Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[triaquasulfatozinc(II)]-μ-3,3′-bis(3-pyridyl)-1,1′-(*m*-phenylene)-diurea] methanol solvate monohydrate]

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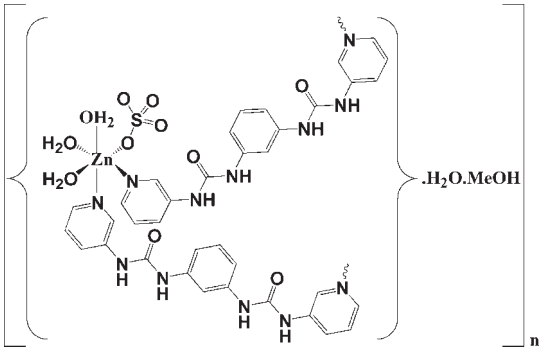
Received 18 January 2010; accepted 11 March 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.031; wR factor = 0.068; data-to-parameter ratio = 10.8.

In the title coordination polymer, $\{[Zn(SO_4)(C_{18}H_{16}N_6O_2)(H_2O)_3]\cdot CH_3OH\cdot H_2O\}_n$, the Zn^{2+} ion adopts a slightly distorted *cis*-ZnN_2O_4 octahedral geometry arising from three coordinated water molecules, one sulfate ion and two bridging 3,3′-bis(3-pyridyl)-1,1′-(*m*-phenylene)diurea (bpmpbu) ligands. The dihedral angles between the central benzene ring and two terminal pyridine rings of the bpmbpu molecule are 10.58 (17) and 34.63 (16)°. In the crystal, the ligands bridge the Zn^{II} ions, thus generating a one-dimensional zigzag coordination polymer propagating in [010]. The crystal structure features extensive N—H···O and O—H···O hydrogen-bonding interactions.

Related literature

For our previous work on related compounds, see: Adarsh *et al.* (2008, 2009),



Experimental

Crystal data

$[Zn(SO_4)(C_{18}H_{16}N_6O_2)(H_2O)_3]\cdot CH_4O\cdot H_2O$
M_r = 613.90
Monoclinic, $P2_1$
a = 6.4831 (7) Å
b = 19.265 (2) Å
c = 9.7062 (11) Å
β = 98.848 (2)°
V = 1197.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 100 K
0.28 × 0.22 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.732, T_{max} = 0.871
5989 measured reflections
3968 independent reflections
3823 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.068
S = 1.02
3968 reflections
369 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1782 Friedel pairs
Flack parameter: 0.049 (10)

Table 1
Selected bond lengths (Å).

Zn1—N1	2.116 (3)	Zn1—O31	2.149 (3)
Zn1—N23^{i}	2.126 (3)	Zn1—O32	2.158 (3)
Zn1—O33	2.062 (2)	Zn1—O27	2.217 (2)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···O29^{ii}	0.86	2.14	2.954 (4)	157
N10—H10···O29^{ii}	0.86	2.25	3.044 (4)	154
N17—H17···O28^{iii}	0.86	2.05	2.875 (4)	160
N20—H20···O30^{iii}	0.86	2.08	2.922 (4)	164
O35—H35···O34	0.82	2.09	2.893 (4)	168
O32—H32*A*···O27^{iv}	0.85 (4)	2.09 (4)	2.942 (3)	179 (4)
O31—H31*A*···O9^{iv}	0.81 (4)	2.09 (4)	2.899 (4)	173 (4)
O33—H33*A*···O29^{iv}	0.85 (4)	1.87 (4)	2.714 (4)	170 (4)
O34—H34*A*···O9	0.90 (5)	2.08 (5)	2.861 (4)	146 (4)
O32—H32*B*···O19^{v}	0.73 (4)	2.08 (4)	2.774 (3)	158 (5)
O31—H31*B*···O34	0.79 (4)	2.11 (4)	2.887 (4)	168 (4)
O33—H33*B*···O28	0.82 (4)	1.84 (4)	2.633 (3)	162 (4)
O34—H34*B*···O30	0.98 (5)	1.90 (5)	2.748 (4)	144 (4)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*, *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

We thank the Department of Science & Technology (DST), New Delhi, India, for financial support. NNA thanks the IACS for research fellowships. The data were collected at the DST-funded National Single Crystal Diffractometer Facility at the Department of Inorganic Chemistry, IACS.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5311).

