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A compressed octahedral cobalt(II) complex in the crystal structure of diaqua[6,6′-sulfanediylbis(2,2′-bipyridine)]cobalt(II) dinitrate

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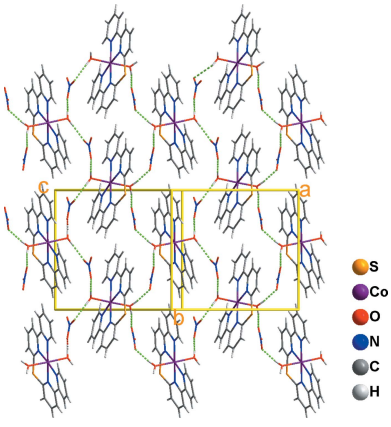
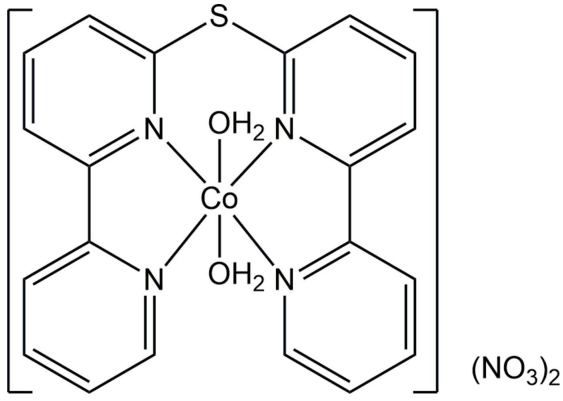
The asymmetric unit of the title salt, $[Co(C_{20}H_{14}N_4S)(H_2O)_2](NO_3)_2$, comprises a $[Co(C_{20}H_{14}N_4S)(H_2O)_2]^{2+}$ cation and two NO_3^- anions. In the complex, $[Co(C_{20}H_{14}N_4S)(H_2O)_2]^{2+}$ cation, the tetradentate 6,6′-sulfanediylbis(2,2′-bipyridine) ligand coordinates to the Co^{II} cation in the equatorial positions, while two water molecules occupy the axial positions, forming a compressed octahedral CoN_4O_2 coordination sphere. The NO_3^- anions are linked to the $[Co(C_{20}H_{14}N_4S)(H_2O)_2]^{2+}$ cations *via* O—H···O hydrogen bonds, yielding a layered arrangement parallel to (001).

1. Chemical context

The control of the molecular structure of coordination compounds is an important task in crystal engineering. It is well known that organic ligands play a significant role in determining the crystal structure of coordination complexes. For example, bidentate 2,2′-bipyridine or its derivatives are common ligands that can be employed to assemble functional compounds (Zhang *et al.*, 2014; Kamdar *et al.*, 2016; Pal *et al.*, 2014). Linking two 2,2′-bipyridine units through a suitable atom leads to a tetradentate ligand (Knight *et al.*, 2010) and, more importantly, the distance of the two 2,2′-bipyridine moieties can then be controlled by the type and size of the bridging atom. As a consequence, the coordination geometry of the metal cation can be affected.





Recently, we obtained the title salt, $[Co(C_{20}H_{14}N_4S)(H_2O)_2](NO_3)_2$, using a tetradentate ligand in which two 2,2′-bipyridine moieties are linked by a sulfur atom. Herein, we report the crystal structure of this cobalt complex.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*WB*···O7^{i}	0.80 (2)	2.02 (2)	2.766 (3)	155 (2)
O2—H2*WA*···O6	0.84 (2)	1.88 (2)	2.698 (2)	168 (3)
O1—H1*WB*···O5^{ii}	0.83 (2)	1.96 (2)	2.789 (2)	179 (3)
O1—H1*WA*···O3	0.80 (2)	1.89 (2)	2.688 (2)	174 (3)

