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trans-Diaquabis(pyridin-2-yl thiophen-2-yl ketone-κ^2N,O)cobalt(II) bis(tetrafluoridoborate)

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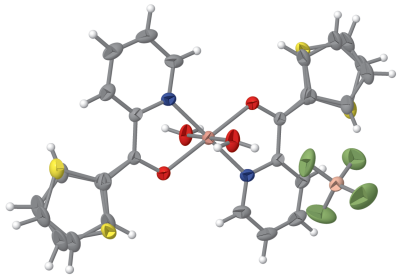
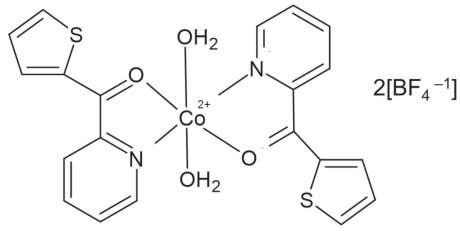
Structural data: full structural data are available from iucrdata.iucr.org

The title salt, $[Co(C_{10}H_7NOS)_2(H_2O)_2](BF_4)_2$, crystallizes in the monoclinic system (space group $P2_1/n$). In the complex cation, the central Co^{II} atom (site symmetry $\overline{1}$) has a pseudo-octahedral coordination environment with bonding to pyridyl N [2.0189 (13) Å] and carbonyl O [2.0869 (11) Å] atoms from the 2-thienyl 2-pyridyl ketone ligands. The remaining bonds are to water molecules [2.0903 (13) Å], which form a hydrogen-bonded extended structure with BF_4^- counter-ions. The thienyl ring shows disorder through an approximate twofold rotation with an occupancy ratio of 0.951 (3):0.049 (3).

3D view



Chemical scheme



Structure description

The complex title salt (Fig. 1) is structurally similar to the previously reported Cu^{II} (Sommerer *et al.*, 1998) and Ni^{II} (Westcott & Nichol, 2026) analogs. The Co^{II} site is located at an inversion center with pseudo-octahedral coordination. The 2-thienyl-2-pyridyl (tpk) ligands coordinate through pyridyl N [2.0189 (13) Å] and carbonyl O [2.0869 (11) Å] atoms in the equatorial plane, and oxygen atoms from water molecules coordinate in the axial positions, leading to an $[O_4N_2]$ coordination set. The Co—O distances with the aqua ligands are significantly shorter than in the Cu^{II} complex [2.0903 (13) Å *versus* 2.409 (3) Å], likely due to the Jahn–Teller distortion seen for octahedral Cu^{II} complexes (Procter *et al.*, 1968).

All other bond lengths and angles are consistent with the previously reported Cu^{II} (Sommerer *et al.*, 1998) and Ni^{II} (Westcott & Nichol, 2026) complexes, and with other Co^{II} complexes with similar ligands, such as di-2-pyridyl ketone (Crundwell *et al.*, 2003) or di-2-pyridyl ketone oxime (Stamou *et al.*, 2025).

The thienyl ring in the title complex is 21.22 (8)° out of the plane defined by the central metal cation and the pyridyl ring, while this value is 19.01 (7)° for the Ni^{II} complex (Westcott & Nichol 2026); however, the rotations are in opposite directions, leading to a difference of ~40° (Fig. 2).

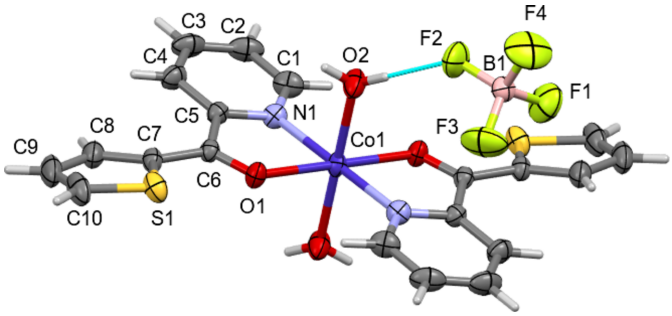


Figure 1
The molecular entities in the crystal structure of the title salt shown with displacement ellipsoids at the 50% probability level. Atoms of the asymmetric unit are labeled and the disordered thienyl ring is shown only for the major component.

