

Chlorido(4'-chloro-2,2':6',2''-terpyridine- κ^3N,N',N'')(trifluoromethanesulfonato- κO)zinc(II) acetonitrile monosolvate

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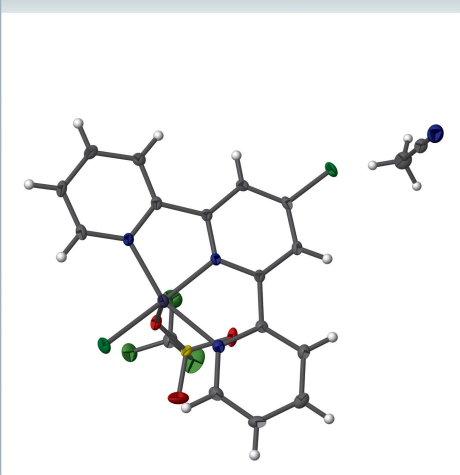
Keywords: crystal structure; zinc atom; chloro-terpyridine ligand; fivefold coordinated; trifluoromethanesulfonate salt.

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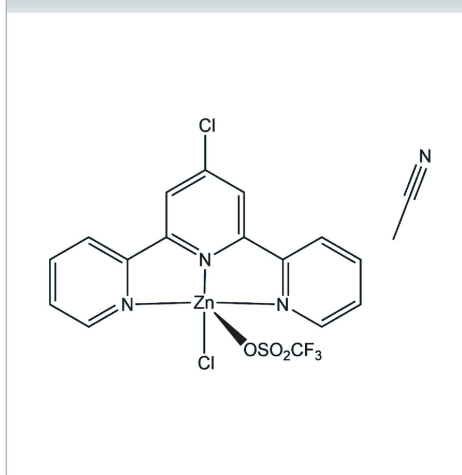
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, $[Zn(CF_3O_3S)Cl(C_{15}H_{10}ClN_3)] \cdot CH_3CN$, the zinc(II) core is fivefold coordinated by one chloride, one trifluoromethanesulfonate O atom and three terpyridine N atoms in a slightly distorted square-pyramidal geometry. The structure provides a distinct example amongst other zinc(II) 4-chloro-terpyridine complexes because of the unusual planarity of the coordinated chloride, the short length of the Zn–N bond opposite to the chloride ligand [1.9572 (15) Å], and the presence of an elongated Zn–O bond [2.3911 (14) Å] in the coordinated trifluoromethanesulfonate ion. A molecule of acetonitrile is also found in the asymmetric unit of the title complex.

3D view



Chemical scheme



Structure description

Substituted terpyridines such as 4'-chloro-2,2':6',2''-terpyridine continue to be recognized as useful chelating ligands for many transition-metal ions, including platinum(II) (Qin *et al.*, 2019), copper(II) (Choroba *et al.*, 2019), cadmium(II) (Li *et al.*, 2020), and zinc(II) (Li *et al.*, 2019). Metal complexes containing zinc(II) and substituted terpyridines as chelating ligand have been shown to have promising antitumor activity (Liang *et al.*, 2019). Our research group interest currently lies in the synthesis of novel terpyridine–metal complexes with potential antitumor activity; as part of our research in this area, herein we describe the synthesis and structure of the title zinc(II) complex.

The asymmetric unit only contains the title compound, with four symmetry-related entities inside each unit cell. The zinc(II) ion shows a distorted square-pyramidal coordination environment defined by a tridentate 4-chloro-terpyridine ligand, a chloride, and an oxygen-coordinated trifluoromethanesulfonate (Fig. 1). The angle N2–Zn1–Cl2

Table 1
Selected geometric parameters (Å, °).