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supporting information

Acta Cryst. (2010). E**66**, m413–m414 [doi:10.1107/S1600536810009268]

catena-Poly[[[triaquasulfatozinc(II)]-μ-3,3′-bis(3-pyridyl)-1,1′-(*m*-phenylene)diurea] methanol solvate monohydrate]

N. N. Adarsh and Parthasarathi Dastidar

S1. Comment

As part of our ongoing studies of functional coordination polymers (CPs) and metal-organic frameworks (MOF) (Adarsh *et al.*, 2008, 2009), we now report a coordination polymer derived from a newly synthesized bis-pyridyl-bis-urea ligand *N*,*N*′-bis(3-pyridyl)meta-phenylene-bis-urea (**BPMPBU**). Suitable single crystals of [{$Zn(H_2O)_3(SO_4)$(μ-**BPMPBU**)}.H_2O.MeOH]$_\infty$, (I), were obtained by layering an methanolic solution of **BPMPBU** over aqueous solution of $ZnSO_4$ in 1:2 metal–ligand ratio (see experimental). It was crystallized in the monoclinic non centrosymmetric space group $P2_1$. In the asymmetric unit, the metal center Zn(II) is found to be hexacoordinated; while euqatorial positions are occupied by pyridyl N atoms of the ligand and water molecules, the apical positions are coordinated by O atoms of water and sulfate. The ORTEP diagram of **1** with 50% probability is given in Fig. 1. The metal center Zn(II) displayed a distorted octahedral geometry [N—Zn—N = 94.72?(12)°; O—Zn—N = 87.4)(12)-93.83 (10)°; O—Zn—O = 87.01 (11)-91.12 (12)°]. In the crystal structure, the ligand **BPMPBU** which displayed *syn-syn-syn* conformation (scheme 1) coordinated to the adjacent Zn(II) metal centres via pyridyl N atoms leading to the formation of a 1D zigzag polymeric chain (Fig. 2). The polymeric chains are further packed in parallel fashion sustained by N–H···O hydrogen bonding interactions involving sulfate and the urea moieties [N···O = 2.875 (4)–3.044 (4) Å; N–H···O =154–164°]. Both the lattice included water and MeOH are occupied within the interstitial space of the chains and are involved in O—H···O hydrogen bonding interactions [O···O = 2.633 (3)–2.942 (3) Å; O–H···O] (Fig. 3).

S2. Experimental

3-Aminopyridine (1 g, 10.6 mmol) and triethylamine (3 ml) were stirred under nitrogen in 150 ml of anhydrous dichloromethane in ice cold condition for 20 min. To this stirring solution, triphosgene (1.57 g, 5.3 mmol) was added and kept stirring for another 20 min at 0°C and to the resultant solution, meta-phenylenediamine (574 mg, 5.3 mmol) in 10 ml of dichloromethane was added dropwise. White precipitate was obtained after 24 hour of stirring at room temperature. The precipitate was filtered, air dried, treated with 5% $NaHCO_3$ solution and washed with distilled water. Pale yellow coloured microcrystalline material of the **BPMPBU** ligand was obtained (880 mg, 55% yield) after recrystallization from H_2O/MeOH (1 : 2 v/v) (880 mg, 55% yield) . mp 265-267°C Anal. data calc. for $C_{18}H_{16}N_6O_2$: C, 62.06; H, 4.63; N, 24.12. Found: C, 61.86, H, 4.24, N, 24.32. ^{1}H NMR (300 MHz, DMSO-d6): δ = 7.09-7.12 (2*H*, d, J = 9 Hz, Ar—H); 7.23-7.18 (1*H*, t, J = 9, 9 Hz, Ar—H); 7.34-7.30 (2*H*, dd, J = 6, 9 Hz, Py—H); 7.70 (1*H*, s, Ar—H); 7.96-7.93 (2*H*, d, J = 9 Hz, Py—H); 8.20-8.19 (2*H*, d, J = 3 Hz, Py—H); 8.62 (2*H*, s, Py—H); 8.78 (2*H*, s, urea N—H); 8.87 (2*H*, s, urea N—H). HRMS(ESI) calcd for $C_{18}H_{16}N_6O_2$ 349.14; found: [M + Na]+ 349.12 F T—IR (KBr, cm-1): 3346 (s, N–H stretch), 3242 (s, O–H stretch), 3059, 3022 (s, aromatic C–H stretch), 2908, 2827 (s, aliphatic C–H stretch), 1710, 1647 (s, urea C=O stretch), 1641 (s, urea N–H bend), 1608, 1595, 1535, 1485, 1425, 1421, 1408, 1327, 1294, 1209, 1186, 1122, 1103, 854, 786, 767, 734, 700, 626, 551.

