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

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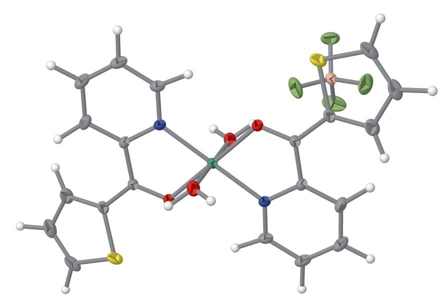
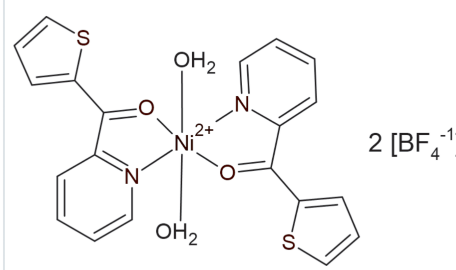
The complex title salt, $[Ni(C_{10}H_7NOS)_2(H_2O)_2](BF_4)_2$, has monoclinic symmetry (space group $P2_1/c$) with the central Ni^{II} atom located at an inversion center. The coordination environment around the Ni^{II} atom is pseudo-octahedral with bonding to pyridyl N [2.0342 (6) Å] and carbonyl O [2.0402 (5) Å] atoms from two chelating 2-thienyl 2-pyridyl ketone ligands. The remaining bonds are to water molecules [2.0989 (7) Å], which are hydrogen-bonded to BF_4^- counter-ions. The crystal structure was refined using nonspherical scattering factors.

3D view



Chemical scheme



Structure description

The ligand di-2-pyridyl ketone (dpk) displays an unusual hydration reaction in the presence of a metal ion allowing this ligand to have three distinct binding sites for metals – the two pyridyl nitrogen atoms and the diol (Efthymiou *et al.*, 2010; Stamatatos & Christou, 2009). Derivatives of dpk, such as di-2-pyridyl ketone oxime (dpko), do not undergo this hydration reaction but can still form multiple binding sites with metals (Stoumpos *et al.*, 2010). The structurally related ligand 2-thienyl-2-pyridyl ketone (tpk) changes the donor of one ring from N to S, which affects the overall electronic and structural capabilities of the compound. To date, only one metal complex with the tpk ligand has been reported (Sommerer *et al.*, 1998). In this complex, only the pyridyl N – not the thienyl S – bonds with the metal ion, and the ketone remains unhydrated despite the presence of water.

The complex title salt (Fig. 1) is structurally and crystallographically similar to the previously reported Cu^{II} analog (Sommerer *et al.*, 1998). The Cu^{II} complex salt was refined in the alternate space group of $P2_1/n$ (*versus* $P2_1/c$) and can be considered as isoconfigurational (Lima de Faria *et al.*, 1990). Both the Ni^{II} atom of the current structure and the Cu^{II} atom from the previous report sit on an inversion center with pseudo-

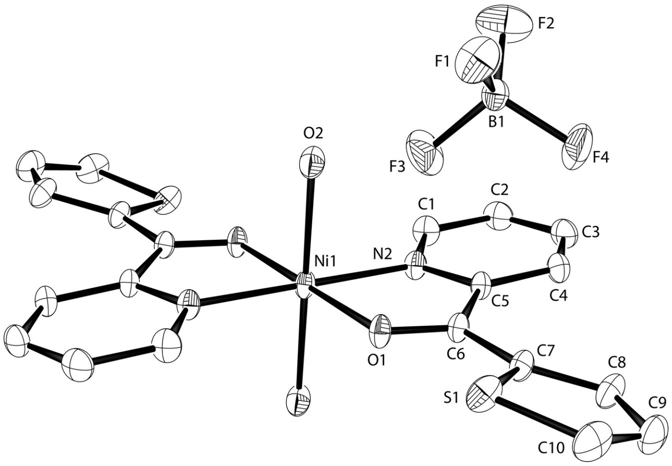


Figure 1
The molecular structures of cation and anion in the complex title salt. Displacement ellipsoids are drawn at the 50% probability level; only atoms of the asymmetric unit are labeled and H atoms omitted for clarity.

octahedral coordination. The tpk ligands coordinate through pyridyl N [2.0342 (6) Å] and carbonyl O [2.0402 (5) Å] atoms in the equatorial plane and through oxygen atoms from water molecules in the axial positions, leading to an $[O_4N_2]$ coordination set. The Ni—O distances with the aqua ligands are significantly shorter than in the Cu^{II} complex [2.0989 (7) 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} complex (Sommerer *et al.*, 1998) and Ni^{II} complexes with similar ligands, such as di-2-pyridyl ketone (Sue-Lein *et al.*, 1986) or di-2-pyridyl ketone oxime (Stamou *et al.*, 2025).

