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Aqua(2,2′-diamino-4,4′-bi-1,3-thiazole-κ^2N,N')(pyridine-2,6-dicarboxylato-κ^3O,N,O')cobalt(II) tetrahydrate

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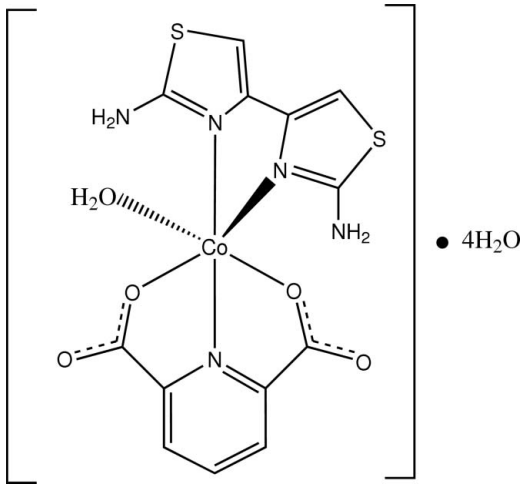
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.112; data-to-parameter ratio = 16.6.

The structure of the title complex, $[Co(C_7H_3NO_4)(C_6H_6N_4S_2)(H_2O)]\cdot 4H_2O$, displays a distorted octahedral coordination geometry around the Co^{II} center, formed by a diaminobithiazole molecule (DABT), one pyridine-2,6-dicarboxylate anion and one water molecule. The pyridine-2,6-dicarboxylate anion chelates the Co^{II} ion with a facial configuration. Within the chelating DABT ligand, the thiazole rings are twisted with respect to each other [dihedral angle 15.10 (5)°]. Uncoordinated water molecules are involved in O—H···O and N—H···O hydrogen bonds, with H···O separations in the range 1.88–2.17 Å, stabilizing the crystal structure.

Related literature

For general background, see Liu *et al.* (2006); For synthesis see Zhang *et al.* (2006). For related structures see: Liu & Xu (2004, 2005); Liu *et al.* (2003, 2005); Sun *et al.* (1997), Ma *et al.* (2002).



Experimental

Crystal data

$[Co(C_7H_3NO_4)(C_6H_6N_4S_2)(H_2O)]\cdot 4H_2O$
M_r = 512.38
Monoclinic, $P2_1/c$
a = 10.0259 (15) Å
b = 7.0956 (11) Å
c = 27.648 (4) Å
β = 93.528 (2)°
V = 1963.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 295 (2) K
0.26 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.76, T_{max} = 0.84
11819 measured reflections
4488 independent reflections
2781 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.112
S = 1.01
4488 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3W	0.81	2.02	2.812 (4)	163
O1—H1B···O22^{i}	0.80	2.01	2.804 (3)	174
O1W—H1WA···O24	0.84	1.88	2.701 (4)	164
O1W—H1WB···O24^{ii}	0.84	2.06	2.883 (4)	167
O2W—H2WA···O4W^{iii}	0.84	1.98	2.816 (4)	171
O2W—H2WB···O22^{i}	0.84	1.88	2.700 (4)	163
O3W—H3WA···O4W	0.81	2.03	2.809 (4)	163
O3W—H3WB···O2W	0.81	2.00	2.784 (4)	165
O4W—H4WA···O1W^{iv}	0.82	1.94	2.760 (4)	173
O4W—H4WB···O2W^{v}	0.84	2.05	2.866 (4)	164
N12—H12B···O3W^{vi}	0.88	2.17	3.047 (4)	173

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

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: BH2116).

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supplementary materials

Acta Cryst. (2007). E**63**, m1964-m1965 [**doi:10.1107/S1600536807029595**]

Aqua(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2N,N')(pyridine-2,6-dicarboxylato-κ^3O,N,O')cobalt(II) tetrahydrate

C.-E. Wei, G.-H. Chen and B.-X. Liu

Comment

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential applications in the field of soft magnetic materials (Sun *et al.*, 1997). As a part of a serial structural investigation of metal complexes with DABT (Liu *et al.*, 2003), 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 has a distorted octahedral coordination geometry formed by one DABT ligand, one pyridine-2,6-dicarboxylate anion and one water molecule. The asymmetric unit is completed with four lattice water molecules.