Zn1—Cl2	2.2206 (6)	Zn1—N2	1.9572 (15)
Zn1—O1	2.3911 (14)	Zn1—N1	2.0468 (17)
Zn1—N3	2.0403 (17)		
Cl2—Zn1—O1	98.13 (4)	N1—Zn1—Cl2	99.19 (5)
N2—Zn1—Cl2	168.69 (5)	N1—Zn1—O1	92.17 (6)
N2—Zn1—O1	93.18 (6)	N3—Zn1—Cl2	99.67 (5)
N2—Zn1—N1	79.97 (7)	N3—Zn1—O1	93.68 (6)
N2—Zn1—N3	79.84 (6)	N3—Zn1—N1	159.24 (6)

of 168.69 (5)° is considerably closer to a planar geometry than the reported value (125.6°) in the only comparable zinc(II) 4-chloroterpyridine structure currently available in the CSD (version 5.41 with update August 2020; Groom *et al.*, 2016; refcode HIVPOS; Huang & Qian, 2008). Another remarkable feature of the structure is that while Zn1—N3 and Zn1—N1 bond lengths [2.0403 (17) and 2.0468 (17) Å, respectively] are well within the values observed in others zinc(II) 4-chloro terpyridine complexes (Huang & Qian, 2008; Dutta *et al.*, 2019; You *et al.*, 2009), the Zn1—N2 bond length, across the chloride, is shorter [1.9572 (15) Å] and not comparable. The structure also features a coordinated trifluoromethanesulfonate anion that includes an elongated Zn—O bond of 2.3911 (14) Å (Gosiewska *et al.*, 2006). All relevant bonds and angles are presented in Table 1.

The packing diagram reveals stacking of the asymmetric unit in columns along the *b* axis. These columns form an alternating pattern with the Cl1 atoms facing away from each other while the trifluoromethanesulfonate ions and acetonitrile molecules occupying the space between the stacked zinc(II) 4-chloroterpyridine units. Adjacent columns also alternate directions in the crystal lattice (Fig. 2).

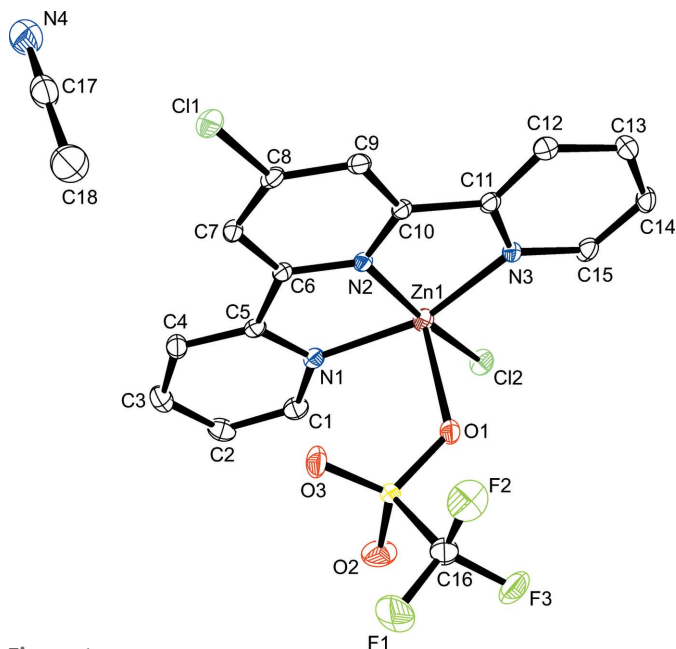


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level; H atoms are omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	[Zn(CF ₃ O ₃ S)Cl(C ₁₅ H ₁₀ ClN ₃)]·C ₂ H ₃ N
<i>M_r</i>	558.65
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>
Temperature (K)	98
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.6550 (14), 15.329 (3), 18.486 (4)
β (°)	92.088 (7)
<i>V</i> (Å ³)	2167.8 (8)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.53
Crystal size (mm)	0.5 × 0.23 × 0.13
Data collection	
Diffractometer	Rigaku Saturn724
Absorption correction	Multi-scan (<i>ABSCOR</i> ; Higashi, 1995)
<i>T_{min}</i> , <i>T_{max}</i>	0.287, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	15157, 4424, 4053
<i>R_{int}</i> (sin θ/λ) _{max} (Å ⁻¹)	0.028 0.625
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.027, 0.075, 1.05
No. of reflections	4424
No. of parameters	290
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.48, -0.46

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *SHELXL* (Sheldrick, 2015).