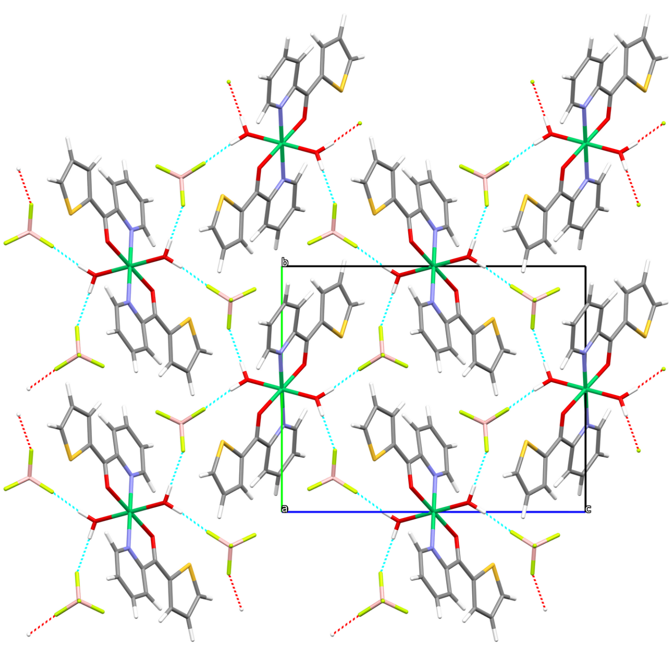


Figure 2
The crystal structure of the complex title salt in a view along the *a* axis. O—H···F hydrogen-bonding is shown by dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*a*···F4^{i}	0.852 (18)	1.862 (18)	2.7091 (10)	172 (2)
O2—H2*b*···F3	0.91 (2)	1.83 (2)	2.7206 (10)	164 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{10}H_7NOS)_2(H_2O)_2](BF_4)_2$
M_r	646.84
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	7.07483 (19), 11.9935 (3), 15.2159 (4)
β (°)	102.760 (3)
V (Å^3)	1259.22 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.03
Crystal size (mm)	0.26 × 0.17 × 0.13 × 0.10 (radius)
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix-Arc 100
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.857, 0.858
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	10509, 10509, 9767
R_{int}	0.048
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.848
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.086, 1.04
No. of reflections	10509
No. of parameters	260
No. of restraints	111
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.02, −0.47

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXS* (Sheldrick, 2008), *OLEX2.refine* (Bourhis *et al.*, 2015), *NoSpherA2* (Kleemiss *et al.*, 2021), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

The BF_4^- anion acts as a hydrogen-bonding acceptor with the coordinating water molecules as donors (Table 1, Fig. 2). These medium–strong O—H···F interactions link adjacent complexes and anions together to form a hydrogen-bonded sheet, which propagates in the *bc* plane.

Synthesis and crystallization

$Ni(BF_4)_2{\cdot}6H_2O$ and acetonitrile were used as received from Thermo-Fisher; 2-thienyl 2-pyridyl ketone was used as received from Rieke Metals. $[Ni(C_{10}H_7NOS)_2(H_2O)_2](BF_4)_2$ was synthesized following a literature procedure (Sommerer *et al.*, 1998): excess $Ni(BF_4)_2{\cdot}6H_2O$ (0.2294 g, 0.675 mmol) was combined with 2-thienyl 2-pyridyl ketone (0.1997 g, 1.10 mmol) in 35 ml of acetonitrile at room temperature affording a dark green solution, which was allowed to slowly evaporate until production and isolation of dark-green crystals suitable for X-ray diffraction (40 d).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal used for data collection was twinned. Non-merohedral twinning was handled with *CrysAlis PRO* (relation between the twin domains by matrix [$\bar{1}$ 0 0 / 0 $\bar{1}$ 0 / 0.9467 0 1]) and refined to a twin scale factor of 0.4990 (6). The crystal structure was refined using nonspherical scattering factors, with all atoms refined anisotropically by using the 'final' default settings of *NoSpherA2* (Kleemiss *et al.*, 2021); *ORCA 5.0* (Neese, 2022) was used for quantum mechanical calculations. The latter programs are implemented in *OLEX2* (Dolomanov *et al.*, 2009). The _olex2_refinement_description section of the CIF gives further details.