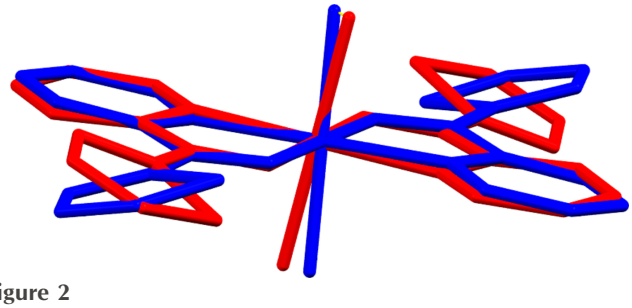


Figure 2
Overlay of the complex cation of the title compound (blue) with the previously reported Ni^{II} complex (red) showing the different orientations of the thienyl moiety.

The BF_4^- anion acts as a hydrogen-bonding acceptor with the coordinating water molecules as donors (Table 1), leading to a hydrogen-bonded layer extending parallel to (10$\bar{1}$), Fig. 3. Additional weak C—H···F interactions between the thiophene moiety and the anion (Table 1) consolidate the packing.

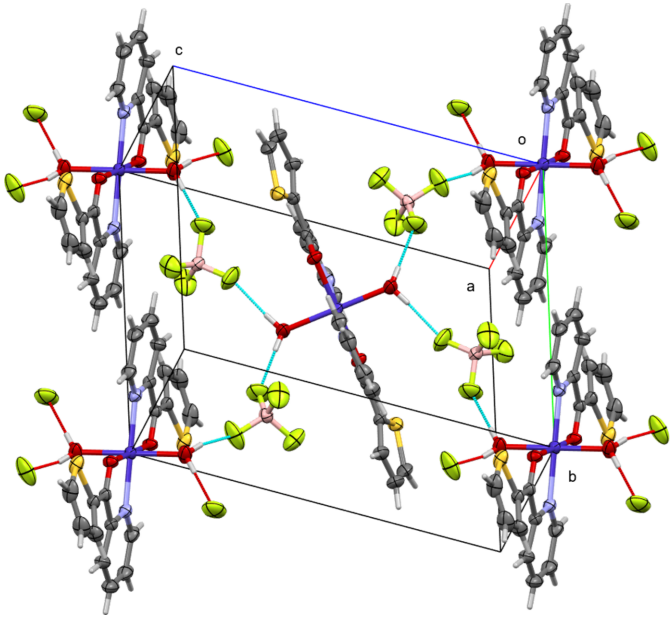


Figure 3
O—H···F hydrogen-bonding interactions (dashed lines) in the title compound showing a layered arrangement parallel to (10$\bar{1}$).

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···F4^{i}	0.81 (1)	1.89 (1)	2.683 (2)	164 (3)
O2—H2B···F2	0.81 (1)	1.86 (1)	2.669 (2)	178 (4)
C2—H2···F1^{ii}	0.95	2.52	3.352 (3)	147
C2—H2···F2^{ii}	0.95	2.55	3.460 (3)	161
C4—H4···F1^{iii}	0.95	2.57	3.207 (3)	124

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{10}H_7NOS)_3(H_2O)_2](BF_4)_2$
M_r	647.03
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	7.2133 (4), 11.9888 (8), 15.2093 (10)
β (°)	103.623 (2)
V (Å^3)	1278.28 (14)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.93
Crystal size (mm)	0.24 × 0.21 × 0.15
Data collection	
Diffractometer	Bruker D8 Quest
Absorption correction	Multi-scan (*TWINABS*; Bruker, 2025)
T_{min}, T_{max}	0.618, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	115558, 4990, 4783
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.099, 1.05
No. of reflections	4990
No. of parameters	231
No. of restraints	168
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.92, −0.58

Computer programs: *APEX6* (Bruker, 2026), *SAINT* (Bruker, 2025), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ShelXle* (Hübschle *et al.*, 2011), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

$Co(BF_4)_2{\cdot}6H_2O$ and acetonitrile were used as received from Thermo-Fisher; 2-thienyl 2-pyridyl ketone (tpk) was used as received from Rieke Metals. The title compound was synthesized following a literature procedure (Sommerer *et al.*, 1998): excess $Co(BF_4)_2{\cdot}6H_2O$ (0.2108 g, 0.620 mmol) was combined with tpk (0.1825 g, 1.00 mmol) in 35 ml of acetonitrile at room temperature affording a dark-red solution, which was allowed to slowly evaporate until production and isolation of dark-orange crystals suitable for X-ray diffraction (30 d).