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

2. Structural commentary

The asymmetric unit of the title salt (Fig. 1) is composed of a $[Co(C_{20}H_{14}N_4S)(H_2O)_2]^{2+}$ cation and two NO_3^- anions. The cobalt(II) atom of the complex $[Co(C_{20}H_{14}N_4S)(H_2O)_2]^{2+}$ cation features a compressed octahedral CoN_4O_2 coordination sphere with the N atoms of the tetradentate ligand in equatorial positions and two water molecules located at the *trans* axial sites. The corresponding Co—O bond lengths are 2.0444 (18) Å and 2.0821 (17) Å, which are obviously shorter than the equatorial Co—N bond lengths [2.1213 (18) −2.1574 (18) Å]. These coordination bond lengths indicate that the Co^{II} cation is in a high-spin state at 123 K, comparable with other high-spin Co^{II} complexes (Li *et al.*, 2016; Knight *et al.*, 2010; Suckert *et al.*, 2017; Zhong *et al.*, 2008; Hathwar *et al.*, 2017). The O—Co—O angle is almost linear at 178.59 (7)°. The four equatorial N atoms and the Co^{II} cation are approximately coplanar, with the largest deviation from the least-squares plane being 0.039 Å for N3.

In a similar Co^{II} complex with the 6,6′-sulfanediylbis(2,2′-bipyridine) ligand replaced by the tetradentate ligand bis(2,2′-bipyrid-6′-yl)ketone (Knight *et al.*, 2010), the Co^{II} cation is slightly convex (0.098 Å) from the plane formed through four coordination N atoms. The Co—O bond lengths of the two axial sites are significantly different at 2.075 (4) Å for that in the convex site and 2.118 (4) Å for that in the concave site. The corresponding O—Co—O bond angle deviates more distinctly from linearity with a value of 172.46 (17)°. The

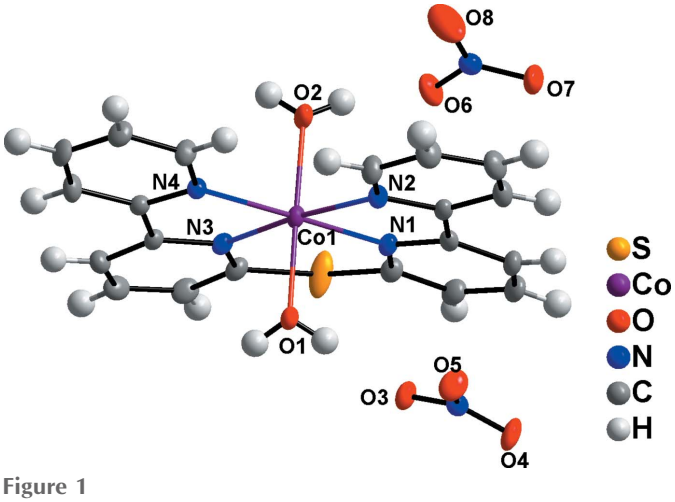


Figure 1
The structures of the molecular entities in the structure of the title salt. Displacement ellipsoids are drawn at the 50% probability level.

