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

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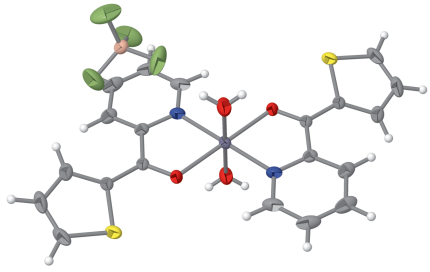
Keywords: crystal structure; zinc; pyridyl ketone; thiophene; isotypism.

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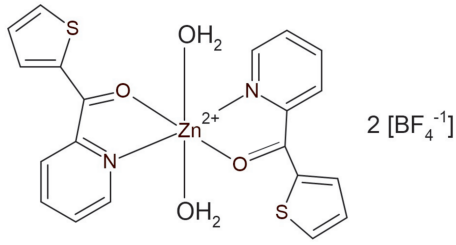
Structural data: full structural data are available from iucrdata.iucr.org

The title salt, $[Zn(C_{10}H_7NOS)_2(H_2O)_2](BF_4)_2$, crystallizes isotypically with the Co^{II} analog in the monoclinic space group $P2_1/n$. In the complex cation, the central Zn^{II} atom (site symmetry $\overline{1}$) has a pseudo-octahedral coordination environment with bonding to pyridyl N [2.0624 (18) Å] and carbonyl O [2.1030 (13) Å] atoms from the 2-thienyl 2-pyridyl ketone ligands. The remaining bonds are to water molecules [2.1598 (16) Å], which form an O—H···F hydrogen-bonded layer with BF_4^- counter-ions.

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. It is isotypic with the Co^{II} complex (Westcott, 2026), but unlike that crystal structure, it has an ordered arrangement of the thiophene units. The title salt also resembles other Zn^{II} complexes with related ligands, such as di-2-pyridyl ketone (Kanaras *et al.*, 2004) and di-2-pyridyl ketone oxime (Westcott *et al.*, 2016).

The zinc atom in the title compound is located at an inversion center with pseudo-octahedral coordination. The 2-thienyl 2-pyridyl ketone (tpk) ligands coordinate through the pyridyl N [2.0624 (18) Å] and carbonyl O [2.1030 (13) Å] atoms in the equatorial plane, and the O atoms from water molecules coordinate in the axial positions, leading to an $[O_4N_2]$ coordination set. The Zn—O distance with the aqua ligands [2.1598 (16) Å] is within the distances seen for the previous three complexes, as are all other bond lengths and angles. The thienyl ring in the title complex is 20.78 (8)° out of the plane defined by the Zn^{II} site and the pyridyl ring, consistent with what is seen for Co^{II} [21.22 (8)°] (Westcott, 2026) and Ni^{II} [19.01 (7)°] (Westcott & Nichol, 2026).

The coordinating water molecules are hydrogen bonded to the BF_4^- anion (Table 1), forming layers extending parallel to $(10\overline{1})$ (Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···F1	0.76	1.97	2.691 (2)	160
O2—H2B···F2^{i}	0.71	2.01	2.709 (2)	171

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Synthesis and crystallization

$Zn(BF_4)_2{\cdot}H_2O$ and acetonitrile were used as received from Thermo Fisher, and di-2-pyridyl ketone (tpk) was used as received from Rieke Metals. The title complex was synthesized following a literature procedure (Sommerer *et al.*, 1998). Excess $Zn(BF_4)_2{\cdot}6H_2O$ (0.2318 g, 0.9019 mmol) was combined with tpk (0.3237 g, 1.711 mmol) in 40 ml of acetonitrile at room temperature, affording a colorless solution, which was allowed to evaporate slowly to facilitate the formation of yellow crystals suitable for X-ray diffraction (18 d).

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. Water H-atom positions were refined maintaining a tetrahedral Zn—O—H angle and allowing O—H distances to obtain the best fit to the observed electron density.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_{10}H_7BF_4NOS)_2(H_2O)_2]$-$(BF_4)_2$
M_r	653.47
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	120
a, b, c (Å)	7.1601 (3), 11.9574 (4), 15.2293 (5)
β (°)	103.519 (2)
V (Å^3)	1267.75 (8)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.73
Crystal size (mm)	0.16 × 0.15 × 0.06
Data collection	
Diffractometer	Bruker Venture
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.632, 0.792
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	50901, 2591, 2426
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.085, 1.05
No. of reflections	2591
No. of parameters	182
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.90, −0.44

Computer programs: *APEX5* (Bruker, 2023), *SAINT* (Bruker, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ShelXle* (Hübschle *et al.*, 2011), *Mercury* (Macrae *et al.*, 2020), and *publCIF* (Westrip, 2010).