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. The unit cell metrically fits an orthorhombic *C*-centered cell, and the crystal under investi-

gation was twinned by a 180° rotation around the reciprocal *c* axis. Refinement as a two-component twin with application of the TWIN transformation matrix [$\overline{1}$ 0 0/ 0 $\overline{1}$ 0/ 1 0 1] gave a BASF value of 0.2138 (8).

The thiophene substituent is disordered by an approximate twofold rotation. The two disordered moieties were restrained to have similar geometries using the SAME restraint of *SHELXL* (Sheldrick, 2015*b*). The minor moiety was restrained to be close to planar, and U^{ij} components for disordered atoms closer to each other than 2.0 Å were restrained to be similar (SIMU 0.01 restraint). Subject to these conditions, the occupancy ratio refined to 0.951 (3):0.049 (3). Water H-atom positions were refined and O—H and H···H distances were restrained to 0.84 (2) and 1.37 (2) Å, respectively.

Acknowledgements

This work was supported by a CSU-AAUP grant. All data were collected at Purdue University by Dr Matthias Zeller as part of the American Crystallographic Association Summer Course (2026). Dr Zeller also assisted with the refinement.

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full crystallographic data

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Crystal data

$[Co(C_{10}H_7NOS)_3(H_2O)_2](BF_4)_2$
M_r = 647.03
Monoclinic, $P2_1/n$
a = 7.2133 (4) Å
b = 11.9888 (8) Å
c = 15.2093 (10) Å
β = 103.623 (2)°
V = 1278.28 (14) Å^3
Z = 2
$F(000)$ = 650
D_x = 1.681 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9155 reflections
θ = 2.2–33.1°
μ = 0.93 mm^{-1}
T = 150 K
Block, orange
0.24 × 0.21 × 0.15 mm

Data collection

Bruker D8 Quest diffractometer
Radiation source: fine focus sealed tube X-ray source
Triumph curved graphite crystal monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans
Absorption correction: multi-scan (*TWINABS*; Bruker, 2025)
T_{min} = 0.618, T_{max} = 0.747
115558 measured reflections
4990 independent reflections
4783 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 33.2°, θ_{min} = 2.8°
h = −11→11
k = −18→18
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.099
S = 1.05
4990 reflections
231 parameters
168 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.4235P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 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.

Refinement. The unit cell does metrically fit an orthorhombic C-centered cell and is twinned by this symmetry (180 degree rotation around reciprocal c (0 0 1). Application of the TWIN transformation matrix -1 0 0 0 -1 0 1 0 1 gave a BASF value of 0.2138 (8).
Refined as a 2-component twin.
The thiophene substituent is disordered by an approximate two-fold rotation. The two disordered moieties were restrained to have similar geometries (SAME restraint of ShelXL). The minor moiety was restrained to be close to planar. Uij components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar (SIMU 0.01 restraint). Subject to these conditions the occupancy ratio refined to 0.951 (3) to 0.049 (3).
Water H atom positions were refined and O-H and H···H distances were restrained to 0.84 (2) and 1.37 (2) Angstrom, respectively. Some water H atom positions were further restrained based on hydrogen bonding considerations.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.500000	0.500000	0.500000	0.02485 (7)	
F1	0.2496 (3)	0.09814 (16)	0.40896 (11)	0.0684 (5)	
F2	0.2007 (3)	0.25203 (12)	0.32495 (14)	0.0682 (5)	
F3	0.4698 (2)	0.1494 (2)	0.33606 (13)	0.0761 (6)	
F4	0.1826 (3)	0.08622 (19)	0.25758 (13)	0.0830 (6)	
N1	0.35744 (18)	0.65047 (11)	0.50282 (9)	0.0272 (2)	
C1	0.2108 (3)	0.66595 (17)	0.54098 (12)	0.0357 (3)	
H1	0.172569	0.606240	0.573802	0.043*	
O1	0.63194 (17)	0.60567 (9)	0.42424 (8)	0.0278 (2)	
O2	0.2908 (2)	0.45919 (11)	0.38414 (9)	0.0413 (3)	
H2A	0.279 (5)	0.503 (2)	0.3424 (15)	0.062*	
H2B	0.266 (5)	0.3962 (13)	0.3655 (19)	0.062*	
C2	0.1118 (3)	0.76632 (19)	0.53445 (13)	0.0422 (4)	
H2	0.010753	0.775885	0.564101	0.051*	
C3	0.1625 (3)	0.85102 (18)	0.48457 (14)	0.0434 (4)	
H3	0.096248	0.920120	0.478913	0.052*	
C4	0.3128 (3)	0.83522 (14)	0.44185 (12)	0.0354 (3)	
H4	0.347505	0.892141	0.405316	0.043*	
C5	0.4095 (2)	0.73449 (12)	0.45430 (9)	0.0252 (2)	
C6	0.5748 (2)	0.70440 (11)	0.41513 (9)	0.0238 (2)	
S1	0.81191 (9)	0.72350 (5)	0.30243 (3)	0.03521 (14)	0.951 (3)
C7	0.6698 (3)	0.78152 (15)	0.36741 (12)	0.0267 (3)	0.951 (3)
C8	0.6793 (5)	0.8966 (3)	0.3668 (2)	0.0385 (6)	0.951 (3)
H8	0.613994	0.943791	0.399664	0.046*	0.951 (3)
C9	0.7978 (4)	0.9359 (2)	0.31144 (17)	0.0475 (5)	0.951 (3)
H9	0.819995	1.012702	0.302468	0.057*	0.951 (3)
C10	0.8764 (4)	0.8518 (2)	0.27245 (15)	0.0457 (5)	0.951 (3)
H10	0.958393	0.863475	0.232761	0.055*	0.951 (3)
S1B	0.641 (3)	0.9146 (15)	0.3538 (13)	0.040 (2)	0.049 (3)
C7B	0.662 (5)	0.772 (2)	0.365 (2)	0.036 (3)	0.049 (3)