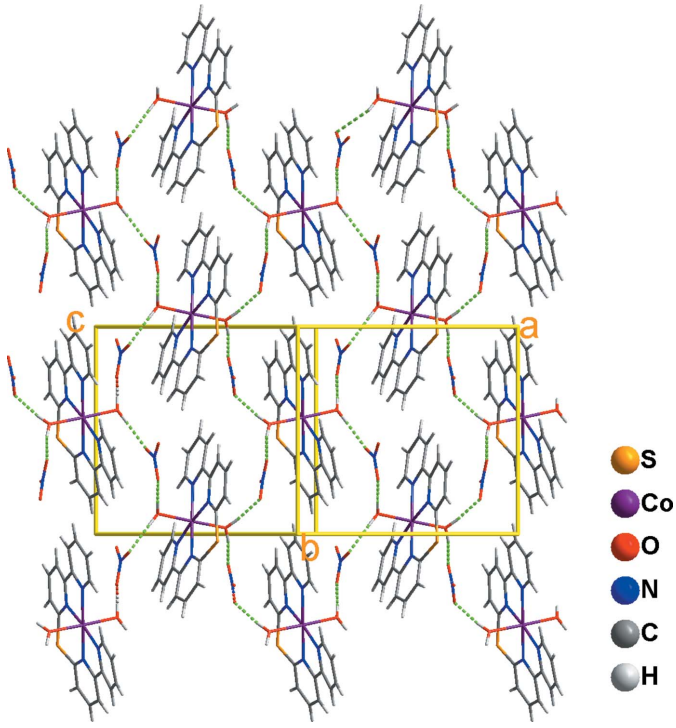


Figure 2
The layer structure in the title salt formed through hydrogen bonds (green dotted lines) between complex cations and nitrate anions.

structural differences between the title complex and the similar reported compound are ascribed to the bridging atom between the two 2,2′-bipyridine moieties, *i.e.* an S atom in the title complex *versus* a C atom of a keto group in the related compound. The bridging bonds [C—S: 1.761 (2) and 1.764 (2) Å] of the title complex are longer than those [C—C: 1.496 (10) and 1.500 (10) Å] in the related complex.

3. Supramolecular features

The coordinating water molecules act as proton donors, forming O—H···O hydrogen bonds with the NO_3^- anions and leading to an extended layer structure parallel to (001) for the title complex (Fig. 2). For these hydrogen bonds, the O···O distances are in the range of 2.688 (2)–2.789 (2) Å, indicating they are of medium strength (Table 1), and are comparable with other hydrogen bonds formed between coordinating water molecules and NO_3^- anions (Kurdziel *et al.*, 2000; Kunz *et al.*, 2007; Wang *et al.*, 2012). There are no intermolecular π–π interactions in the molecular packing of the title complex.

4. Synthesis and crystallization

The ligand 6,6′-sulfanediylbis(2,2′-bipyridine) was synthesized by a method analogous to that for the preparation of 2,2′-sulfanediylbis(1,10-phenanthroline) (Krapcho *et al.*, 2007). The title complex was obtained as follows: An ethanolic solution (10 ml) of $Co^{II}(NO_3)_2{\cdot}6H_2O$ (29.1 mg, 0.1 mmol) was added to a ethanolic solution (10 ml) of 6,6′-sulfane-

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{20}H_{14}N_4S)(H_2O)_2](NO_3)_2$
M_r	561.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	123
a, b, c (Å)	13.412 (3), 11.421 (2), 15.441 (3)
β (°)	110.50 (3)
V (Å^3)	2215.4 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.93
Crystal size (mm)	0.15 × 0.14 × 0.11
Data collection	
Diffractometer	Rigaku Saturn724
Absorption correction	Multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min}, T_{max}	0.893, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17851, 5045, 3984
R_{int}	0.044
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.090, 1.06
No. of reflections	5045
No. of parameters	337
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.42

Computer programs: *CrystalClear* (Rigaku, 2008), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

diylbis(2,2′-bipyridine) (34.4 mg, 0.1 mmol), which afforded a light-yellow solution, which was stored at ambient conditions. Yellow crystals of the title compound were obtained by slow evaporation of the solvent, yield: *ca*. 50%.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms bound to carbon atoms were placed geometrically, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atoms of water molecules were found from difference-Fourier maps and their O—H bond lengths were normalized to 0.82 Å and refined with a common U_{iso}(H) parameter.

