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Bis(μ-pyridine-2,3-dicarboxylato)-bis[aqua(2,2′-diamino-4,4′-bi-1,3-thiazole)cobalt(II)] decahydrate

Yuan-Yuan Lin, Guang-Hua Chen, Yan-Ping Yu and Bing-Xin Liu*

Department of Chemistry, Shanghai University, People's Republic of China
Correspondence e-mail: r5744011@yahoo.com.cn

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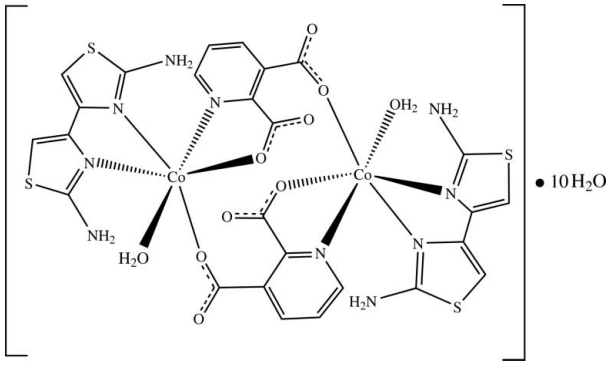
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.094; data-to-parameter ratio = 13.0.

In the centrosymmetric title dimeric Co^{II} complex, $[Co_2(C_7H_3NO_4)_2(C_6H_6N_4OS_2)_2(H_2O)_2].10H_2O$, each Co^{II} cation has a distorted octahedral coordination geometry formed by a diaminobithiazole (DABT) ligand, two pyridine-2,3-dicarboxylate anions and a coordinated water molecule. With its two carboxylate groups, the pyridine-2,3-dicarboxylate anion bridges two Co^{II} ions to form the dimeric complex. Within the chelating DABT ligand, the two thiazole rings are twisted with respect to each other [dihedral angle = 3.29 (19)°]. Extensive N—H···O, O—H···O and O—H···N hydrogen bonding helps to stabilize the crystal structure.

Related literature

For general background, see: Waring (1981); Fisher *et al.* (1985). For related structures, see: Liu & Xu (2004); Liu *et al.* (2004); Liu & Xu (2005); Luo *et al.* (2004); Wu *et al.* (2003).



Experimental

Crystal data

$[Co_2(C_7H_3NO_4)_2(C_6H_6N_4OS_2)_2(H_2O)_2]\cdot10H_2O$
M_r = 1060.80
Triclinic, $P\overline{1}$
a = 8.1415 (12) Å
b = 11.2685 (17) Å
c = 12.0084 (18) Å
α = 74.269 (2)°
β = 82.864 (2)°
γ = 87.713 (2)°
V = 1052.2 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 295 (2) K
0.20 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.785, T_{max} = 0.850
5510 measured reflections
3653 independent reflections
2911 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.094
S = 1.06
3653 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co—O1	2.100 (2)	Co—N1	2.119 (2)
Co—O11	2.077 (2)	Co—N3	2.151 (3)
Co—O13^{i}	2.119 (2)	Co—N11	2.152 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O4W	0.91	1.79	2.694 (4)	177
O1—H1B···O5W	0.97	2.04	2.943 (4)	153
N2—H2A···O13^{i}	0.87	2.08	2.853 (4)	149
N2—H2B···O3W^{ii}	0.84	2.14	2.968 (4)	167
N4—H4A···O11	0.86	2.21	2.869 (4)	133
N4—H4B···O5W^{iii}	0.87	2.25	3.105 (4)	165
O1W—H1WA···O12	0.85	1.90	2.690 (3)	156
O1W—H1WB···O2W	0.82	1.99	2.796 (4)	166
O2W—H2WA···O14	0.85	2.01	2.839 (3)	167
O2W—H2WB···O14^{iv}	0.83	2.01	2.817 (3)	165
O3W—H3WA···O1W^{v}	0.84	2.02	2.823 (4)	158
O3W—H3WB···O14	0.82	2.10	2.878 (4)	159
O4W—H4WA···O2W^{ii}	0.86	2.01	2.814 (4)	155
O4W—H4WB···O1W^{vi}	0.83	2.08	2.884 (5)	164
O5W—H5WB···O3W^{vii}	0.86	1.99	2.854 (4)	175

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2294).

