)	162
C5—H5···S1$^{\text{iii}}$	0.93	2.77	3.695 (4)	173
C12—H12···S1$^{\text{iv}}$	0.93	2.85	3.768 (4)	170
O3—H1···O2	0.82	1.81	2.527 (2)	145
O3—H1···N2	0.82	2.46	2.878 (2)	113
O5—H2···O4	0.82	1.72	2.460 (3)	150
O5—H2···N3	0.82	2.34	2.796 (3)	116

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

Fig. 1

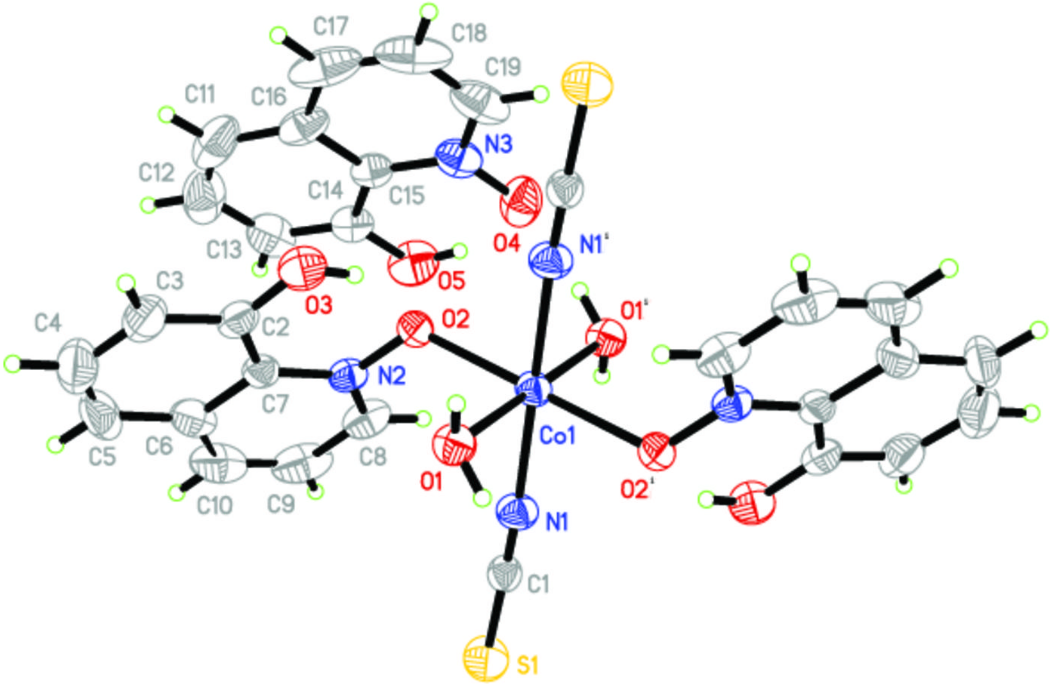

C17
C18
C19
C11
C16
N3
C12
C14
C15
C13
O4
N1ⁱ
O5
C3
O3
O1ⁱ
C4
C2
O2
N2
C7
C6
Co1
C5
C8
O1
O2ⁱ
C10
C9
N1
C1
S1

Fig. 2