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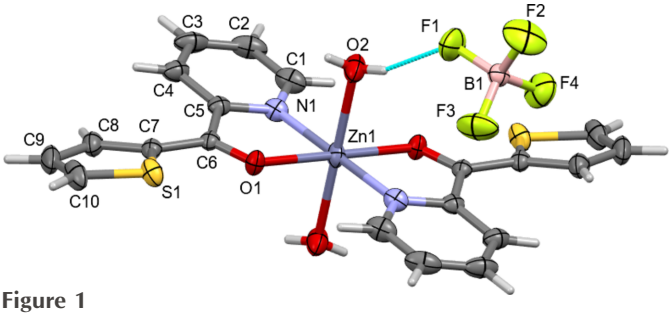


Figure 1
The molecular entities in the asymmetric unit of the title salt shown with displacement ellipsoids at the 50% probability level. O—H···F hydrogen bonding is shown by a dashed line. Atoms of the asymmetric unit are labeled and non-labeled atoms are generated by the symmetry code (−x + 1, −y + 1, −z + 1).

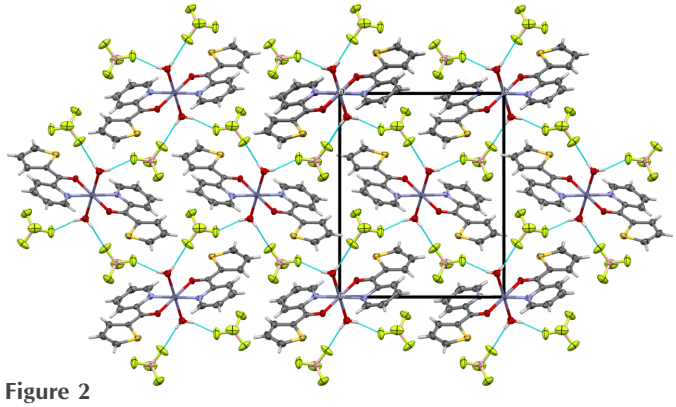


Figure 2
The crystal structure of the title salt viewed along the a-axis direction. O—H···F hydrogen bonding is shown by dashed lines.

full crystallographic data

IUCrData (2026). **11**, x261036 [https://doi.org/10.1107/S2414314626010369]

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Crystal data

$[Zn(C_{10}H_7BF_4NOS)_2(H_2O)_2](BF_4)_2$
M_r = 653.47
Monoclinic, $P2_1/n$
a = 7.1601 (3) Å
b = 11.9574 (4) Å
c = 15.2293 (5) Å
β = 103.519 (2)°
V = 1267.75 (8) Å^3
Z = 2
$F(000)$ = 656
D_x = 1.712 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9706 reflections
θ = 4.8–74.6°
μ = 3.73 mm^{-1}
T = 120 K
Block, colourless
0.16 × 0.15 × 0.06 mm