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supplementary materials

Acta Cryst. (2007). E**63**, m2178-m2179 [**doi:10.1107/S160053680703454X**]

Bis(μ-pyridine-2,3-dicarboxylato)bis[aqua(2,2'-diamino-4,4'-bi-1,3-thiazole)cobalt(II)] decahydrate

Y.-Y. Lin, G.-H. Chen, Y.-P. Yu and B.-X. Liu

Comment

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown biological activities such as the effective inhibitors of DNA synthesis of the tumor cells (Waring, 1981; Fisher *et al.*, 1985). As part of serial structural investigation of metal complexes with DABT (Liu & Xu, 2004), the title Co^{II} complex was recently prepared and its X-ray structure is presented here.

The molecular structure of the title compound is shown in Fig. 1. The complex of Co^{II} has a distorted octahedral coordination geometry (Table 1) formed by one of DABT ligand, one of pyridine-2,3-dicarboxylate anion, one of coordinated water and one of adjacent pyridine-2,3-dicarboxylate anion.

Within the complex, the DABT molecule shows approximately coplanar configuration with the dihedral angle of 3.29 (19)° between thiazole rings defined by C1, C2, C3, S1, N1 and C4, C5, C6, S2, N3. This is compare to 4.57 (7)° found in [Mn(DABT)(oxydiacetate)] (Luo *et al.*, 2004) and 6.52 (9)° found in [Cu(DABT)(oxydiacetato)] (Wu *et al.*, 2003), but different from the 17.23 (7)° found in $[Cr(C_4H_5NO_4)(C_6H_6N_4S_2)(H_2O)]Cl$ (Liu *et al.*, 2004) and 20.02 (8)° in [Ni(DABT)(iminodiacetate)] (Liu & Xu, 2005). Bond lengths C6—N4 [1.334 (4) Å] and C3—N2 [1.326 (4) Å] imply the existence of electron delocalization between thiazole rings and amino groups.

Within the pyridine-2,3-dicarboxylate anion, one oxygen atom (O11) of one carboxyl group of the pyridine-2,3-dicarboxylate anion and the nitrogen atom (N11) of pyridine ring chelate to Co^{II} atom and one oxygen atom (O13) of another carboxyl group of the pyridine-2,3-dicarboxylate anion chelates to another neighboring Co^{II} atom to form the dimeric complex across an inversion centre. The dihedral angles between the pyridine ring and two carboxyl group plans are 5.84 (7) and 84.82 (11)° for the plan formed by C11, C16, O11, O12 and the plan formed by C12, C17, O13, O14 respectively. Otherwise, another uncoordinated oxygen atom (O12 and O14) hydrogen bonded to the lattice water within the complex (Fig. 1 and Table 2), which helps to stabilize the crystal structure.

Experimental

An aqua solution (20 ml) containing DABT (0.20 g, 1 mmol) and $CoCl_2{\cdot}6H_2O$ (0.23 g, 1 mmol) was mixed with an aqueous solution (10 ml) of pyridine-2,3-dicarboxylic acid (0.17 g, 1 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 6 h. After cooling to room temperature the solution was filtered. Single crystals of the title compound were obtained from the filtrate after 3 d.

Refinement

H atoms on carbon atoms were placed in calculated positions with C—H distances = 0.93 Å (aromatic), and were included in the final cycles of refinement in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of amino groups and coordinated water molecule were located in a difference Fourier map and included in the structure factor calculations in riding mode with $U_{iso}(H) = 1.2U_{eq}(N,O)$. H atoms of lattice water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions, $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

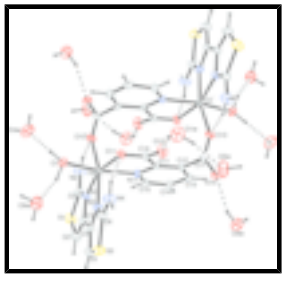


Fig. 1. The molecular structure of the title compound with 30% probability displacement ellipsoids (arbitrary spheres for H atoms), dashed lines showing the hydrogen bonding [symmetry code: (ii) $1-x,2-y,1-z$].