The title compound was synthesized by layering a methanolic solution of **BPMPBU** (40 mg, 0.1149 mmol) over an aqueous solution of $ZnSO_4.7H_2O$ (16.5 mg, 0.0575 mmol). After three days, colourless blocks of (I) were obtained (yield = 20 mg, 57 %). Anal. data calc. for $C_{19}H_{28}N_6O_{11}SZn$: C, 37.17; H, 4.60; N, 13.69, found: C, 37.12, H, 4.28, N, 13.66. F T —IR (KBr, cm-1): 3323 (b, N–H stretch), 3219 (b, O–H stretch), 3090 (b, aromatic C–H stretch), 1693 (s, urea C=O stretch), 1610 (s, urea N–H bend), 1589, 1570, 1552, 1496, 1483, 1431, 1330, 1294, 1217, 1193, 1130, 1089, 1066, 1035, 945, 900, 850, 819, 775, 704.

S3. Refinement

Whenever possible, the hydrogen atoms were located on a difference Fourier map and refined. In other cases, the hydrogen atoms were geometrically fixed. The positional parameters of hydrogen atoms of the water molecules and methanol molecule were refined with the constraint $U_{iso}(H) = 1.2$ or $1.5U_{eq}$(carrier) applied.

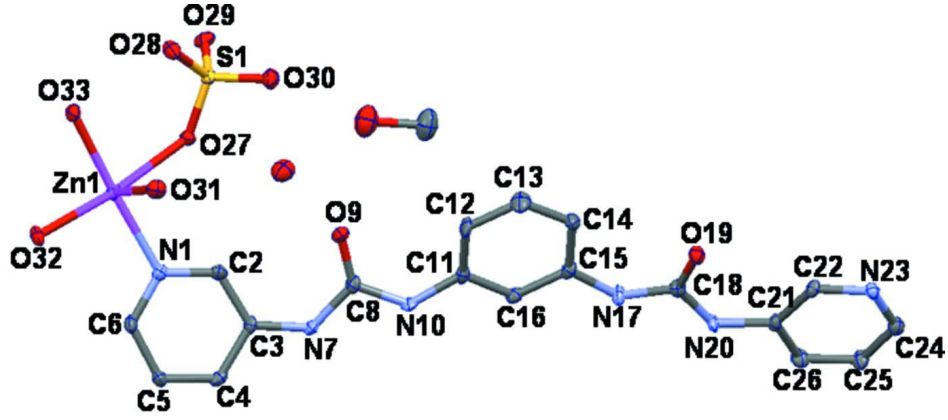

Figure 1

Fragment of the structure of (I) with displacement ellipsoids drawn at 50% probability level