C8B	0.788 (6)	0.731 (3)	0.316 (3)	0.037 (3)	0.049 (3)
H8B	0.816978	0.653858	0.312593	0.044*	0.049 (3)
C9B	0.867 (6)	0.816 (3)	0.273 (3)	0.041 (3)	0.049 (3)
H9B	0.958416	0.803783	0.238039	0.050*	0.049 (3)
C10B	0.797 (5)	0.918 (3)	0.286 (2)	0.041 (3)	0.049 (3)
H10B	0.831310	0.983895	0.259243	0.049*	0.049 (3)
B1	0.2782 (3)	0.14565 (15)	0.33038 (12)	0.0294 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03299 (13)	0.02138 (11)	0.02170 (11)	−0.00081 (9)	0.00948 (10)	0.00206 (9)
F1	0.0812 (12)	0.0736 (11)	0.0577 (9)	0.0076 (9)	0.0306 (8)	0.0260 (8)
F2	0.0762 (11)	0.0261 (5)	0.0926 (12)	0.0049 (6)	0.0007 (10)	0.0003 (7)
F3	0.0369 (7)	0.1274 (17)	0.0669 (10)	0.0009 (9)	0.0183 (7)	0.0025 (11)
F4	0.0865 (13)	0.0901 (14)	0.0624 (9)	−0.0011 (11)	−0.0025 (9)	−0.0491 (10)
N1	0.0301 (5)	0.0292 (5)	0.0239 (5)	0.0016 (4)	0.0095 (4)	−0.0016 (4)
C1	0.0336 (7)	0.0469 (9)	0.0293 (6)	0.0015 (6)	0.0127 (6)	−0.0051 (6)
O1	0.0345 (5)	0.0221 (4)	0.0295 (5)	0.0034 (4)	0.0131 (4)	0.0039 (3)
O2	0.0612 (8)	0.0278 (5)	0.0286 (5)	−0.0070 (6)	−0.0018 (5)	0.0033 (4)
C2	0.0302 (7)	0.0576 (12)	0.0388 (8)	0.0089 (7)	0.0082 (6)	−0.0153 (8)
C3	0.0336 (7)	0.0439 (9)	0.0490 (10)	0.0135 (7)	0.0022 (7)	−0.0126 (8)
C4	0.0358 (7)	0.0284 (7)	0.0395 (8)	0.0078 (6)	0.0037 (6)	−0.0016 (6)
C5	0.0278 (6)	0.0232 (5)	0.0239 (5)	0.0018 (5)	0.0046 (4)	−0.0017 (4)
C6	0.0284 (6)	0.0221 (5)	0.0207 (5)	−0.0007 (4)	0.0050 (4)	0.0008 (4)
S1	0.0430 (3)	0.0378 (2)	0.0284 (2)	−0.01227 (17)	0.01575 (17)	−0.00512 (16)
C7	0.0345 (7)	0.0227 (6)	0.0224 (6)	−0.0030 (5)	0.0059 (5)	0.0016 (5)
C8	0.0442 (14)	0.0280 (11)	0.0403 (13)	−0.0046 (9)	0.0037 (10)	0.0059 (8)
C9	0.0605 (12)	0.0359 (9)	0.0427 (11)	−0.0152 (9)	0.0054 (10)	0.0131 (8)
C10	0.0578 (12)	0.0489 (12)	0.0317 (8)	−0.0223 (10)	0.0132 (8)	0.0083 (8)
S1B	0.048 (4)	0.032 (4)	0.038 (4)	−0.009 (4)	0.005 (4)	0.002 (4)
C7B	0.043 (5)	0.030 (5)	0.033 (5)	−0.006 (5)	0.006 (5)	−0.002 (5)
C8B	0.046 (5)	0.036 (5)	0.029 (5)	−0.014 (5)	0.010 (5)	0.000 (5)
C9B	0.051 (5)	0.039 (5)	0.033 (5)	−0.014 (5)	0.008 (5)	0.003 (5)
C10B	0.050 (5)	0.036 (5)	0.035 (5)	−0.014 (5)	0.009 (5)	0.008 (5)
B1	0.0329 (7)	0.0273 (7)	0.0283 (7)	−0.0003 (6)	0.0080 (6)	−0.0047 (5)