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References

Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Efthymiou, C. J., Stamatatos, T. C., Papatriantafyllopoulou, C., Tasiopoulos, A. J., Wernsdorfer, W., Perlepes, S. P. & Christou, G. (2010). *Inorg. Chem.* **49**, 9737–9739.
Kleemiss, F., Dolomanov, O. V., Bodensteiner, M., Peyerimhoff, N., Midgley, L., Bourhis, L. J., Genoni, A., Malaspina, L. A., Jayatilaka, D., Spencer, J. L., White, F., Grundkötter-Stock, B., Steinhauer, S., Lentz, D., Puschmann, H. & Grabowsky, S. (2021). *Chem. Sci.* **12**, 1675–1692.
Lima-de-Faria, J., Hellner, E., Liebau, F., Makovicky, E. & Parthé, E. (1990). *Acta Cryst.* A**46**, 1–11.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Neese, F. (2022). *WIREs Comput. Mol. Sci.* **12**, e1606.
Procter, I. M., Hathaway, B. J. & Nicholls, P. (1968). *J. Chem. Soc. A* pp. 1678–1684.
Rigaku OD (2024). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sommerer, S. O., Friebe, T. L., Jircitano, A. J., MacBeth, C. E. & Abboud, K. A. (1998). *Acta Cryst.* C**54**, 178–179.
Stamatatos, T. C. & Christou, C. (2009). *Inorg. Chem.* **48**, 3308–3322.
Stamou, C., Polyzou, C. D., Lada, Z. G., Konidaris, K. F. & Perlepes, S. P. (2025). *Molecules* **30**, 791–872.
Stoumpos, T. C., Inglis, R., Roubeau, O., Sartzi, H., Kitos, A. A., Milios, C. J., Aromí, G., Tasiopoulos, A. J., Nastopoulos, V., Brechin, E. K. & Perlepes, S. P. (2010). *Inorg. Chem.* **49**, 4388–4390.
Sue-Lein, W., Richardson, J. W., Briggs, S. J., Jacobson, R. A. & Jensen, W. P. (1986). *Inorg. Chim. Acta* **111**, 67–72.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2026). **11**, x260240 [https://doi.org/10.1107/S2414314626002403]