Data collection

Bruker Venture diffractometer
Radiation source: micro-focus, Incoatec Diamond
HELIOS Multi-layer monochromator
Detector resolution: 7.41 pixels mm^{-1}
combination of ω and φ–scans
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.632, T_{max} = 0.792
50901 measured reflections
2591 independent reflections
2426 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 74.6°, θ_{min} = 4.8°
h = −8→8
k = −14→14
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.085
S = 1.05
2591 reflections
182 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 1.6051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 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}
Zn1	0.500000	0.500000	0.500000	0.02437 (12)
S1	0.18759 (8)	0.72375 (5)	0.69959 (3)	0.03012 (14)
F1	0.8022 (3)	0.24775 (13)	0.67903 (14)	0.0624 (5)
F2	0.8089 (3)	0.07751 (18)	0.73899 (13)	0.0714 (6)
F3	0.5264 (2)	0.15039 (18)	0.66175 (11)	0.0608 (5)
F4	0.7480 (3)	0.09858 (16)	0.58875 (11)	0.0579 (5)
C1	0.7890 (3)	0.6652 (2)	0.45821 (15)	0.0344 (5)
H1	0.826771	0.605726	0.424795	0.041*
O1	0.3691 (2)	0.60322 (11)	0.58006 (9)	0.0244 (3)
O2	0.7274 (3)	0.45695 (15)	0.61534 (11)	0.0389 (4)
H2A	0.725 (2)	0.395 (2)	0.6240 (11)	0.052 (10)*
H2B	0.724 (2)	0.4932 (17)	0.6516 (13)	0.068 (13)*
N1	0.6421 (2)	0.64948 (15)	0.49702 (11)	0.0252 (4)
C2	0.8881 (3)	0.7654 (2)	0.46508 (16)	0.0397 (6)
H2	0.989151	0.775495	0.435059	0.048*
C3	0.8378 (3)	0.8496 (2)	0.51593 (17)	0.0395 (6)
H3	0.904055	0.919023	0.521513	0.047*
C4	0.6892 (3)	0.83319 (19)	0.55943 (15)	0.0310 (5)
H4	0.656277	0.889617	0.597064	0.037*
C5	0.5907 (3)	0.73282 (17)	0.54654 (13)	0.0232 (4)
C6	0.4250 (3)	0.70198 (16)	0.58704 (12)	0.0207 (4)
C7	0.3300 (3)	0.78074 (16)	0.63380 (13)	0.0230 (4)
C8	0.3224 (3)	0.89730 (18)	0.63450 (15)	0.0315 (5)
H8	0.390280	0.944439	0.602466	0.038*
C9	0.2018 (4)	0.9361 (2)	0.68855 (17)	0.0418 (6)
H9	0.178309	1.013201	0.696706	0.050*
C10	0.1221 (4)	0.8528 (2)	0.72797 (15)	0.0400 (6)
H10	0.038714	0.865221	0.767203	0.048*
B1	0.7191 (3)	0.14287 (19)	0.66790 (16)	0.0245 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0334 (2)	0.0206 (2)	0.0211 (2)	0.00279 (15)	0.01042 (15)	−0.00211 (14)
S1	0.0370 (3)	0.0322 (3)	0.0241 (3)	0.0106 (2)	0.0131 (2)	0.00448 (19)
F1	0.0648 (11)	0.0253 (7)	0.0870 (13)	−0.0074 (7)	−0.0029 (9)	−0.0029 (8)
F2	0.0715 (12)	0.0805 (14)	0.0575 (11)	0.0102 (10)	0.0054 (9)	0.0448 (10)
F3	0.0303 (8)	0.1036 (15)	0.0507 (9)	0.0004 (8)	0.0138 (7)	−0.0034 (9)
F4	0.0630 (10)	0.0683 (11)	0.0479 (9)	−0.0027 (9)	0.0242 (8)	−0.0216 (8)
C1	0.0295 (11)	0.0502 (14)	0.0257 (10)	0.0037 (10)	0.0110 (9)	0.0086 (10)
O1	0.0304 (7)	0.0194 (7)	0.0265 (7)	−0.0024 (5)	0.0131 (6)	−0.0030 (5)
O2	0.0571 (11)	0.0268 (9)	0.0273 (8)	0.0076 (8)	−0.0009 (7)	−0.0034 (7)
N1	0.0262 (8)	0.0301 (9)	0.0205 (8)	0.0013 (7)	0.0083 (7)	0.0042 (7)
C2	0.0251 (11)	0.0616 (16)	0.0326 (12)	−0.0038 (11)	0.0071 (9)	0.0184 (11)
C3	0.0273 (11)	0.0456 (14)	0.0408 (13)	−0.0125 (10)	−0.0018 (10)	0.0167 (11)

C4	0.0277 (11)	0.0302 (11)	0.0317 (11)	−0.0055 (9)	0.0004 (8)	0.0057 (9)
C5	0.0237 (9)	0.0245 (10)	0.0199 (9)	−0.0003 (8)	0.0017 (7)	0.0047 (7)
C6	0.0238 (9)	0.0203 (9)	0.0162 (8)	0.0008 (7)	0.0012 (7)	0.0003 (7)
C7	0.0280 (10)	0.0215 (10)	0.0180 (9)	0.0019 (7)	0.0026 (7)	−0.0001 (7)
C8	0.0376 (12)	0.0233 (10)	0.0304 (11)	0.0049 (9)	0.0019 (9)	−0.0013 (8)
C9	0.0525 (15)	0.0299 (12)	0.0383 (13)	0.0132 (11)	0.0013 (11)	−0.0125 (10)
C10	0.0493 (14)	0.0466 (14)	0.0244 (11)	0.0210 (11)	0.0092 (10)	−0.0058 (10)
B1	0.0264 (11)	0.0221 (11)	0.0249 (11)	0.0003 (9)	0.0059 (9)	0.0031 (9)