Thiazole rings of DABT are not coplanar, as observed in other complexes we have reported. The dihedral angle between thiazole rings is 15.10 (5) °, the rings being defined as C11/C12/C13/S11/N11 and C14/C15/C16/S12/N13. This angle is similar to the dihedral angle of 17.23 (7)° found in $[Cr(C_4H_5NO_4)(C_6H_6N_4S_2)(H_2O)]Cl\cdot H_2O$, (Liu & Xu, 2004). Bond lengths C16—N14 [1.335 (4) Å] and C16—N13 [1.324 (4) Å] imply the existence of electron delocalization between thiazole rings and amino groups. This feature for DABT can be found in other DABT complexes based on Mn^{II} (Liu & Xu, 2005) and Co^{II} (Liu, Yu & Xu, 2005) we have reported. Other DABT complexes have been reported (Liu *et al.*, 2006; Zhang *et al.*, 2006).

The tridentate pyridine-2,6-dicarboxylate anion chelates to the Co^{II} ion with a facial configuration (Ma *et al.*, 2002). The maximum deviation from the mean plane defined by C21···C27/N21/O21···O24 is 0.082 (3) Å, for atom N21.

The extensive hydrogen bonding scheme involving lattice water molecules and complex helps to stabilize the crystal structure, as shown in Fig. 1. and Table reporting intermolecular contacts..

Experimental

The complex was prepared following a procedure similar to that previously used for a Ni^{II} compound (Zhang *et al.*, 2006). An aqueous solution (20 ml) containing DABT (1 mmol) and $CoCl_2$ (1 mmol) was mixed with an aqueous solution (10 ml) of pyridine-2,6-dicarboxylic acid (1 mmol) and NaOH (2 mmol). The mixture was refluxed for 5 h. After cooling to room temperature the solution was filtered. Red single crystals of the title complex were obtained from the filtrate after 30 d.

Refinement

C-bonded H atoms were placed in calculated positions, and were included in the refinement in riding mode with C—H distances constrained to 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$(carrier C atom). H atoms of amino groups of DABT were located in a difference map and included in the refinement with fixed positions and isotropic displacement parameters $U_{iso}(H)$ =

0.05 Å^2. Finally, H atoms of water molecules were located in a difference map and included in the refinement as riding with O—H bond lengths constrained to the found distances and U_{iso}(H) = 1.5U_{eq}(carrier O atom).

Figures

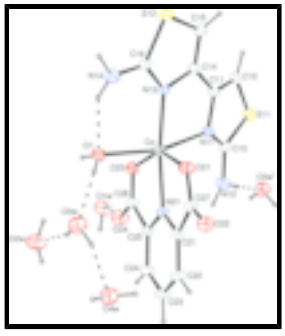


Fig. 1. The molecular structure of the title complex with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines show the hydrogen bonds [symmetry code: (i) $x-1, y, z$].

Aqua(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2*N*,*N*')(pyridine- 2,6-dicarboxylato-κ^3*O*,*N*,*O*')cobalt(II) tetrahydrate