Synthesis and crystallization

4'-Chloro-2,2':6',2''-terpyridine (0.200 g, 0.747 mmol) was suspended in 30 ml of acetonitrile and stirred for 10 min. ZnCl₂ (0.102 g, 0.747 mmol) was added to the suspension and heated under stirring at 323 K for 1 h. AgOTf (0.384 g,

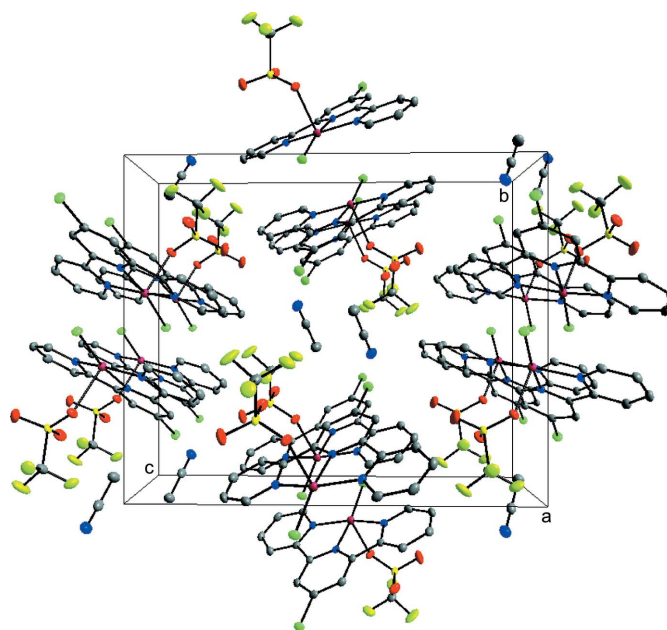


Figure 2
Perspective view of the packing structure of the title complex along the *a* axis.

1.49 mmol) was added to the mixture and stirred without heating for 30 min. After the removal of AgCl by filtration using a 0.45 μm PTFE syringe filter, the resulting clear solution was used to grow crystals by vapor diffusion with diethyl ether at 278 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2020). 5, x201292 [https://doi.org/10.1107/S2414314620012924]

Chlorido(4'-chloro-2,2':6',2''-terpyridine- κ^3N,N',N'')(trifluoromethanesulfonato- κO)zinc(II) acetonitrile monosolvate

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Crystal data

$[\text{Zn}(\text{CF}_3\text{O}_3\text{S})\text{Cl}(\text{C}_{15}\text{H}_{10}\text{ClN}_3)] \cdot \text{C}_2\text{H}_3\text{N}$

$M_r = 558.65$

Monoclinic, $P2_1/n$

$a = 7.6550$ (14) Å

$b = 15.329$ (3) Å

$c = 18.486$ (4) Å

$\beta = 92.088$ (7)°

$V = 2167.8$ (8) Å³

$Z = 4$

$F(000) = 1120$

$D_x = 1.712$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 10648 reflections

$\theta = 3.0\text{--}27.4^\circ$

$\mu = 1.53$ mm⁻¹

$T = 98$ K

Chunk, blue

$0.5 \times 0.23 \times 0.13$ mm

Data collection

Rigaku Saturn724

diffractometer

Radiation source: Sealed Tube

Graphite Monochromator monochromator

Detector resolution: 28.5714 pixels mm⁻¹

profile data from ω -scans

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

$T_{\min} = 0.287$, $T_{\max} = 1.000$

15157 measured reflections

4424 independent reflections

4053 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -9 \rightarrow 9$

$k = -19 \rightarrow 19$

$l = -23 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.075$

$S = 1.05$

4424 reflections

290 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 1.6585P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.48$ e Å⁻³