Geometric parameters (Å, º)

Zn1—N1^{i}	2.0624 (18)	O2—H2B	0.71 (2)
Zn1—N1	2.0624 (18)	N1—C5	1.352 (3)
Zn1—O1^{i}	2.1030 (13)	C2—C3	1.369 (4)
Zn1—O1	2.1030 (13)	C2—H2	0.9500
Zn1—O2	2.1598 (16)	C3—C4	1.392 (3)
Zn1—O2^{i}	2.1598 (16)	C3—H3	0.9500
S1—C10	1.697 (2)	C4—C5	1.383 (3)
S1—C7	1.728 (2)	C4—H4	0.9500
F1—B1	1.381 (3)	C5—C6	1.506 (3)
F2—B1	1.368 (3)	C6—C7	1.443 (3)
F3—B1	1.364 (3)	C7—C8	1.395 (3)
F4—B1	1.376 (3)	C8—C9	1.404 (3)
C1—N1	1.335 (3)	C8—H8	0.9500
C1—C2	1.383 (4)	C9—C10	1.357 (4)
C1—H1	0.9500	C9—H9	0.9500
O1—C6	1.243 (2)	C10—H10	0.9500
O2—H2A	0.76 (2)		
N1^{i}—Zn1—N1	180.0	C2—C3—H3	120.1
N1^{i}—Zn1—O1^{i}	78.06 (6)	C4—C3—H3	120.1
N1—Zn1—O1^{i}	101.94 (6)	C5—C4—C3	118.4 (2)
N1^{i}—Zn1—O1	101.94 (6)	C5—C4—H4	120.8
N1—Zn1—O1	78.06 (6)	C3—C4—H4	120.8
O1^{i}—Zn1—O1	180.00 (6)	N1—C5—C4	121.54 (19)
N1^{i}—Zn1—O2	93.30 (7)	N1—C5—C6	113.04 (17)
N1—Zn1—O2	86.70 (7)	C4—C5—C6	125.39 (19)
O1^{i}—Zn1—O2	88.75 (6)	O1—C6—C7	118.84 (18)
O1—Zn1—O2	91.25 (6)	O1—C6—C5	117.80 (17)
N1^{i}—Zn1—O2^{i}	86.70 (7)	C7—C6—C5	123.35 (17)
N1—Zn1—O2^{i}	93.30 (7)	C8—C7—C6	132.8 (2)
O1^{i}—Zn1—O2^{i}	91.25 (6)	C8—C7—S1	111.11 (16)
O1—Zn1—O2^{i}	88.75 (6)	C6—C7—S1	116.03 (15)
O2—Zn1—O2^{i}	180.0	C7—C8—C9	111.4 (2)
C10—S1—C7	91.42 (12)	C7—C8—H8	124.3
N1—C1—C2	122.1 (2)	C9—C8—H8	124.3
N1—C1—H1	118.9	C10—C9—C8	113.4 (2)
C2—C1—H1	118.9	C10—C9—H9	123.3

C6—O1—Zn1	115.38 (12)	C8—C9—H9	123.3
Zn1—O2—H2A	109.5	C9—C10—S1	112.67 (18)
Zn1—O2—H2B	109.5	C9—C10—H10	123.7
H2A—O2—H2B	117.4	S1—C10—H10	123.7
C1—N1—C5	119.2 (2)	F3—B1—F2	111.9 (2)
C1—N1—Zn1	125.16 (16)	F3—B1—F4	108.78 (19)
C5—N1—Zn1	115.26 (13)	F2—B1—F4	109.5 (2)
C3—C2—C1	118.8 (2)	F3—B1—F1	110.4 (2)
C3—C2—H2	120.6	F2—B1—F1	108.2 (2)
C1—C2—H2	120.6	F4—B1—F1	108.0 (2)
C2—C3—C4	119.8 (2)		

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*···F1	0.76	1.97	2.691 (2)	160
O2—H2*B*···F2^{ii}	0.71	2.01	2.709 (2)	171

Symmetry code: (ii) −*x*+3/2, *y*+1/2, −*z*+3/2.