Acknowledgements

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Guo-Ling Li and Osamu Sato

Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Diaqua[6,6′-sulfanediylbis(2,2′-bipyridine)]cobalt(II) dinitrate

Crystal data

$[Co(C_{20}H_{14}N_4S)(H_2O)_2](NO_3)_2$
M_r = 561.39
Monoclinic, $P2_1/c$
a = 13.412 (3) Å
b = 11.421 (2) Å
c = 15.441 (3) Å
β = 110.50 (3)°
V = 2215.4 (9) Å^3
Z = 4
$F(000)$ = 1148
D_x = 1.683 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5682 reflections
θ = 3.1–27.5°
μ = 0.93 mm^{-1}
T = 123 K
Block, yellow
0.15 × 0.14 × 0.11 mm

Data collection

Rigaku Saturn724 diffractometer
Radiation source: Rotating Anode
Detector resolution: 28.5714 pixels mm^{-1}
dtprofit.ref scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.893, T_{max} = 1.000
17851 measured reflections
5045 independent reflections
3984 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −17→17
k = −14→10
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.090
S = 1.06
5045 reflections
337 parameters
4 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S2	0.34784 (7)	0.53580 (6)	0.48067 (4)	0.0421 (2)
Co1	0.24302 (2)	0.43855 (2)	0.24018 (2)	0.01606 (9)
O1	0.39231 (13)	0.40239 (14)	0.23348 (10)	0.0187 (3)
O2	0.09507 (14)	0.47032 (15)	0.24506 (13)	0.0285 (4)
O3	0.50179 (13)	0.23807 (13)	0.35394 (10)	0.0236 (4)
O4	0.54960 (14)	0.06402 (14)	0.40822 (11)	0.0300 (4)
O6	0.05056 (14)	0.33139 (14)	0.36815 (11)	0.0292 (4)
O5	0.47102 (14)	0.08860 (15)	0.26072 (10)	0.0297 (4)
O7	0.02144 (15)	0.14605 (15)	0.36918 (13)	0.0393 (5)
O8	−0.06083 (17)	0.2472 (2)	0.24938 (13)	0.0593 (7)
N5	0.50719 (15)	0.12943 (16)	0.34121 (13)	0.0198 (4)
N6	0.00328 (15)	0.24137 (17)	0.32853 (13)	0.0212 (4)
N2	0.19761 (15)	0.26188 (16)	0.19352 (12)	0.0186 (4)
N4	0.20317 (14)	0.55097 (15)	0.12099 (12)	0.0166 (4)
N3	0.29863 (14)	0.60458 (15)	0.29886 (12)	0.0172 (4)
N1	0.28384 (14)	0.34360 (15)	0.36610 (12)	0.0175 (4)
C7	0.18108 (19)	0.0673 (2)	0.24432 (16)	0.0238 (5)
H7A	0.1923	0.0149	0.2929	0.029*
C8	0.1315 (2)	0.0304 (2)	0.15461 (17)	0.0276 (6)
H8A	0.1085	−0.0466	0.1419	0.033*
C6	0.21437 (17)	0.18271 (19)	0.26220 (14)	0.0176 (5)
C4	0.30035 (18)	0.1515 (2)	0.43295 (15)	0.0229 (5)
H4A	0.2909	0.0711	0.4245	0.027*
C10	0.15035 (19)	0.2232 (2)	0.10636 (16)	0.0250 (5)
H10A	0.1398	0.2763	0.0583	0.030*
C9	0.1167 (2)	0.1098 (2)	0.08414 (16)	0.0280 (6)
H9A	0.0846	0.0871	0.0227	0.034*
C5	0.26838 (17)	0.22627 (19)	0.35760 (15)	0.0179 (5)
C2	0.36036 (19)	0.3163 (2)	0.53060 (16)	0.0242 (5)
H2A	0.3905	0.3495	0.5890	0.029*
C1	0.32874 (18)	0.3862 (2)	0.45197 (15)	0.0214 (5)
C3	0.34627 (19)	0.1974 (2)	0.52047 (16)	0.0262 (5)
H3A	0.3674	0.1486	0.5719	0.031*
C14	0.33856 (18)	0.8009 (2)	0.26565 (16)	0.0220 (5)
H14A	0.3370	0.8578	0.2221	0.026*
C16	0.23741 (17)	0.66245 (19)	0.13919 (14)	0.0175 (5)
C19	0.11790 (19)	0.6048 (2)	−0.03804 (15)	0.0236 (5)
H19A	0.0759	0.5828	−0.0977	0.028*
C17	0.21498 (19)	0.7466 (2)	0.07011 (15)	0.0232 (5)