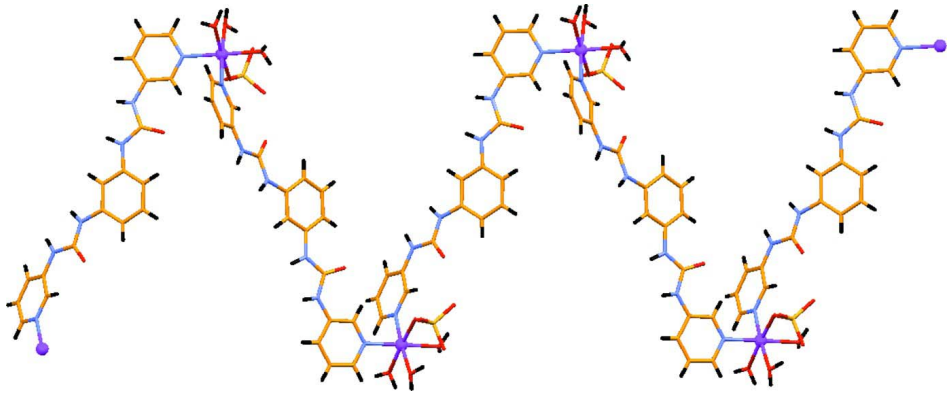

Figure 2

1D zig-zag coordination polymer in (I).

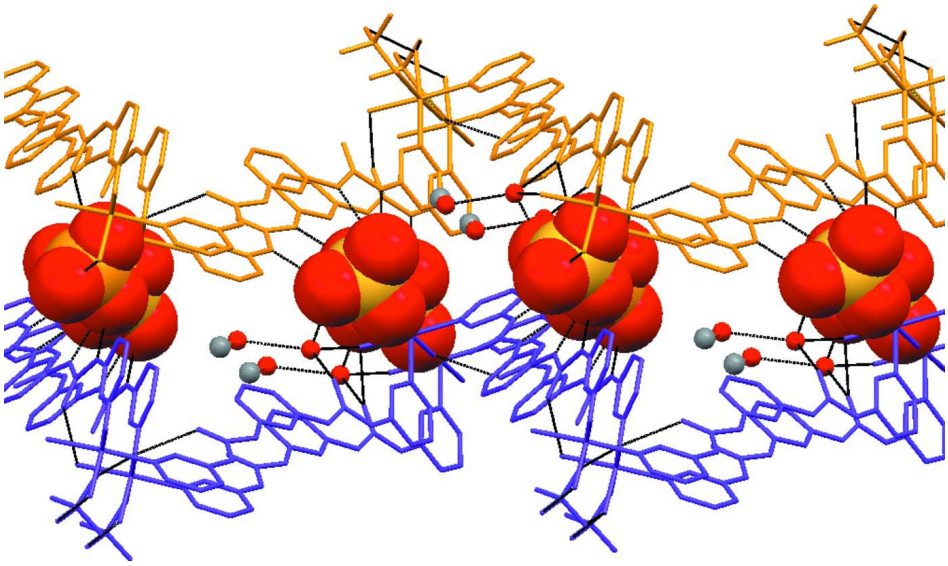

Figure 3

Parallel packing of 1D zigzag chains in (I) (shown in orange and purple colour) displaying various hydrogen bonding (dotted lines) intearctions (dotted lines).

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Crystal data

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$M_r = 613.90$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 6.4831\ (7)$ Å
$b = 19.265\ (2)$ Å
$c = 9.7062\ (11)$ Å
$\beta = 98.848\ (2)°$
$V = 1197.8\ (2)$ Å^3
$Z = 2$
$F(000) = 636$
$D_x = 1.702$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 144 reflections
$\theta = 2.3–26.0°$
$\mu = 1.19$ mm^{-1}
$T = 100$ K
Block, colourless
0.28 × 0.22 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 3 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min} = 0.732$, $T_{max} = 0.871$
5989 measured reflections
3968 independent reflections
3823 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -7\rightarrow6$
$k = -22\rightarrow22$
$l = -7\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.068$
$S = 1.02$
3968 reflections
369 parameters
1 restraint

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0188P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Absolute structure: Flack (1983), 1782 Friedel pairs
Absolute structure parameter: 0.049 (10)