Crystal data

$[Co(C_7H_3NO_4)(C_6H_6N_4S_2)(H_2O)]\cdot 4H_2O$	F_{000} = 1052
M_r = 512.38	D_x = 1.734 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4380 reflections
a = 10.0259 (15) Å	θ = 2.0–27.5º
b = 7.0956 (11) Å	μ = 1.15 mm^{-1}
c = 27.648 (4) Å	T = 295 (2) K
β = 93.528 (2)º	Prism, red
V = 1963.2 (5) Å^3	0.26 × 0.20 × 0.15 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	4488 independent reflections
Radiation source: fine-focus sealed tube	2781 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 2.0º
ω scans	h = −12→13
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −7→9
T_{min} = 0.76, T_{max} = 0.84	l = −34→35
11819 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
4488 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
271 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co	0.70981 (5)	0.52542 (7)	0.673116 (16)	0.02505 (15)
N11	0.5102 (3)	0.5782 (4)	0.69340 (9)	0.0249 (7)
N12	0.3703 (3)	0.5793 (5)	0.62170 (11)	0.0416 (9)
H12A	0.4206	0.5889	0.5964	0.050*
H12B	0.2843	0.5756	0.6136	0.050*
N13	0.7381 (3)	0.5238 (4)	0.74861 (9)	0.0246 (7)
N14	0.9684 (3)	0.4777 (5)	0.76659 (11)	0.0393 (8)
H14A	0.9778	0.4265	0.7394	0.050*
H14B	1.0317	0.4637	0.7900	0.050*
N21	0.7092 (3)	0.6023 (4)	0.60086 (9)	0.0238 (7)
O1	0.9027 (2)	0.3886 (3)	0.66627 (8)	0.0322 (6)
H1A	0.9571	0.4446	0.6511	0.048*
H1B	0.8962	0.2837	0.6563	0.048*
O21	0.8075 (2)	0.8037 (3)	0.67166 (8)	0.0318 (6)
O22	0.8782 (2)	1.0307 (3)	0.62364 (9)	0.0349 (6)
O23	0.6270 (2)	0.2834 (3)	0.63337 (8)	0.0315 (6)
O24	0.5645 (3)	0.1782 (4)	0.55884 (9)	0.0449 (7)
O1W	0.4090 (3)	−0.1295 (4)	0.54364 (10)	0.0501 (8)
H1WA	0.4614	−0.0438	0.5535	0.075*
H1WB	0.4072	−0.1294	0.5134	0.075*
O2W	0.9974 (3)	0.2014 (4)	0.55043 (9)	0.0520 (8)
H2WA	0.9544	0.1987	0.5232	0.078*
H2WB	0.9475	0.1632	0.5717	0.078*
O3W	1.0712 (3)	0.5351 (4)	0.59782 (10)	0.0482 (7)
H3WA	1.0734	0.6325	0.5828	0.072*
H3WB	1.0465	0.4509	0.5799	0.072*
O4W	1.1338 (3)	0.8492 (4)	0.54165 (9)	0.0470 (7)
H4WA	1.2153	0.8601	0.5443	0.070*
H4WB	1.0993	0.9507	0.5499	0.070*
S11	0.26088 (9)	0.55446 (15)	0.70815 (4)	0.0358 (3)

S12	0.80820 (10)	0.54847 (16)	0.83941 (3)	0.0378 (3)
C11	0.4991 (4)	0.5664 (5)	0.74335 (12)	0.0263 (8)
C12	0.3732 (4)	0.5532 (5)	0.75708 (13)	0.0329 (9)
H12	0.3502	0.5446	0.7891	0.039*
C13	0.3914 (4)	0.5722 (5)	0.67035 (13)	0.0293 (8)
C14	0.6233 (3)	0.5582 (5)	0.77352 (12)	0.0268 (8)
C15	0.6420 (4)	0.5770 (5)	0.82163 (13)	0.0332 (9)
H15	0.5748	0.6020	0.8425	0.040*