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

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Crystal data

$[Ni(C_{10}H_7NOS)_2(H_2O)_2](BF_4)_2$
M_r = 646.84
Monoclinic, $P2_1/c$
a = 7.07483 (19) Å
b = 11.9935 (3) Å
c = 15.2159 (4) Å
β = 102.760 (3)°
V = 1259.22 (6) Å^3
Z = 2
$F(000)$ = 653.806
D_x = 1.706 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 13596 reflections
θ = 2.2–37.0°
μ = 1.03 mm^{-1}
T = 100 K
Block, dark yellow
0.26 × 0.17 × 0.13 × 0.10 (radius) mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix-Arc 100 diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2024)
T_{min} = 0.857, T_{max} = 0.858
10509 measured reflections
10509 independent reflections
9767 reflections with $I \geq 2u(I)$
R_{int} = 0.048
θ_{max} = 37.1°, θ_{min} = 2.2°
$h = -11 \rightarrow 11$
$k = -20 \rightarrow 20$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.086
S = 1.04
10509 reflections
260 parameters
111 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.1359P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = −0.001
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Refinement. NoSpherA2 refinement, some displacement ellipsoid restraints used. Non-merohedral twinning was handled with CrysAlisPro, twin law [-1 0 0 / 0 -1 0 / 0.9467 0 1] and refined twin scale factor 0.4990 (6).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.0	0.5	0.0	0.01554 (3)
S1	0.51294 (3)	0.714938 (19)	0.195111 (15)	0.02452 (4)
O1	0.20854 (7)	0.60036 (5)	0.07412 (4)	0.01866 (9)
O2	−0.10841 (9)	0.46202 (6)	0.11422 (5)	0.02351 (10)
H2a	−0.122 (3)	0.3961 (16)	0.1328 (14)	0.051 (4)
H2b	−0.062 (3)	0.5008 (14)	0.1661 (14)	0.038 (5)
N2	−0.14605 (7)	0.64682 (5)	−0.00535 (5)	0.01763 (10)
C1	−0.33236 (9)	0.66168 (7)	−0.04418 (6)	0.02221 (13)
H1	−0.407 (2)	0.5867 (17)	−0.0779 (14)	0.051 (5)
C2	−0.42673 (10)	0.76294 (8)	−0.03927 (6)	0.02484 (15)
H2	−0.5776 (18)	0.7711 (16)	−0.0713 (13)	0.040 (4)
C3	−0.32397 (11)	0.84908 (7)	0.01029 (7)	0.02557 (15)
H3	−0.3928 (19)	0.9261 (14)	0.0201 (12)	0.035 (4)
C4	−0.13057 (10)	0.83255 (6)	0.05346 (6)	0.02240 (13)
H4	−0.047 (2)	0.8930 (16)	0.0989 (13)	0.043 (4)
C5	−0.04442 (9)	0.73122 (6)	0.04249 (5)	0.01673 (10)
C6	0.16137 (8)	0.69937 (6)	0.08269 (5)	0.01650 (10)
C7	0.30595 (9)	0.77502 (6)	0.13156 (5)	0.01887 (11)
C8	0.31606 (11)	0.89175 (7)	0.13509 (6)	0.02567 (14)
H8	0.217 (2)	0.9425 (13)	0.1003 (12)	0.059 (5)
C9	0.49357 (14)	0.92843 (9)	0.18999 (8)	0.03150 (18)
H9	0.527 (3)	1.0200 (18)	0.206 (2)	0.080 (9)
C10	0.61176 (13)	0.84113 (9)	0.22691 (7)	0.03060 (17)
H10	0.754 (2)	0.8531 (17)	0.2664 (15)	0.059 (6)
F1	0.16379 (8)	0.59372 (6)	0.40965 (5)	0.03488 (13)
F2	−0.13872 (8)	0.63709 (9)	0.33296 (5)	0.04540 (19)
F3	0.08886 (10)	0.58187 (7)	0.25713 (6)	0.04152 (17)
F4	0.11487 (11)	0.75000 (6)	0.32510 (6)	0.03963 (15)
B1	0.05459 (10)	0.63984 (7)	0.33141 (6)	0.01851 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01687 (5)	0.01203 (5)	0.01510 (6)	0.00016 (3)	−0.00211 (4)	−0.00188 (4)
S1	0.02372 (7)	0.02472 (9)	0.02122 (9)	−0.00632 (5)	−0.00344 (6)	0.00232 (7)
O1	0.01799 (17)	0.0133 (2)	0.0212 (2)	0.00127 (13)	−0.00320 (15)	−0.00312 (18)
O2	0.0323 (2)	0.0169 (3)	0.0205 (3)	−0.00054 (18)	0.0039 (2)	−0.0011 (2)
H2a	0.081 (11)	0.026 (4)	0.040 (8)	−0.014 (3)	0.002 (6)	0.004 (2)
H2b	0.074 (12)	0.017 (7)	0.018 (5)	−0.007 (5)	−0.001 (4)	0.003 (3)
N2	0.01724 (19)	0.0151 (2)	0.0179 (3)	0.00239 (15)	−0.00166 (16)	0.0000 (2)
C1	0.0179 (2)	0.0233 (3)	0.0222 (3)	0.00361 (19)	−0.0023 (2)	0.0012 (3)
H1	0.036 (7)	0.034 (6)	0.071 (14)	0.002 (3)	−0.013 (6)	−0.014 (4)
C2	0.0200 (2)	0.0272 (4)	0.0264 (4)	0.0085 (2)	0.0031 (2)	0.0062 (3)
H2	0.023 (4)	0.043 (8)	0.050 (10)	0.012 (2)	−0.003 (2)	0.002 (5)
C3	0.0258 (3)	0.0207 (3)	0.0317 (4)	0.0097 (2)	0.0094 (3)	0.0045 (3)