Bis(μ-pyridine-2,3-dicarboxylato)bis[aqua(2,2'-diamino-4,4'-bi-1,3-\ thiazole)cobalt(II)] decahydrate

Crystal data

$[Co_2(C_7H_3NO_4)_2(C_6H_6N_4OS_2)_2(H_2O)_2]\cdot 10H_2O$	$Z = 1$
$M_r = 1060.80$	$F_{000} = 546$
Triclinic, $P\overline{1}$	$D_x = 1.674$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1415$ (12) Å	Cell parameters from 3550 reflections
$b = 11.2685$ (17) Å	$\theta = 2.2$–25.0º
$c = 12.0084$ (18) Å	$\mu = 1.08$ mm^{-1}
$\alpha = 74.269$ (2)º	$T = 295$ (2) K
$\beta = 82.864$ (2)º	Prism, red
$\gamma = 87.713$ (2)º	0.20 × 0.18 × 0.15 mm
$V = 1052.2$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	3653 independent reflections
Radiation source: fine-focus sealed tube	2911 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 25.0$º
$T = 295(2)$ K	$\theta_{min} = 2.2$º
ω scans	$h = -9\rightarrow 9$

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

T_{min} = 0.785, T_{max} = 0.850

5510 measured reflections

k = −12→13

l = −10→14

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.041

$wR(F^2)$ = 0.094

S = 1.06

3653 reflections

280 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.1585P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.35 e Å^{-3}

$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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}
Co	0.60678 (5)	0.75306 (4)	0.67792 (3)	0.02432 (14)
O1	0.8327 (3)	0.7076 (2)	0.74704 (18)	0.0352 (6)
H1A	0.8672	0.7344	0.8051	0.042*
H1B	0.8511	0.6202	0.7539	0.042*
O11	0.7251 (2)	0.84018 (19)	0.51418 (18)	0.0283 (5)
O12	0.6872 (3)	0.9176 (2)	0.32782 (19)	0.0430 (7)
O13	0.4141 (3)	1.10459 (19)	0.23638 (17)	0.0310 (5)
O14	0.3918 (3)	0.9300 (2)	0.18751 (18)	0.0346 (6)
O1W	0.9293 (3)	0.9688 (3)	0.1480 (2)	0.0643 (8)
H1WA	0.8766	0.9545	0.2156	0.096*
H1WB	0.8631	0.9621	0.1036	0.096*
O2W	0.6777 (3)	0.9173 (3)	0.0296 (2)	0.0668 (9)
H2WA	0.6010	0.9136	0.0851	0.100*
H2WB	0.6404	0.9555	−0.0317	0.100*