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. Refinement of F^2 against ALL reflections. The weighted *R*-factor wR and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) etc. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	1.01818 (5)	0.83531 (2)	0.15530 (4)	0.01276 (10)
S1	0.59561 (13)	0.76119 (4)	−0.03921 (8)	0.01383 (19)
N1	0.9621 (4)	0.84335 (19)	0.3638 (3)	0.0137 (6)
C2	0.7909 (5)	0.81484 (16)	0.4027 (3)	0.0159 (8)
H2	0.6967	0.7916	0.3365	0.019*
C3	0.7500 (5)	0.81905 (15)	0.5399 (3)	0.0133 (8)
C4	0.8923 (5)	0.85448 (16)	0.6356 (4)	0.0157 (8)
H4	0.8676	0.8592	0.7270	0.019*
C5	1.0682 (5)	0.88257 (18)	0.5975 (4)	0.0159 (8)
H5	1.1653	0.9056	0.6622	0.019*
C6	1.0987 (5)	0.87587 (18)	0.4585 (4)	0.0164 (8)
H6	1.2183	0.8947	0.4315	0.020*
N7	0.5748 (4)	0.79042 (15)	0.5860 (3)	0.0174 (7)
H7	0.5445	0.8065	0.6631	0.021*
C8	0.4459 (5)	0.73982 (18)	0.5225 (4)	0.0147 (8)
O9	0.4570 (4)	0.71652 (12)	0.4060 (2)	0.0177 (5)
N10	0.3052 (5)	0.71747 (15)	0.6036 (3)	0.0165 (6)
H10	0.3019	0.7402	0.6796	0.020*
C11	0.1645 (5)	0.66159 (17)	0.5776 (3)	0.0138 (7)
C12	0.1858 (6)	0.60887 (19)	0.4839 (4)	0.0185 (8)
H12	0.2956	0.6091	0.4325	0.022*
C13	0.0411 (6)	0.5561 (2)	0.4683 (4)	0.0248 (9)
H13	0.0552	0.5208	0.4051	0.030*
C14	−0.1251 (6)	0.55336 (19)	0.5430 (4)	0.0193 (9)
H14	−0.2232	0.5179	0.5282	0.023*
C15	−0.1405 (5)	0.60492 (17)	0.6399 (3)	0.0145 (7)
C16	0.0004 (5)	0.65929 (17)	0.6551 (3)	0.0142 (7)
H16	−0.0144	0.6948	0.7178	0.017*