C16	0.8444 (4)	0.5117 (5)	0.77936 (12)	0.0274 (8)
C21	0.7622 (3)	0.7664 (5)	0.58793 (12)	0.0246 (8)
C22	0.7694 (4)	0.8154 (5)	0.53997 (12)	0.0324 (9)
H22	0.8062	0.9302	0.5315	0.039*
C23	0.7210 (4)	0.6913 (6)	0.50479 (13)	0.0363 (9)
H23	0.7231	0.7225	0.4722	0.044*
C24	0.6693 (4)	0.5201 (5)	0.51834 (13)	0.0332 (9)
H24	0.6381	0.4337	0.4950	0.040*
C25	0.6647 (3)	0.4792 (5)	0.56717 (12)	0.0249 (8)
C26	0.6130 (4)	0.2984 (5)	0.58774 (13)	0.0298 (8)
C27	0.8201 (3)	0.8784 (5)	0.63080 (13)	0.0269 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0258 (3)	0.0284 (3)	0.0209 (3)	−0.0019 (2)	0.00102 (19)	0.0000 (2)
N11	0.0250 (17)	0.0282 (18)	0.0219 (15)	−0.0007 (12)	0.0037 (12)	0.0019 (13)
N12	0.0281 (18)	0.069 (3)	0.0275 (17)	0.0025 (16)	−0.0039 (14)	−0.0014 (17)
N13	0.0236 (16)	0.0279 (17)	0.0222 (15)	−0.0020 (13)	0.0008 (12)	0.0033 (13)
N14	0.0272 (18)	0.063 (2)	0.0273 (17)	0.0008 (16)	−0.0065 (13)	−0.0040 (16)
N21	0.0253 (16)	0.0238 (17)	0.0221 (15)	−0.0044 (12)	−0.0006 (12)	−0.0020 (13)
O1	0.0344 (15)	0.0291 (15)	0.0330 (14)	0.0013 (11)	0.0023 (11)	−0.0048 (12)
O21	0.0390 (16)	0.0353 (16)	0.0209 (13)	−0.0092 (12)	−0.0005 (11)	−0.0014 (12)
O22	0.0403 (16)	0.0300 (15)	0.0341 (15)	−0.0124 (12)	0.0012 (12)	−0.0024 (12)
O23	0.0394 (16)	0.0256 (14)	0.0295 (14)	−0.0043 (11)	0.0039 (11)	0.0027 (12)
O24	0.0606 (19)	0.0334 (16)	0.0397 (16)	−0.0197 (14)	−0.0044 (14)	−0.0087 (14)
O1W	0.062 (2)	0.0436 (18)	0.0450 (17)	−0.0232 (15)	0.0053 (14)	−0.0062 (15)
O2W	0.058 (2)	0.060 (2)	0.0384 (16)	−0.0206 (16)	0.0055 (14)	−0.0009 (15)
O3W	0.0499 (18)	0.0456 (18)	0.0491 (18)	−0.0084 (14)	0.0023 (14)	0.0041 (15)
O4W	0.0489 (18)	0.0468 (18)	0.0451 (17)	−0.0039 (14)	0.0018 (14)	0.0022 (14)
S11	0.0258 (5)	0.0401 (6)	0.0420 (6)	−0.0004 (4)	0.0045 (4)	−0.0018 (5)
S12	0.0423 (6)	0.0492 (7)	0.0214 (5)	−0.0010 (5)	−0.0027 (4)	−0.0007 (5)
C11	0.032 (2)	0.0211 (19)	0.0265 (19)	−0.0015 (15)	0.0054 (15)	0.0001 (15)
C12	0.032 (2)	0.037 (2)	0.030 (2)	0.0015 (17)	0.0068 (16)	0.0007 (18)
C13	0.028 (2)	0.033 (2)	0.027 (2)	0.0002 (16)	0.0000 (16)	−0.0020 (17)
C14	0.031 (2)	0.025 (2)	0.0254 (19)	−0.0041 (16)	0.0038 (15)	0.0015 (16)
C15	0.033 (2)	0.040 (2)	0.027 (2)	0.0002 (17)	0.0027 (16)	−0.0010 (18)
C16	0.031 (2)	0.027 (2)	0.0235 (18)	−0.0018 (16)	−0.0027 (15)	0.0025 (16)
C21	0.0219 (18)	0.024 (2)	0.0277 (19)	−0.0013 (15)	0.0001 (15)	−0.0019 (16)
C22	0.040 (2)	0.029 (2)	0.028 (2)	−0.0080 (17)	−0.0019 (17)	0.0065 (17)