O3W	0.1478 (3)	0.7661 (3)	0.1589 (2)	0.0578 (8)
H3WA	0.0658	0.8144	0.1503	0.087*
H3WB	0.2164	0.7997	0.1845	0.087*
O4W	0.9238 (4)	0.7896 (3)	0.9211 (2)	0.0692 (9)
H4WA	0.8313	0.8099	0.9535	0.104*
H4WB	0.9765	0.8543	0.8905	0.104*
O5W	0.9981 (3)	0.4713 (3)	0.7438 (2)	0.0580 (8)
H5WA	1.0817	0.4715	0.7758	0.087*
H5WB	0.9498	0.4013	0.7758	0.087*
N1	0.4475 (3)	0.6361 (2)	0.8125 (2)	0.0277 (6)
N2	0.3392 (4)	0.7576 (3)	0.9341 (3)	0.0496 (9)
H2A	0.4010	0.8200	0.8967	0.060*
H2B	0.2718	0.7646	0.9912	0.060*
N3	0.6356 (3)	0.5797 (2)	0.6344 (2)	0.0292 (6)
N4	0.8368 (4)	0.6102 (3)	0.4712 (3)	0.0466 (8)
H4A	0.8628	0.6849	0.4660	0.056*
H4B	0.8918	0.5762	0.4206	0.056*
N11	0.4028 (3)	0.8234 (2)	0.5804 (2)	0.0244 (6)
S1	0.24658 (13)	0.52066 (9)	0.98787 (8)	0.0504 (3)
S2	0.69105 (13)	0.38950 (9)	0.55697 (9)	0.0494 (3)
C1	0.4354 (4)	0.5161 (3)	0.8048 (3)	0.0318 (8)
C2	0.3348 (4)	0.4416 (3)	0.8901 (3)	0.0461 (10)
H2	0.3153	0.3593	0.8958	0.055*
C3	0.3536 (4)	0.6516 (3)	0.9056 (3)	0.0343 (8)
C4	0.5369 (4)	0.4850 (3)	0.7072 (3)	0.0315 (8)
C5	0.5490 (5)	0.3779 (3)	0.6782 (3)	0.0451 (10)
H5	0.4892	0.3073	0.7179	0.054*
C6	0.7259 (4)	0.5416 (3)	0.5516 (3)	0.0347 (8)
C11	0.4513 (4)	0.8779 (3)	0.4665 (2)	0.0219 (7)
C12	0.3387 (4)	0.9247 (3)	0.3874 (3)	0.0225 (7)
C13	0.1700 (4)	0.9115 (3)	0.4278 (3)	0.0287 (7)
H13	0.0912	0.9400	0.3768	0.034*
C14	0.1218 (4)	0.8561 (3)	0.5432 (3)	0.0292 (8)
H14	0.0101	0.8466	0.5715	0.035*
C15	0.2420 (4)	0.8144 (3)	0.6168 (3)	0.0294 (8)
H15	0.2086	0.7785	0.6953	0.035*
C16	0.6369 (4)	0.8799 (3)	0.4317 (3)	0.0251 (7)
C17	0.3888 (4)	0.9916 (3)	0.2608 (3)	0.0267 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0253 (2)	0.0238 (3)	0.0231 (2)	−0.00139 (18)	−0.00092 (17)	−0.00574 (18)
O1	0.0353 (13)	0.0335 (14)	0.0382 (14)	−0.0013 (10)	−0.0107 (10)	−0.0090 (11)
O11	0.0217 (12)	0.0335 (13)	0.0282 (12)	−0.0005 (10)	−0.0003 (9)	−0.0071 (10)
O12	0.0309 (14)	0.0640 (18)	0.0259 (13)	0.0036 (12)	0.0064 (10)	−0.0032 (12)
O13	0.0436 (14)	0.0247 (13)	0.0244 (12)	−0.0022 (10)	−0.0013 (10)	−0.0070 (10)
O14	0.0486 (15)	0.0332 (14)	0.0252 (12)	−0.0035 (11)	−0.0032 (10)	−0.0132 (10)