H17A	0.2403	0.8226	0.0844	0.028*
C20	0.14367 (18)	0.5253 (2)	0.03312 (15)	0.0224 (5)
H20A	0.1184	0.4492	0.0197	0.027*
C11	0.34248 (18)	0.63032 (19)	0.38876 (15)	0.0202 (5)
C15	0.29568 (17)	0.69114 (18)	0.23791 (14)	0.0166 (5)
C18	0.15527 (19)	0.7174 (2)	−0.01954 (15)	0.0242 (5)
H18A	0.1405	0.7726	−0.0666	0.029*
C13	0.38377 (18)	0.8247 (2)	0.35920 (16)	0.0249 (5)
H13A	0.4132	0.8979	0.3793	0.030*
C12	0.38477 (19)	0.7396 (2)	0.42191 (16)	0.0240 (5)
H12B	0.4130	0.7544	0.4851	0.029*
H1WA	0.4237 (19)	0.3504 (18)	0.2663 (15)	0.029*
H1WB	0.4339 (18)	0.4572 (18)	0.2351 (17)	0.029*
H2WA	0.072 (2)	0.430 (2)	0.2791 (15)	0.029*
H2WB	0.0665 (19)	0.5317 (17)	0.2273 (17)	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S2	0.0871 (6)	0.0210 (3)	0.0148 (3)	0.0028 (4)	0.0135 (3)	−0.0002 (3)
Co1	0.02039 (16)	0.01296 (16)	0.01403 (17)	0.00085 (12)	0.00502 (12)	0.00167 (12)
O1	0.0214 (9)	0.0152 (8)	0.0188 (8)	0.0018 (7)	0.0061 (7)	0.0044 (6)
O2	0.0270 (10)	0.0227 (10)	0.0398 (11)	0.0072 (8)	0.0165 (8)	0.0158 (8)
O3	0.0325 (10)	0.0146 (8)	0.0223 (9)	0.0043 (7)	0.0077 (7)	0.0010 (7)
O4	0.0419 (11)	0.0178 (9)	0.0241 (9)	0.0056 (8)	0.0038 (8)	0.0073 (7)
O6	0.0407 (11)	0.0191 (9)	0.0325 (9)	−0.0100 (8)	0.0186 (8)	−0.0077 (7)
O5	0.0388 (11)	0.0276 (10)	0.0172 (9)	0.0020 (8)	0.0030 (8)	−0.0066 (7)
O7	0.0359 (11)	0.0206 (9)	0.0598 (12)	0.0024 (8)	0.0148 (9)	0.0163 (9)
O8	0.0515 (14)	0.0879 (18)	0.0237 (11)	−0.0330 (13)	−0.0057 (10)	0.0093 (11)
N5	0.0200 (10)	0.0177 (10)	0.0228 (10)	−0.0004 (8)	0.0087 (8)	−0.0011 (8)
N6	0.0193 (10)	0.0231 (11)	0.0231 (11)	0.0000 (8)	0.0097 (9)	0.0003 (9)
N2	0.0214 (10)	0.0158 (9)	0.0173 (10)	−0.0014 (8)	0.0052 (8)	0.0008 (8)
N4	0.0178 (9)	0.0159 (9)	0.0149 (9)	−0.0006 (8)	0.0041 (7)	0.0011 (7)
N3	0.0192 (9)	0.0161 (9)	0.0150 (9)	0.0023 (8)	0.0045 (8)	−0.0006 (8)
N1	0.0206 (10)	0.0162 (10)	0.0164 (9)	0.0025 (8)	0.0075 (8)	0.0027 (8)
C7	0.0293 (13)	0.0169 (12)	0.0281 (13)	−0.0005 (10)	0.0139 (11)	0.0028 (10)
C8	0.0337 (14)	0.0179 (12)	0.0329 (14)	−0.0062 (11)	0.0138 (11)	−0.0031 (10)
C6	0.0184 (11)	0.0155 (11)	0.0213 (12)	0.0029 (9)	0.0102 (9)	0.0037 (9)
C4	0.0254 (12)	0.0184 (12)	0.0254 (13)	0.0023 (10)	0.0095 (10)	0.0076 (10)
C10	0.0328 (14)	0.0204 (12)	0.0197 (12)	−0.0018 (11)	0.0064 (10)	0.0029 (10)
C9	0.0340 (14)	0.0250 (13)	0.0227 (13)	−0.0054 (11)	0.0071 (11)	−0.0035 (10)
C5	0.0188 (11)	0.0164 (11)	0.0219 (12)	0.0012 (9)	0.0113 (9)	0.0032 (9)
C2	0.0275 (13)	0.0272 (13)	0.0172 (12)	0.0040 (11)	0.0069 (10)	0.0031 (10)
C1	0.0252 (12)	0.0202 (12)	0.0198 (12)	0.0029 (10)	0.0091 (10)	0.0011 (10)
C3	0.0288 (13)	0.0283 (14)	0.0207 (12)	0.0032 (11)	0.0079 (10)	0.0112 (10)
C14	0.0214 (12)	0.0185 (12)	0.0251 (13)	−0.0028 (10)	0.0070 (10)	0.0014 (10)
C16	0.0165 (11)	0.0173 (12)	0.0182 (11)	0.0013 (9)	0.0055 (9)	0.0021 (9)
C19	0.0265 (13)	0.0253 (13)	0.0149 (11)	0.0013 (10)	0.0019 (10)	0.0008 (10)