$\Delta\rho_{\min} = -0.46$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.57879 (3)	0.10461 (2)	0.54368 (2)	0.01503 (8)
Cl2	0.77504 (6)	0.00527 (3)	0.57903 (3)	0.01862 (11)
S1	0.66102 (6)	0.27610 (3)	0.66109 (3)	0.01438 (11)
Cl1	-0.06371 (6)	0.33529 (3)	0.41880 (3)	0.02027 (12)
F3	0.96127 (16)	0.36209 (9)	0.66388 (8)	0.0307 (3)
F2	0.75796 (19)	0.41967 (9)	0.59444 (8)	0.0354 (3)
O1	0.71851 (17)	0.22976 (9)	0.59695 (8)	0.0176 (3)
F1	0.7465 (2)	0.43216 (10)	0.71074 (9)	0.0462 (4)
O3	0.48031 (18)	0.30461 (10)	0.65635 (9)	0.0249 (3)
N2	0.38097 (19)	0.17251 (10)	0.50413 (9)	0.0119 (3)
N1	0.4111 (2)	0.09391 (10)	0.62698 (9)	0.0137 (3)
N3	0.66449 (19)	0.13089 (10)	0.44275 (9)	0.0132 (3)
O2	0.7203 (2)	0.23764 (11)	0.72904 (9)	0.0312 (4)
C6	0.2382 (2)	0.18139 (12)	0.54416 (10)	0.0127 (4)
C11	0.5531 (2)	0.18136 (12)	0.40107 (11)	0.0135 (4)
C10	0.3898 (2)	0.20620 (12)	0.43760 (10)	0.0125 (4)
N4	-0.4601 (3)	0.42556 (13)	0.40405 (11)	0.0290 (4)
C5	0.2542 (2)	0.13511 (12)	0.61493 (11)	0.0129 (4)
C7	0.0949 (2)	0.23059 (12)	0.51838 (11)	0.0147 (4)
H7	-0.0047	0.2369	0.5452	0.018*
C15	0.8157 (2)	0.10331 (12)	0.41444 (11)	0.0163 (4)
H15	0.8913	0.0686	0.4425	0.020*
C8	0.1082 (2)	0.26963 (12)	0.45068 (11)	0.0144 (4)
C1	0.4419 (2)	0.05299 (12)	0.69072 (11)	0.0177 (4)
H1	0.5490	0.0256	0.6994	0.021*
C4	0.1227 (2)	0.13329 (12)	0.66510 (11)	0.0167 (4)
H4	0.0155	0.1601	0.6552	0.020*
C9	0.2528 (2)	0.25749 (12)	0.40792 (10)	0.0143 (4)
H9	0.2582	0.2821	0.3621	0.017*
C12	0.5901 (2)	0.20541 (13)	0.33050 (11)	0.0170 (4)
H12	0.5120	0.2394	0.3030	0.020*
C14	0.8612 (2)	0.12554 (13)	0.34456 (11)	0.0183 (4)
H14	0.9661	0.1062	0.3264	0.022*
C3	0.1562 (3)	0.09007 (13)	0.73072 (12)	0.0204 (4)
H3	0.0710	0.0878	0.7653	0.024*
C2	0.3178 (3)	0.05051 (13)	0.74399 (11)	0.0204 (4)
H2	0.3427	0.0227	0.7879	0.024*
C17	-0.3767 (3)	0.48293 (14)	0.42493 (12)	0.0227 (4)
C13	0.7479 (3)	0.17715 (13)	0.30196 (11)	0.0191 (4)
H13	0.7765	0.1926	0.2552	0.023*
C16	0.7872 (3)	0.37808 (14)	0.65711 (12)	0.0224 (4)
C18	-0.2688 (3)	0.55655 (15)	0.45103 (14)	0.0304 (5)
H18A	-0.2941	0.6070	0.4217	0.046*
H18B	-0.1474	0.5418	0.4480	0.046*
H18C	-0.2944	0.5690	0.5004	0.046*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01194 (12)	0.01654 (12)	0.01657 (13)	0.00242 (8)	-0.00006 (9)	-0.00003 (9)