C23	0.049 (3)	0.041 (2)	0.0189 (19)	−0.0058 (19)	−0.0007 (17)	0.0024 (18)
C24	0.043 (2)	0.033 (2)	0.0228 (19)	−0.0084 (18)	0.0011 (16)	−0.0070 (17)
C25	0.0285 (19)	0.0220 (19)	0.0237 (18)	−0.0005 (15)	−0.0006 (14)	−0.0003 (15)
C26	0.029 (2)	0.031 (2)	0.029 (2)	−0.0037 (16)	0.0025 (16)	0.0000 (17)
C27	0.025 (2)	0.026 (2)	0.029 (2)	−0.0039 (15)	0.0016 (15)	−0.0050 (17)

Geometric parameters (Å, °)

Co—N21	2.070 (3)	O1W—H1WB	0.8346
Co—N13	2.089 (3)	O2W—H2WA	0.8437
Co—N11	2.144 (3)	O2W—H2WB	0.8397
Co—O23	2.176 (2)	O3W—H3WA	0.8077
Co—O1	2.182 (2)	O3W—H3WB	0.8042
Co—O21	2.206 (2)	O4W—H4WA	0.8198
N11—C13	1.316 (4)	O4W—H4WB	0.8369
N11—C11	1.395 (4)	S11—C12	1.706 (4)
N12—C13	1.350 (4)	S11—C13	1.729 (4)
N12—H12A	0.8902	S12—C15	1.720 (4)
N12—H12B	0.8774	S12—C16	1.741 (3)
N13—C16	1.324 (4)	C11—C12	1.344 (5)
N13—C14	1.399 (4)	C11—C14	1.457 (5)
N14—C16	1.335 (4)	C12—H12	0.9300
N14—H14A	0.8454	C14—C15	1.338 (5)
N14—H14B	0.8832	C15—H15	0.9300
N21—C25	1.334 (4)	C21—C22	1.377 (4)
N21—C21	1.338 (4)	C21—C27	1.513 (4)
O1—H1A	0.8126	C22—C23	1.379 (5)
O1—H1B	0.7954	C22—H22	0.9300
O21—C27	1.261 (4)	C23—C24	1.381 (5)
O22—C27	1.250 (4)	C23—H23	0.9300
O23—C26	1.265 (4)	C24—C25	1.385 (5)
O24—C26	1.247 (4)	C24—H24	0.9300
O1W—H1WA	0.8383	C25—C26	1.508 (5)
N21—Co—N13	163.25 (11)	C15—S12—C16	90.01 (17)
N21—Co—N11	105.01 (11)	C12—C11—N11	114.7 (3)
N13—Co—N11	79.13 (10)	C12—C11—C14	128.3 (3)
N21—Co—O23	75.06 (10)	N11—C11—C14	116.8 (3)
N13—Co—O23	121.63 (10)	C11—C12—S11	111.2 (3)
N11—Co—O23	86.38 (10)	C11—C12—H12	124.4
N21—Co—O1	89.05 (10)	S11—C12—H12	124.4
N13—Co—O1	91.00 (10)	N11—C13—N12	124.3 (3)
N11—Co—O1	161.20 (10)	N11—C13—S11	113.9 (3)
O23—Co—O1	85.27 (9)	N12—C13—S11	121.8 (3)
N21—Co—O21	73.83 (10)	C15—C14—N13	116.0 (3)
N13—Co—O21	89.42 (10)	C15—C14—C11	128.9 (3)
N11—Co—O21	105.71 (10)	N13—C14—C11	115.2 (3)
O23—Co—O21	148.60 (9)	C14—C15—S12	110.2 (3)
O1—Co—O21	90.00 (9)	C14—C15—H15	124.9
C13—N11—C11	110.6 (3)	S12—C15—H15	124.9