C17	0.0315 (13)	0.0155 (11)	0.0222 (12)	−0.0021 (10)	0.0089 (10)	0.0022 (9)
C20	0.0271 (13)	0.0169 (12)	0.0187 (12)	−0.0019 (10)	0.0023 (10)	−0.0008 (9)
C11	0.0227 (12)	0.0185 (12)	0.0183 (12)	0.0050 (10)	0.0057 (9)	0.0006 (9)
C15	0.0176 (11)	0.0145 (11)	0.0174 (11)	0.0024 (9)	0.0059 (9)	0.0017 (9)
C18	0.0296 (13)	0.0239 (13)	0.0172 (12)	0.0022 (10)	0.0059 (10)	0.0091 (10)
C13	0.0235 (12)	0.0196 (12)	0.0284 (13)	−0.0027 (10)	0.0051 (10)	−0.0065 (10)
C12	0.0264 (13)	0.0244 (13)	0.0172 (12)	0.0011 (10)	0.0027 (10)	−0.0068 (10)

Geometric parameters (Å, º)

S2—C1	1.761 (2)	N1—C1	1.341 (3)
S2—C11	1.764 (2)	N1—C5	1.355 (3)
Co1—O2	2.0444 (18)	C7—C8	1.376 (3)
Co1—O1	2.0821 (17)	C7—C6	1.388 (3)
Co1—N3	2.1213 (18)	C8—C9	1.376 (3)
Co1—N1	2.1238 (17)	C6—C5	1.481 (3)
Co1—N4	2.1523 (18)	C4—C3	1.377 (3)
Co1—N2	2.1574 (18)	C4—C5	1.384 (3)
O3—N5	1.262 (2)	C10—C9	1.375 (3)
O4—N5	1.241 (2)	C2—C3	1.373 (3)
O6—N6	1.250 (2)	C2—C1	1.390 (3)
O5—N5	1.255 (2)	C14—C15	1.383 (3)
O7—N6	1.238 (2)	C14—C13	1.384 (3)
O8—N6	1.225 (2)	C16—C17	1.388 (3)
N2—C10	1.346 (3)	C16—C15	1.486 (3)
N2—C6	1.351 (3)	C19—C20	1.373 (3)
N4—C20	1.344 (3)	C19—C18	1.373 (3)
N4—C16	1.349 (3)	C17—C18	1.376 (3)
N3—C11	1.337 (3)	C11—C12	1.392 (3)
N3—C15	1.356 (3)	C13—C12	1.369 (3)
C1—S2—C11	115.45 (11)	C5—N1—Co1	115.76 (14)
O2—Co1—O1	178.59 (7)	C8—C7—C6	120.0 (2)
O2—Co1—N3	91.50 (7)	C7—C8—C9	118.6 (2)
O1—Co1—N3	89.90 (7)	N2—C6—C7	121.7 (2)
O2—Co1—N1	89.95 (7)	N2—C6—C5	116.40 (19)
O1—Co1—N1	90.02 (7)	C7—C6—C5	121.9 (2)