Cl2	0.0152 (2)	0.0169 (2)	0.0236 (3)	0.00591 (16)	-0.00090 (18)	0.00110 (18)
S1	0.0125 (2)	0.0189 (2)	0.0118 (2)	-0.00271 (16)	0.00134 (17)	-0.00214 (18)
Cl1	0.0152 (2)	0.0225 (2)	0.0228 (3)	0.00850 (17)	-0.00349 (18)	0.00070 (19)
F3	0.0176 (6)	0.0366 (7)	0.0377 (8)	-0.0105 (5)	-0.0020 (5)	-0.0001 (6)
F2	0.0393 (8)	0.0246 (6)	0.0420 (9)	-0.0027 (6)	-0.0007 (7)	0.0113 (6)
O1	0.0132 (6)	0.0204 (7)	0.0196 (7)	-0.0014 (5)	0.0044 (5)	-0.0056 (6)
F1	0.0517 (9)	0.0371 (8)	0.0507 (10)	-0.0152 (7)	0.0157 (8)	-0.0296 (8)
O3	0.0139 (7)	0.0297 (8)	0.0315 (9)	0.0014 (6)	0.0075 (6)	-0.0083 (7)
N2	0.0093 (7)	0.0134 (7)	0.0128 (8)	0.0009 (5)	-0.0005 (6)	-0.0020 (6)
N1	0.0120 (7)	0.0142 (7)	0.0149 (8)	-0.0011 (6)	-0.0003 (6)	-0.0004 (6)
N3	0.0105 (7)	0.0160 (7)	0.0131 (8)	0.0005 (6)	0.0006 (6)	-0.0029 (6)
O2	0.0346 (9)	0.0410 (9)	0.0174 (8)	-0.0117 (7)	-0.0057 (7)	0.0080 (7)
C6	0.0100 (8)	0.0147 (8)	0.0135 (9)	-0.0009 (7)	-0.0003 (7)	-0.0031 (7)
C11	0.0107 (8)	0.0143 (8)	0.0155 (9)	-0.0009 (7)	-0.0004 (7)	-0.0036 (7)
C10	0.0104 (8)	0.0137 (8)	0.0133 (9)	-0.0005 (7)	-0.0005 (7)	-0.0022 (7)
N4	0.0269 (10)	0.0310 (10)	0.0293 (11)	0.0007 (8)	0.0027 (8)	-0.0062 (9)
C5	0.0122 (8)	0.0123 (8)	0.0141 (9)	-0.0018 (7)	-0.0015 (7)	-0.0015 (7)
C7	0.0102 (8)	0.0176 (9)	0.0164 (10)	0.0006 (7)	0.0010 (7)	-0.0039 (8)
C15	0.0111 (8)	0.0166 (9)	0.0212 (10)	0.0019 (7)	-0.0004 (7)	-0.0041 (8)
C8	0.0104 (8)	0.0147 (8)	0.0177 (10)	0.0021 (7)	-0.0035 (7)	-0.0028 (7)
C1	0.0173 (9)	0.0169 (9)	0.0186 (10)	0.0015 (7)	-0.0027 (8)	0.0014 (8)
C4	0.0142 (9)	0.0177 (9)	0.0182 (10)	-0.0001 (7)	0.0030 (7)	-0.0019 (8)
C9	0.0139 (8)	0.0160 (9)	0.0127 (9)	-0.0004 (7)	-0.0022 (7)	-0.0006 (7)
C12	0.0155 (9)	0.0198 (9)	0.0156 (10)	0.0006 (7)	-0.0011 (7)	-0.0003 (8)
C14	0.0123 (9)	0.0222 (10)	0.0207 (11)	0.0011 (7)	0.0047 (8)	-0.0065 (8)
C3	0.0232 (10)	0.0200 (9)	0.0183 (11)	-0.0015 (8)	0.0066 (8)	-0.0013 (8)
C2	0.0275 (10)	0.0200 (9)	0.0134 (10)	0.0001 (8)	-0.0011 (8)	0.0031 (8)
C17	0.0219 (10)	0.0262 (11)	0.0203 (11)	0.0057 (9)	0.0044 (8)	0.0005 (9)
C13	0.0181 (9)	0.0247 (10)	0.0147 (10)	-0.0025 (8)	0.0037 (8)	-0.0033 (8)
C16	0.0220 (10)	0.0210 (10)	0.0242 (12)	-0.0037 (8)	0.0023 (9)	-0.0062 (9)
C18	0.0314 (12)	0.0291 (12)	0.0309 (13)	-0.0062 (9)	0.0034 (10)	-0.0023 (10)