O1W	0.0445 (17)	0.096 (2)	0.0495 (18)	−0.0068 (16)	0.0110 (13)	−0.0213 (16)
O2W	0.0565 (18)	0.104 (3)	0.0370 (16)	0.0172 (17)	−0.0063 (13)	−0.0152 (16)
O3W	0.0556 (18)	0.068 (2)	0.0555 (18)	0.0012 (15)	−0.0085 (14)	−0.0250 (15)
O4W	0.064 (2)	0.079 (2)	0.078 (2)	0.0005 (17)	−0.0182 (16)	−0.0410 (18)
O5W	0.0528 (18)	0.070 (2)	0.0552 (18)	0.0086 (15)	−0.0105 (14)	−0.0224 (15)
N1	0.0281 (15)	0.0266 (15)	0.0251 (15)	0.0004 (12)	−0.0002 (12)	−0.0030 (12)
N2	0.057 (2)	0.045 (2)	0.0430 (19)	−0.0086 (16)	0.0228 (16)	−0.0177 (16)
N3	0.0276 (15)	0.0267 (15)	0.0347 (16)	0.0009 (12)	−0.0036 (12)	−0.0107 (13)
N4	0.050 (2)	0.0421 (19)	0.048 (2)	−0.0006 (15)	0.0140 (16)	−0.0209 (16)
N11	0.0244 (14)	0.0229 (14)	0.0249 (14)	−0.0020 (11)	0.0007 (11)	−0.0057 (11)
S1	0.0504 (6)	0.0504 (6)	0.0390 (6)	−0.0131 (5)	0.0117 (5)	0.0015 (5)
S2	0.0630 (7)	0.0339 (6)	0.0588 (7)	0.0044 (5)	−0.0069 (5)	−0.0261 (5)
C1	0.0314 (19)	0.0279 (19)	0.0337 (19)	−0.0034 (15)	−0.0088 (15)	−0.0013 (15)
C2	0.049 (2)	0.033 (2)	0.051 (2)	−0.0106 (18)	−0.0011 (19)	−0.0032 (18)
C3	0.0319 (19)	0.037 (2)	0.0279 (19)	0.0003 (16)	0.0003 (15)	−0.0006 (16)
C4	0.036 (2)	0.0237 (18)	0.036 (2)	0.0004 (15)	−0.0118 (15)	−0.0067 (15)
C5	0.056 (3)	0.028 (2)	0.053 (2)	−0.0035 (18)	−0.0084 (19)	−0.0115 (18)
C6	0.038 (2)	0.030 (2)	0.042 (2)	0.0078 (16)	−0.0081 (16)	−0.0182 (16)
C11	0.0256 (17)	0.0191 (16)	0.0233 (17)	−0.0011 (13)	−0.0037 (13)	−0.0090 (13)
C12	0.0271 (17)	0.0187 (16)	0.0241 (17)	0.0005 (13)	−0.0022 (13)	−0.0103 (13)
C13	0.0276 (18)	0.0292 (19)	0.0326 (19)	0.0040 (14)	−0.0079 (14)	−0.0124 (15)
C14	0.0216 (17)	0.0306 (19)	0.0352 (19)	−0.0021 (14)	0.0032 (14)	−0.0111 (15)
C15	0.0287 (18)	0.0311 (19)	0.0267 (18)	−0.0028 (14)	0.0026 (14)	−0.0073 (14)
C16	0.0267 (17)	0.0217 (17)	0.0282 (19)	−0.0007 (13)	0.0004 (14)	−0.0101 (14)
C17	0.0240 (17)	0.030 (2)	0.0266 (18)	0.0013 (14)	−0.0055 (13)	−0.0071 (15)

Geometric parameters (Å, °)

Co—O1	2.100 (2)	N2—H2B	0.8421
Co—O11	2.077 (2)	N3—C6	1.319 (4)
Co—O13^{i}	2.119 (2)	N3—C4	1.392 (4)
Co—N1	2.119 (2)	N4—C6	1.334 (4)
Co—N3	2.151 (3)	N4—H4A	0.8603
Co—N11	2.152 (3)	N4—H4B	0.8727
O1—H1A	0.9091	N11—C15	1.326 (4)
O1—H1B	0.9730	N11—C11	1.354 (4)
O11—C16	1.268 (4)	S1—C2	1.730 (4)
O12—C16	1.226 (4)	S1—C3	1.735 (3)
O13—C17	1.246 (4)	S2—C5	1.721 (4)
O13—Co^{i}	2.119 (2)	S2—C6	1.731 (3)
O14—C17	1.258 (4)	C1—C2	1.344 (4)
O1W—H1WA	0.8476	C1—C4	1.462 (4)
O1W—H1WB	0.8222	C2—H2	0.9300
O2W—H2WA	0.8481	C4—C5	1.342 (5)
O2W—H2WB	0.8324	C5—H5	0.9300
O3W—H3WA	0.8428	C11—C12	1.388 (4)
O3W—H3WB	0.8205	C11—C16	1.517 (4)
O4W—H4WA	0.8557	C12—C13	1.398 (4)
O4W—H4WB	0.8309	C12—C17	1.515 (4)