Geometric parameters (Å, º)

Co1—N1	2.0819 (13)	C4—C5	1.385 (2)
Co1—N1^{i}	2.0819 (13)	C4—H4	0.9500
Co1—O1	2.0869 (11)	C5—C6	1.497 (2)
Co1—O1^{i}	2.0869 (11)	C6—C7B	1.36 (3)
Co1—O2	2.0902 (13)	C6—C7	1.444 (2)
Co1—O2^{i}	2.0903 (13)	S1—C10	1.700 (2)
F1—B1	1.383 (2)	S1—C7	1.729 (2)
F2—B1	1.387 (2)	C7—C8	1.382 (4)
F3—B1	1.365 (2)	C8—C9	1.414 (4)

F4—B1	1.360 (2)	C8—H8	0.9500
N1—C1	1.334 (2)	C9—C10	1.359 (4)
N1—C5	1.3531 (19)	C9—H9	0.9500
C1—C2	1.391 (3)	C10—H10	0.9500
C1—H1	0.9500	S1B—C10B	1.698 (19)
O1—C6	1.2502 (17)	S1B—C7B	1.73 (2)
O2—H2A	0.811 (13)	C7B—C8B	1.39 (2)
O2—H2B	0.812 (13)	C8B—C9B	1.413 (19)
C2—C3	1.368 (3)	C8B—H8B	0.9500
C2—H2	0.9500	C9B—C10B	1.345 (19)
C3—C4	1.402 (3)	C9B—H9B	0.9500
C3—H3	0.9500	C10B—H10B	0.9500