Geometric parameters (\AA , $^\circ$)

Zn1—Cl2	2.2206 (6)	N4—C17	1.145 (3)
Zn1—O1	2.3911 (14)	C5—C4	1.394 (3)
Zn1—N3	2.0403 (17)	C7—H7	0.9300
Zn1—N2	1.9572 (15)	C7—C8	1.394 (3)
Zn1—N1	2.0468 (17)	C15—H15	0.9300
S1—O1	1.4636 (14)	C15—C14	1.393 (3)
S1—O3	1.4503 (15)	C8—C9	1.396 (3)
S1—O2	1.4455 (16)	C1—H1	0.9300
S1—C16	1.840 (2)	C1—C2	1.394 (3)
Cl1—C8	1.7420 (18)	C4—H4	0.9300

F3—C16	1.357 (2)	C4—C3	1.398 (3)
F2—C16	1.334 (3)	C9—H9	0.9300
F1—C16	1.338 (3)	C12—H12	0.9300
N2—C6	1.349 (2)	C12—C13	1.404 (3)
N2—C10	1.338 (2)	C14—H14	0.9300
N1—C5	1.368 (2)	C14—C13	1.396 (3)
N1—C1	1.348 (3)	C3—H3	0.9300
N3—C11	1.368 (2)	C3—C2	1.391 (3)
N3—C15	1.356 (2)	C2—H2	0.9300
C6—C5	1.489 (3)	C17—C18	1.470 (3)
C6—C7	1.400 (3)	C13—H13	0.9300
C11—C10	1.491 (3)	C18—H18A	0.9600
C11—C12	1.395 (3)	C18—H18B	0.9600
C10—C9	1.406 (3)	C18—H18C	0.9600
C12—Zn1—O1	98.13 (4)	N3—C15—C14	121.86 (18)
N2—Zn1—C12	168.69 (5)	C14—C15—H15	119.1
N2—Zn1—O1	93.18 (6)	C7—C8—C11	118.23 (14)
N2—Zn1—N1	79.97 (7)	C7—C8—C9	122.42 (17)
N2—Zn1—N3	79.84 (6)	C9—C8—C11	119.36 (15)
N1—Zn1—C12	99.19 (5)	N1—C1—H1	119.0
N1—Zn1—O1	92.17 (6)	N1—C1—C2	121.91 (18)
N3—Zn1—C12	99.67 (5)	C2—C1—H1	119.0
N3—Zn1—O1	93.68 (6)	C5—C4—H4	120.9
N3—Zn1—N1	159.24 (6)	C5—C4—C3	118.23 (18)
O1—S1—C16	101.90 (9)	C3—C4—H4	120.9
O3—S1—O1	114.30 (9)	C10—C9—H9	121.7
O3—S1—C16	104.02 (10)	C8—C9—C10	116.70 (18)
O2—S1—O1	114.32 (10)	C8—C9—H9	121.7
O2—S1—O3	116.35 (10)	C11—C12—H12	120.8
O2—S1—C16	103.45 (10)	C11—C12—C13	118.47 (18)
S1—O1—Zn1	125.44 (8)	C13—C12—H12	120.8
C6—N2—Zn1	118.69 (13)	C15—C14—H14	120.3
C10—N2—Zn1	118.96 (12)	C15—C14—C13	119.38 (18)
C10—N2—C6	122.32 (16)	C13—C14—H14	120.3
C5—N1—Zn1	114.29 (13)	C4—C3—H3	120.2
C1—N1—Zn1	126.91 (13)	C2—C3—C4	119.56 (19)
C1—N1—C5	118.78 (17)	C2—C3—H3	120.2
C11—N3—Zn1	114.34 (12)	C1—C2—H2	120.4
C15—N3—Zn1	126.80 (13)	C3—C2—C1	119.22 (19)
C15—N3—C11	118.86 (17)	C3—C2—H2	120.4
N2—C6—C5	113.06 (16)	N4—C17—C18	179.4 (3)
N2—C6—C7	120.53 (18)	C12—C13—H13	120.4
C7—C6—C5	126.41 (17)	C14—C13—C12	119.24 (19)
N3—C11—C10	113.87 (17)	C14—C13—H13	120.4
N3—C11—C12	122.19 (17)	F3—C16—S1	110.98 (14)
C12—C11—C10	123.93 (17)	F2—C16—S1	111.67 (14)
N2—C10—C11	112.90 (16)	F2—C16—F3	107.43 (17)