O5W—H5WA	0.8221	C13—C14	1.371 (4)
O5W—H5WB	0.8637	C13—H13	0.9300
N1—C3	1.322 (4)	C14—C15	1.383 (4)
N1—C1	1.388 (4)	C14—H14	0.9300
N2—C3	1.326 (4)	C15—H15	0.9300
N2—H2A	0.8659		
O11—Co—O1	92.19 (8)	C5—S2—C6	89.78 (17)
O11—Co—O13^{i}	102.79 (8)	C2—C1—N1	115.8 (3)
O1—Co—O13^{i}	86.43 (9)	C2—C1—C4	127.8 (3)
O11—Co—N1	161.66 (10)	N1—C1—C4	116.3 (3)
O1—Co—N1	99.38 (9)	C1—C2—S1	110.3 (3)
O13^{i}—Co—N1	92.16 (9)	C1—C2—H2	124.9
O11—Co—N3	89.33 (9)	S1—C2—H2	124.9
O1—Co—N3	85.08 (9)	N1—C3—N2	123.7 (3)
O13^{i}—Co—N3	165.46 (9)	N1—C3—S1	114.1 (3)
N1—Co—N3	77.62 (10)	N2—C3—S1	122.2 (3)
O11—Co—N11	77.37 (8)	C5—C4—N3	115.4 (3)
O1—Co—N11	169.15 (9)	C5—C4—C1	129.1 (3)
O13^{i}—Co—N11	92.97 (9)	N3—C4—C1	115.5 (3)
N1—Co—N11	91.47 (9)	C4—C5—S2	110.4 (3)
N3—Co—N11	97.56 (10)	C4—C5—H5	124.8
Co—O1—H1A	125.8	S2—C5—H5	124.8
Co—O1—H1B	106.3	N3—C6—N4	124.8 (3)
H1A—O1—H1B	114.7	N3—C6—S2	113.6 (3)
C16—O11—Co	118.08 (19)	N4—C6—S2	121.6 (3)
C17—O13—Co^{i}	138.2 (2)	N11—C11—C12	122.3 (3)
H1WA—O1W—H1WB	107.0	N11—C11—C16	114.9 (3)
H2WA—O2W—H2WB	107.4	C12—C11—C16	122.8 (3)
H3WA—O3W—H3WB	106.3	C11—C12—C13	118.0 (3)
H4WA—O4W—H4WB	107.1	C11—C12—C17	123.6 (3)
H5WA—O5W—H5WB	107.3	C13—C12—C17	118.5 (3)
C3—N1—C1	110.5 (3)	C14—C13—C12	119.5 (3)
C3—N1—Co	133.9 (2)	C14—C13—H13	120.3
C1—N1—Co	115.6 (2)	C12—C13—H13	120.3
C3—N2—H2A	121.2	C13—C14—C15	118.9 (3)
C3—N2—H2B	120.2	C13—C14—H14	120.6
H2A—N2—H2B	118.5	C15—C14—H14	120.6
C6—N3—C4	110.9 (3)	N11—C15—C14	122.9 (3)
C6—N3—Co	134.3 (2)	N11—C15—H15	118.5
C4—N3—Co	114.8 (2)	C14—C15—H15	118.5
C6—N4—H4A	125.9	O12—C16—O11	126.4 (3)
C6—N4—H4B	118.0	O12—C16—C11	117.7 (3)
H4A—N4—H4B	116.0	O11—C16—C11	115.9 (3)
C15—N11—C11	118.4 (3)	O13—C17—O14	124.9 (3)
C15—N11—Co	128.4 (2)	O13—C17—C12	117.7 (3)
C11—N11—Co	113.05 (19)	O14—C17—C12	117.2 (3)
C2—S1—C3	89.32 (17)		