N1—Co1—N1^{i}	180.0	O1—C6—C7B	116.0 (15)
N1—Co1—O1	77.12 (5)	O1—C6—C7	118.63 (14)
N1^{i}—Co1—O1	102.88 (5)	O1—C6—C5	117.16 (12)
N1—Co1—O1^{i}	102.88 (5)	C7B—C6—C5	126.7 (15)
N1^{i}—Co1—O1^{i}	77.12 (5)	C7—C6—C5	124.21 (14)
O1—Co1—O1^{i}	180.0	C10—S1—C7	91.47 (11)
N1—Co1—O2	87.60 (6)	C8—C7—C6	132.3 (2)
N1^{i}—Co1—O2	92.40 (6)	C8—C7—S1	111.14 (19)
O1—Co1—O2	90.53 (5)	C6—C7—S1	116.43 (13)
O1^{i}—Co1—O2	89.48 (5)	C7—C8—C9	112.0 (3)
N1—Co1—O2^{i}	92.40 (6)	C7—C8—H8	124.0
N1^{i}—Co1—O2^{i}	87.60 (6)	C9—C8—H8	124.0
O1—Co1—O2^{i}	89.47 (5)	C10—C9—C8	112.7 (2)
O1^{i}—Co1—O2^{i}	90.52 (5)	C10—C9—H9	123.7
O2—Co1—O2^{i}	180.00 (5)	C8—C9—H9	123.7
C1—N1—C5	118.95 (15)	C9—C10—S1	112.68 (17)
C1—N1—Co1	125.15 (12)	C9—C10—H10	123.7
C5—N1—Co1	115.59 (9)	S1—C10—H10	123.7
N1—C1—C2	122.40 (18)	C10B—S1B—C7B	91.6 (13)
N1—C1—H1	118.8	C6—C7B—C8B	122 (3)
C2—C1—H1	118.8	C6—C7B—S1B	127 (3)
C6—O1—Co1	117.04 (9)	C8B—C7B—S1B	110.4 (17)
Co1—O2—H2A	115 (2)	C7B—C8B—C9B	112 (2)
Co1—O2—H2B	125 (2)	C7B—C8B—H8B	123.8
H2A—O2—H2B	111 (2)	C9B—C8B—H8B	123.8
C3—C2—C1	118.82 (17)	C10B—C9B—C8B	112 (2)
C3—C2—H2	120.6	C10B—C9B—H9B	123.8
C1—C2—H2	120.6	C8B—C9B—H9B	123.8
C2—C3—C4	119.58 (17)	C9B—C10B—S1B	113.2 (18)
C2—C3—H3	120.2	C9B—C10B—H10B	123.4
C4—C3—H3	120.2	S1B—C10B—H10B	123.4
C5—C4—C3	118.29 (18)	F4—B1—F3	112.37 (18)
C5—C4—H4	120.9	F4—B1—F1	109.74 (19)
C3—C4—H4	120.9	F3—B1—F1	108.29 (17)
N1—C5—C4	121.89 (15)	F4—B1—F2	108.26 (18)

N1—C5—C6	112.77 (12)	F3—B1—F2	111.16 (19)
C4—C5—C6	125.32 (14)	F1—B1—F2	106.87 (17)
C5—N1—C1—C2	−1.5 (2)	C5—C6—C7—C8	21.1 (3)
Co1—N1—C1—C2	−174.79 (14)	O1—C6—C7—S1	16.1 (2)
N1—C1—C2—C3	2.2 (3)	C5—C6—C7—S1	−163.28 (11)
C1—C2—C3—C4	−0.4 (3)	C10—S1—C7—C8	−1.8 (2)
C2—C3—C4—C5	−2.1 (3)	C10—S1—C7—C6	−178.32 (15)
C1—N1—C5—C4	−1.1 (2)	C6—C7—C8—C9	177.5 (2)
Co1—N1—C5—C4	172.80 (12)	S1—C7—C8—C9	1.7 (3)
C1—N1—C5—C6	−179.52 (13)	C7—C8—C9—C10	−0.7 (3)
Co1—N1—C5—C6	−5.59 (15)	C8—C9—C10—S1	−0.7 (3)
C3—C4—C5—N1	2.9 (2)	C7—S1—C10—C9	1.4 (2)
C3—C4—C5—C6	−178.94 (15)	O1—C6—C7B—C8B	9.1 (17)
Co1—O1—C6—C7B	−179.8 (12)	C5—C6—C7B—C8B	−166.4 (15)
Co1—O1—C6—C7	176.64 (11)	O1—C6—C7B—S1B	−170.0 (15)
Co1—O1—C6—C5	−3.91 (16)	C5—C6—C7B—S1B	15 (3)
N1—C5—C6—O1	6.33 (18)	C10B—S1B—C7B—C6	179 (2)
C4—C5—C6—O1	−171.99 (15)	C10B—S1B—C7B—C8B	−0.2 (13)
N1—C5—C6—C7B	−178.3 (14)	C6—C7B—C8B—C9B	−178 (3)
C4—C5—C6—C7B	3.4 (14)	S1B—C7B—C8B—C9B	1.4 (18)
N1—C5—C6—C7	−174.25 (14)	C7B—C8B—C9B—C10B	−2 (3)
C4—C5—C6—C7	7.4 (2)	C8B—C9B—C10B—S1B	2 (4)
O1—C6—C7—C8	−159.5 (3)	C7B—S1B—C10B—C9B	−1 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···F4^{ii}	0.81 (1)	1.89 (1)	2.683 (2)	164 (3)
O2—H2*B*···F2	0.81 (1)	1.86 (1)	2.669 (2)	178 (4)
C2—H2···F1^{iii}	0.95	2.52	3.352 (3)	147
C2—H2···F2^{iii}	0.95	2.55	3.460 (3)	161
C4—H4···F1^{iv}	0.95	2.57	3.207 (3)	124

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