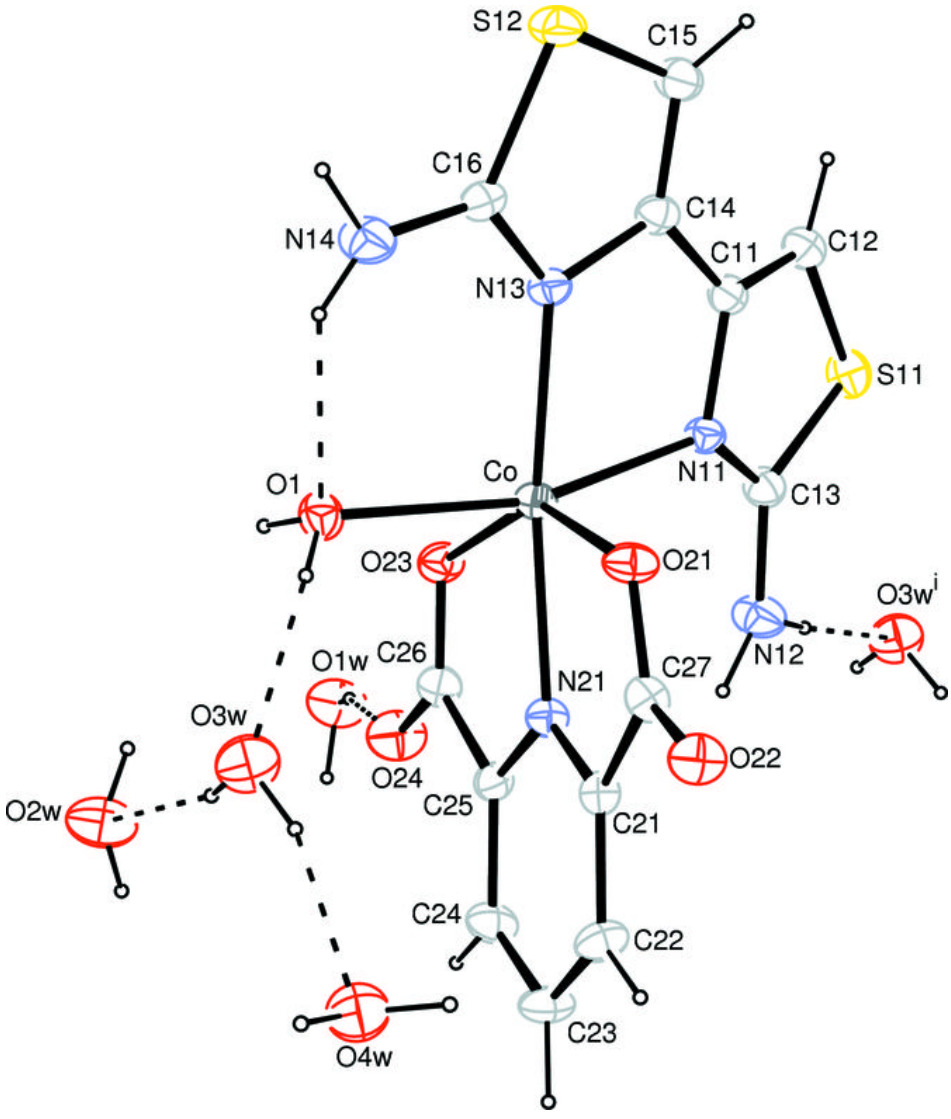
C13—N11—Co	134.3 (2)	N13—C16—N14	124.6 (3)
C11—N11—Co	112.4 (2)	N13—C16—S12	113.3 (3)
C13—N12—H12A	136.5	N14—C16—S12	122.1 (3)
C13—N12—H12B	110.3	N21—C21—C22	121.5 (3)
H12A—N12—H12B	113.3	N21—C21—C27	112.8 (3)
C16—N13—C14	110.4 (3)	C22—C21—C27	125.6 (3)
C16—N13—Co	134.1 (2)	C21—C22—C23	118.7 (3)
C14—N13—Co	115.2 (2)	C21—C22—H22	120.6
C16—N14—H14A	118.0	C23—C22—H22	120.6
C16—N14—H14B	117.7	C22—C23—C24	119.5 (3)
H14A—N14—H14B	119.3	C22—C23—H23	120.3
C25—N21—C21	120.3 (3)	C24—C23—H23	120.3
C25—N21—Co	118.8 (2)	C23—C24—C25	119.0 (3)
C21—N21—Co	120.6 (2)	C23—C24—H24	120.5
Co—O1—H1A	117.0	C25—C24—H24	120.5
Co—O1—H1B	113.1	N21—C25—C24	120.9 (3)
H1A—O1—H1B	108.7	N21—C25—C26	113.7 (3)
C27—O21—Co	117.5 (2)	C24—C25—C26	125.4 (3)
C26—O23—Co	116.9 (2)	O24—C26—O23	126.6 (3)
H1WA—O1W—H1WB	107.5	O24—C26—C25	118.0 (3)
H2WA—O2W—H2WB	108.8	O23—C26—C25	115.3 (3)
H3WA—O3W—H3WB	109.6	O22—C27—O21	125.4 (3)
H4WA—O4W—H4WB	108.7	O22—C27—C21	119.4 (3)
C12—S11—C13	89.57 (17)	O21—C27—C21	115.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O3W	0.81	2.02	2.812 (4)	163
O1—H1B···O22^{i}	0.80	2.01	2.804 (3)	174
O1W—H1WA···O24	0.84	1.88	2.701 (4)	164
O1W—H1WB···O24^{ii}	0.84	2.06	2.883 (4)	167
O2W—H2WA···O4W^{iii}	0.84	1.98	2.816 (4)	171
O2W—H2WB···O22^{i}	0.84	1.88	2.700 (4)	163
O3W—H3WA···O4W	0.81	2.03	2.809 (4)	163
O3W—H3WB···O2W	0.81	2.00	2.784 (4)	165
O4W—H4WA···O1W^{iv}	0.82	1.94	2.760 (4)	173
O4W—H4WB···O2W^{v}	0.84	2.05	2.866 (4)	164
N12—H12A···O1W^{v}	0.89	2.47	3.030 (4)	121
N12—H12B···O3W^{vi}	0.88	2.17	3.047 (4)	173
N14—H14A···O1	0.85	2.13	2.881 (4)	148
N14—H14B···O21^{vii}	0.88	2.19	3.003 (4)	152
N14—H14B···O22^{vii}	0.88	2.55	3.338 (4)	150

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

Fig. 1


S12
C15
C16
C14
N14
C11
C12
N13
S11
N11
Co
C13
O1
O23
O21
O3w^{i}
O1w
C26
N21
C27
N12
O3w
O24
O22
O2w
C25
C21
C24
C22
C23
O4w