H3	0.031 (5)	0.028 (5)	0.044 (9)	0.014 (2)	0.003 (4)	−0.001 (3)
C4	0.0249 (3)	0.0150 (3)	0.0280 (4)	0.0045 (2)	0.0072 (2)	−0.0007 (3)
H4	0.043 (6)	0.024 (7)	0.056 (10)	0.005 (3)	0.001 (4)	−0.016 (4)
C5	0.0192 (2)	0.0119 (2)	0.0180 (3)	0.00215 (16)	0.00177 (18)	−0.0002 (2)
C6	0.0182 (2)	0.0127 (3)	0.0167 (3)	−0.00050 (16)	−0.00035 (18)	−0.0018 (2)
C7	0.0222 (2)	0.0147 (3)	0.0178 (3)	−0.00397 (17)	0.0005 (2)	−0.0022 (2)
C8	0.0301 (3)	0.0187 (3)	0.0265 (4)	−0.0087 (2)	0.0025 (3)	−0.0015 (3)
H8	0.059 (4)	0.030 (4)	0.074 (10)	−0.0002 (16)	−0.018 (3)	0.003 (2)
C9	0.0372 (4)	0.0239 (4)	0.0328 (5)	−0.0133 (3)	0.0064 (3)	−0.0097 (3)
H9	0.062 (8)	0.027 (2)	0.12 (2)	−0.0111 (14)	−0.039 (6)	−0.0161 (16)
C10	0.0308 (3)	0.0348 (5)	0.0225 (4)	−0.0144 (3)	−0.0020 (3)	−0.0054 (3)
H10	0.042 (3)	0.035 (6)	0.080 (13)	−0.0138 (15)	−0.025 (3)	−0.006 (3)
F1	0.0359 (2)	0.0336 (3)	0.0294 (3)	0.0018 (2)	−0.0050 (2)	0.0100 (3)
F2	0.0210 (2)	0.0763 (6)	0.0379 (4)	−0.0031 (2)	0.0043 (2)	0.0044 (4)
F3	0.0493 (3)	0.0429 (4)	0.0327 (3)	−0.0044 (3)	0.0096 (3)	−0.0207 (3)
F4	0.0557 (3)	0.0152 (3)	0.0485 (5)	−0.0017 (2)	0.0129 (3)	0.0015 (3)
B1	0.0191 (2)	0.0171 (3)	0.0180 (3)	−0.00108 (19)	0.0011 (2)	−0.0020 (3)

Geometric parameters (Å, º)

Ni1—O1^{i}	2.0402 (5)	C3—H3	1.070 (15)
Ni1—O1	2.0402 (5)	C3—C4	1.3950 (11)
Ni1—O2^{i}	2.0989 (7)	C4—H4	1.082 (17)
Ni1—O2	2.0989 (7)	C4—C5	1.3861 (10)
Ni1—N2^{i}	2.0342 (6)	C5—C6	1.4987 (9)
Ni1—N2	2.0342 (6)	C6—C7	1.4445 (9)
S1—C7	1.7243 (7)	C7—C8	1.4022 (11)
S1—C10	1.6924 (9)	C8—H8	0.989 (15)
O1—C6	1.2481 (8)	C8—C9	1.4160 (12)
O2—H2a	0.852 (18)	C9—H9	1.14 (2)
O2—H2b	0.91 (2)	C9—C10	1.3797 (16)
N2—C1	1.3321 (8)	C10—H10	1.060 (15)
N2—C5	1.3565 (9)	F1—B1	1.3833 (11)
C1—H1	1.109 (19)	F2—B1	1.3734 (9)
C1—C2	1.3958 (11)	F3—B1	1.3931 (11)
C2—H2	1.075 (13)	F4—B1	1.3982 (11)
C2—C3	1.3865 (14)		
O1^{i}—Ni1—O1	180.0	C4—C3—C2	119.48 (7)
O2—Ni1—O1	91.27 (2)	C4—C3—H3	119.1 (9)
O2—Ni1—O1^{i}	88.73 (2)	H4—C4—C3	123.0 (9)
O2^{i}—Ni1—O1	88.73 (2)	C5—C4—C3	118.66 (8)
O2^{i}—Ni1—O1^{i}	91.27 (2)	C5—C4—H4	118.2 (9)
O2^{i}—Ni1—O2	180.0	C4—C5—N2	121.58 (6)
N2^{i}—Ni1—O1^{i}	79.07 (2)	C6—C5—N2	112.38 (6)
N2^{i}—Ni1—O1	100.93 (2)	C6—C5—C4	125.99 (7)
N2—Ni1—O1	79.07 (2)	C5—C6—O1	117.25 (6)
N2—Ni1—O1^{i}	100.93 (2)	C7—C6—O1	118.43 (6)