N2—C10—C9	120.82 (17)	F2—C16—F1	108.14 (18)
C9—C10—C11	126.26 (18)	F1—C16—S1	111.11 (15)
N1—C5—C6	113.98 (16)	F1—C16—F3	107.33 (17)
N1—C5—C4	122.25 (18)	C17—C18—H18A	109.5
C4—C5—C6	123.78 (17)	C17—C18—H18B	109.5
C6—C7—H7	121.5	C17—C18—H18C	109.5
C8—C7—C6	117.06 (17)	H18A—C18—H18B	109.5
C8—C7—H7	121.5	H18A—C18—H18C	109.5
N3—C15—H15	119.1	H18B—C18—H18C	109.5
Zn1—N2—C6—C5	-0.7 (2)	O2—S1—C16—F3	55.57 (17)
Zn1—N2—C6—C7	178.98 (13)	O2—S1—C16—F2	175.40 (15)
Zn1—N2—C10—C11	3.2 (2)	O2—S1—C16—F1	-63.78 (18)
Zn1—N2—C10—C9	-178.17 (13)	C6—N2—C10—C11	-174.71 (16)
Zn1—N1—C5—C6	-1.36 (19)	C6—N2—C10—C9	3.9 (3)
Zn1—N1—C5—C4	178.72 (14)	C6—C5—C4—C3	-177.78 (17)
Zn1—N1—C1—C2	179.44 (14)	C6—C7—C8—C11	-177.17 (13)
Zn1—N3—C11—C10	-0.70 (19)	C6—C7—C8—C9	3.2 (3)
Zn1—N3—C11—C12	-179.68 (14)	C11—N3—C15—C14	0.6 (3)
Zn1—N3—C15—C14	-179.87 (14)	C11—C10—C9—C8	177.31 (17)
C11—C8—C9—C10	177.93 (13)	C11—C12—C13—C14	0.6 (3)
O1—S1—C16—F3	-63.33 (16)	C10—N2—C6—C5	177.25 (16)
O1—S1—C16—F2	56.51 (16)	C10—N2—C6—C7	-3.1 (3)
O1—S1—C16—F1	177.33 (16)	C10—C11—C12—C13	-179.40 (17)
O3—S1—O1—Zn1	-54.32 (13)	C5—N1—C1—C2	0.9 (3)
O3—S1—C16—F3	177.58 (14)	C5—C6—C7—C8	179.16 (17)
O3—S1—C16—F2	-62.58 (17)	C5—C4—C3—C2	0.0 (3)
O3—S1—C16—F1	58.24 (18)	C7—C6—C5—N1	-178.30 (17)
N2—C6—C5—N1	1.3 (2)	C7—C6—C5—C4	1.6 (3)
N2—C6—C5—C4	-178.75 (17)	C7—C8—C9—C10	-2.4 (3)
N2—C6—C7—C8	-0.4 (3)	C15—N3—C11—C10	178.92 (15)
N2—C10—C9—C8	-1.1 (3)	C15—N3—C11—C12	-0.1 (3)
N1—C5—C4—C3	2.1 (3)	C15—C14—C13—C12	-0.1 (3)
N1—C1—C2—C3	1.1 (3)	C1—N1—C5—C6	177.34 (16)
N3—C11—C10—N2	-1.5 (2)	C1—N1—C5—C4	-2.6 (3)
N3—C11—C10—C9	179.96 (17)	C4—C3—C2—C1	-1.5 (3)
N3—C11—C12—C13	-0.5 (3)	C12—C11—C10—N2	177.45 (17)
N3—C15—C14—C13	-0.5 (3)	C12—C11—C10—C9	-1.1 (3)
O2—S1—O1—Zn1	83.30 (11)	C16—S1—O1—Zn1	-165.84 (10)