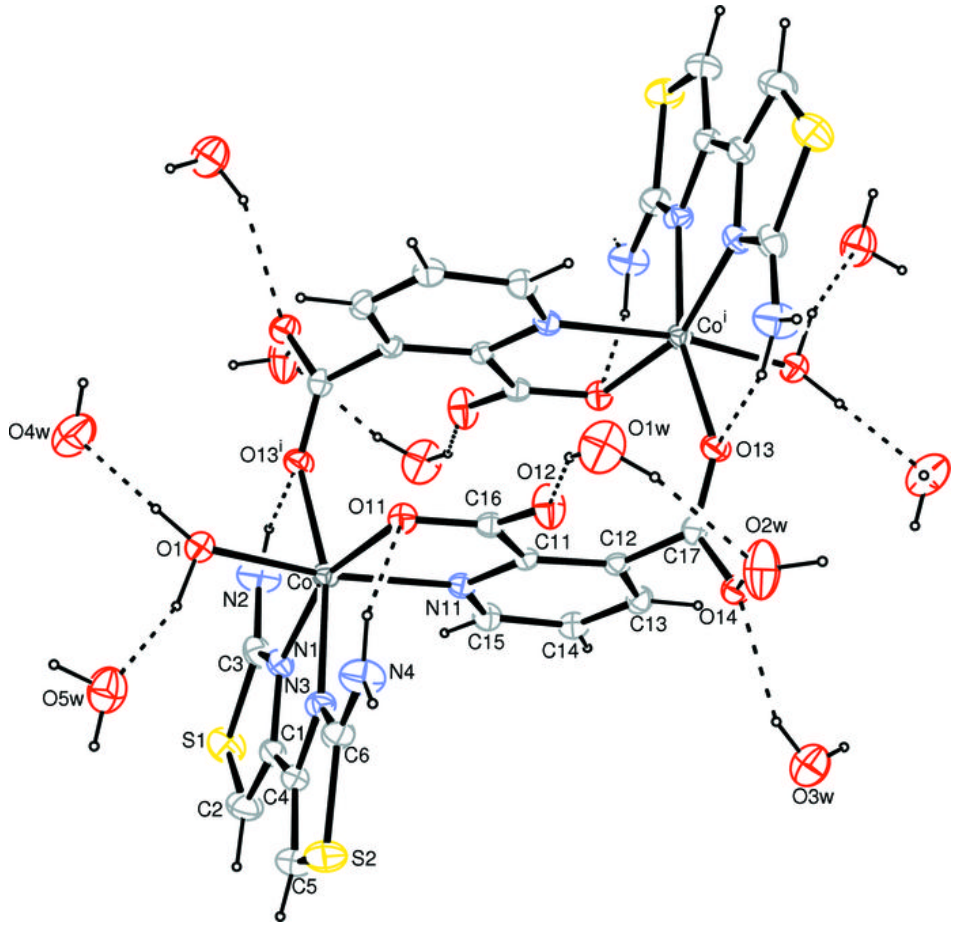
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O4W	0.91	1.79	2.694 (4)	177
O1—H1B···O5W	0.97	2.04	2.943 (4)	153
N2—H2A···O13^{i}	0.87	2.08	2.853 (4)	149
N2—H2B···O3W^{ii}	0.84	2.14	2.968 (4)	167
N4—H4A···O11	0.86	2.21	2.869 (4)	133
N4—H4B···O5W^{iii}	0.87	2.25	3.105 (4)	165
O1W—H1WA···O12	0.85	1.90	2.690 (3)	156
O1W—H1WB···O2W	0.82	1.99	2.796 (4)	166
O2W—H2WA···O14	0.85	2.01	2.839 (3)	167
O2W—H2WB···O14^{iv}	0.83	2.01	2.817 (3)	165
O3W—H3WA···O1W^{v}	0.84	2.02	2.823 (4)	158
O3W—H3WB···O14	0.82	2.10	2.878 (4)	159
O4W—H4WA···O2W^{ii}	0.86	2.01	2.814 (4)	155
O4W—H4WB···O1W^{vi}	0.83	2.08	2.884 (5)	164
O5W—H5WB···O3W^{vii}	0.86	1.99	2.854 (4)	175

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

Fig. 1


Co^{i}
O1w
O13
O12
O13^{i}
O4w
O11
C16
C11
C12
C17
O2w
O1
Co
N2
N11
C13
O14
C15
C14
C3
N1
N4
N3
O5w
S1
C1
C6
C2
C4
S2
C5
O3w