N2^{i}—Ni1—O2^{i}	86.89 (3)	C7—C6—C5	124.31 (6)
N2—Ni1—O2	86.89 (3)	C6—C7—S1	116.32 (5)
N2^{i}—Ni1—O2	93.11 (3)	C8—C7—S1	111.46 (5)
N2—Ni1—O2^{i}	93.11 (3)	C8—C7—C6	132.16 (7)
N2^{i}—Ni1—N2	180.0	H8—C8—C7	124.7 (9)
C10—S1—C7	91.87 (4)	C9—C8—C7	111.34 (8)
C6—O1—Ni1	116.21 (4)	C9—C8—H8	123.8 (9)
H2a—O2—Ni1^{i}	124.3 (14)	H9—C9—C8	122.7 (11)
H2b—O2—Ni1^{i}	118.7 (13)	C10—C9—C8	112.53 (8)
H2b—O2—H2a	103.4 (17)	C10—C9—H9	124.6 (12)
C1—N2—Ni1	125.28 (5)	C9—C10—S1	112.79 (6)
C5—N2—Ni1	114.84 (4)	H10—C10—S1	124.3 (12)
C5—N2—C1	119.58 (6)	H10—C10—C9	122.8 (12)
H1—C1—N2	114.8 (9)	F2—B1—F1	110.16 (8)
C2—C1—N2	122.06 (8)	F3—B1—F1	109.54 (7)
C2—C1—H1	123.1 (9)	F3—B1—F2	110.76 (8)
H2—C2—C1	119.6 (10)	F4—B1—F1	108.43 (7)
C3—C2—C1	118.55 (6)	F4—B1—F2	110.11 (8)
C3—C2—H2	121.8 (10)	F4—B1—F3	107.79 (8)
H3—C3—C2	121.3 (8)		

Ni1—O1—C6—C5	3.44 (6)	N2—C5—C6—C7	175.51 (6)
Ni1—O1—C6—C7	−177.61 (5)	C1—N2—C5—C4	1.14 (9)
Ni1—N2—C1—C2	175.01 (7)	C1—N2—C5—C6	179.00 (7)
Ni1—N2—C5—C4	−172.91 (6)	C1—C2—C3—C4	0.11 (10)
Ni1—N2—C5—C6	4.95 (6)	C2—C1—N2—C5	1.63 (10)
S1—C7—C6—O1	−14.34 (7)	C2—C3—C4—C5	2.48 (10)
S1—C7—C6—C5	164.53 (5)	C3—C4—C5—C6	179.26 (7)
S1—C7—C8—C9	−0.05 (7)	C4—C5—C6—C7	−6.74 (10)
S1—C10—C9—C8	0.81 (8)	C5—C6—C7—C8	−18.60 (10)
O1—C6—C5—N2	−5.61 (8)	C6—C7—S1—C10	177.93 (7)
O1—C6—C5—C4	172.14 (7)	C6—C7—C8—C9	−177.03 (10)
O1—C6—C7—C8	162.53 (7)	C7—S1—C10—C9	−0.71 (6)
N2—C1—C2—C3	−2.25 (10)	C7—C8—C9—C10	−0.48 (9)
N2—C5—C4—C3	−3.18 (9)	C8—C7—S1—C10	0.43 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*a*···F4^{ii}	0.852 (18)	1.862 (18)	2.7091 (10)	172 (2)
O2—H2*b*···F3	0.91 (2)	1.83 (2)	2.7206 (10)	164 (2)

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