N3—Co1—N1	97.24 (7)	C3—C4—C5	119.4 (2)
O2—Co1—N4	88.40 (7)	N2—C10—C9	123.9 (2)
O1—Co1—N4	91.77 (7)	C10—C9—C8	118.7 (2)
N3—Co1—N4	77.10 (7)	N1—C5—C4	122.4 (2)
N1—Co1—N4	174.06 (7)	N1—C5—C6	115.68 (18)
O2—Co1—N2	90.81 (7)	C4—C5—C6	121.9 (2)
O1—Co1—N2	87.81 (7)	C3—C2—C1	118.8 (2)
N3—Co1—N2	174.08 (7)	N1—C1—C2	123.3 (2)
N1—Co1—N2	77.31 (7)	N1—C1—S2	125.20 (17)
N4—Co1—N2	108.41 (7)	C2—C1—S2	111.39 (17)
O4—N5—O5	120.48 (18)	C2—C3—C4	119.0 (2)

O4—N5—O3	119.77 (18)	C15—C14—C13	119.0 (2)
O5—N5—O3	119.74 (18)	N4—C16—C17	121.8 (2)
O8—N6—O7	119.9 (2)	N4—C16—C15	116.12 (18)
O8—N6—O6	120.1 (2)	C17—C16—C15	122.0 (2)
O7—N6—O6	119.96 (19)	C20—C19—C18	118.8 (2)
C10—N2—C6	117.12 (19)	C18—C17—C16	119.9 (2)
C10—N2—Co1	128.32 (15)	N4—C20—C19	123.9 (2)
C6—N2—Co1	114.45 (14)	N3—C11—C12	123.6 (2)
C20—N4—C16	117.03 (18)	N3—C11—S2	125.44 (17)
C20—N4—Co1	127.97 (15)	C12—C11—S2	110.88 (16)
C16—N4—Co1	114.86 (13)	N3—C15—C14	122.5 (2)
C11—N3—C15	117.11 (19)	N3—C15—C16	115.36 (19)
C11—N3—Co1	126.95 (15)	C14—C15—C16	122.0 (2)
C15—N3—Co1	115.77 (14)	C19—C18—C17	118.6 (2)
C1—N1—C5	117.09 (18)	C12—C13—C14	119.4 (2)
C1—N1—Co1	127.03 (15)	C13—C12—C11	118.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*WB*···O7^{i}	0.80 (2)	2.02 (2)	2.766 (3)	155 (2)
O2—H2*WA*···O6	0.84 (2)	1.88 (2)	2.698 (2)	168 (3)
O1—H1*WB*···O5^{ii}	0.83 (2)	1.96 (2)	2.789 (2)	179 (3)
O1—H1*WA*···O3	0.80 (2)	1.89 (2)	2.688 (2)	174 (3)

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