N17	−0.2982 (4)	0.60722 (14)	0.7258 (3)	0.0164 (6)
H17	−0.3135	0.6464	0.7656	0.020*
C18	−0.4296 (5)	0.55496 (17)	0.7538 (4)	0.0144 (8)
O19	−0.4347 (4)	0.49686 (12)	0.7017 (2)	0.0166 (5)
N20	−0.5554 (4)	0.57575 (15)	0.8485 (3)	0.0154 (6)
H20	−0.5270	0.6156	0.8867	0.018*
C21	−0.7245 (6)	0.54001 (18)	0.8903 (4)	0.0144 (7)
C22	−0.7849 (5)	0.47290 (18)	0.8489 (3)	0.0140 (7)
H22	−0.7116	0.4495	0.7879	0.017*
N23	−0.9455 (4)	0.44088 (14)	0.8943 (3)	0.0129 (6)
C24	−1.0544 (5)	0.47467 (19)	0.9809 (4)	0.0181 (8)
H24	−1.1646	0.4523	1.0134	0.022*
C25	−1.0052 (6)	0.54219 (19)	1.0225 (4)	0.0197 (8)
H25	−1.0843	0.5653	1.0803	0.024*
C26	−0.8391 (5)	0.57487 (18)	0.9779 (4)	0.0185 (8)
H26	−0.8039	0.6200	1.0063	0.022*
O27	0.6905 (4)	0.80524 (12)	0.0790 (2)	0.0142 (5)
O28	0.7580 (4)	0.73351 (12)	−0.1150 (3)	0.0204 (6)
O29	0.4479 (4)	0.80304 (13)	−0.1355 (2)	0.0198 (6)
O30	0.4820 (4)	0.70339 (12)	0.0130 (3)	0.0231 (6)
O31	1.0881 (4)	0.72757 (13)	0.1965 (3)	0.0185 (6)
O32	1.3440 (4)	0.86231 (13)	0.2068 (3)	0.0167 (6)
O33	1.0745 (4)	0.81868 (13)	−0.0455 (2)	0.0175 (6)
O34	0.7276 (5)	0.64800 (13)	0.2427 (3)	0.0277 (7)
O35	0.6380 (5)	0.50133 (16)	0.2090 (3)	0.0393 (8)
H35	0.6448	0.5437	0.2152	0.059*
C36	0.4550 (7)	0.4779 (2)	0.2561 (5)	0.0385 (11)
H36A	0.4866	0.4655	0.3529	0.058*
H36B	0.4017	0.4380	0.2029	0.058*
H36C	0.3522	0.5141	0.2446	0.058*
H31A	1.194 (7)	0.722 (2)	0.251 (4)	0.027*
H31B	1.000 (7)	0.704 (2)	0.220 (4)	0.027*
H32A	1.445 (6)	0.846 (2)	0.170 (4)	0.026*
H32B	1.386 (7)	0.898 (2)	0.215 (4)	0.026*
H33A	1.198 (7)	0.8143 (19)	−0.063 (4)	0.027*
H33B	0.995 (6)	0.786 (2)	−0.063 (4)	0.027*
H34A	0.691 (7)	0.667 (2)	0.320 (5)	0.043*
H34B	0.615 (7)	0.648 (2)	0.163 (5)	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01308 (19)	0.01284 (18)	0.01308 (19)	0.00027 (18)	0.00425 (13)	−0.00021 (18)
S1	0.0139 (4)	0.0144 (4)	0.0138 (4)	−0.0007 (3)	0.0043 (3)	−0.0030 (3)
N1	0.0149 (14)	0.0138 (16)	0.0132 (14)	0.0001 (14)	0.0047 (10)	0.0015 (14)
C2	0.0147 (18)	0.019 (2)	0.0137 (18)	−0.0010 (14)	−0.0003 (14)	0.0010 (13)
C3	0.0111 (17)	0.014 (2)	0.0162 (17)	0.0010 (13)	0.0056 (13)	0.0011 (13)
C4	0.0222 (19)	0.014 (2)	0.0119 (17)	0.0028 (14)	0.0068 (14)	0.0002 (13)

C5	0.0147 (19)	0.0166 (18)	0.0159 (19)	−0.0050 (15)	0.0007 (14)	−0.0001 (15)
C6	0.017 (2)	0.0138 (18)	0.0197 (19)	−0.0057 (15)	0.0074 (15)	−0.0018 (15)
N7	0.0183 (17)	0.0237 (17)	0.0119 (15)	−0.0061 (14)	0.0076 (12)	−0.0029 (13)
C8	0.0115 (18)	0.0167 (19)	0.0166 (19)	0.0038 (14)	0.0046 (14)	0.0024 (15)
O9	0.0190 (14)	0.0218 (13)	0.0133 (13)	−0.0022 (11)	0.0054 (10)	−0.0024 (11)
N10	0.0210 (17)	0.0184 (16)	0.0115 (15)	−0.0037 (13)	0.0073 (12)	−0.0062 (12)
C11	0.0122 (18)	0.0136 (17)	0.0165 (18)	0.0018 (14)	0.0048 (14)	0.0049 (14)
C12	0.0171 (19)	0.020 (2)	0.022 (2)	−0.0037 (16)	0.0133 (15)	−0.0011 (16)
C13	0.031 (2)	0.020 (2)	0.027 (2)	−0.0029 (17)	0.0151 (17)	−0.0104 (16)
C14	0.022 (2)	0.019 (2)	0.017 (2)	−0.0087 (17)	0.0053 (16)	−0.0029 (15)
C15	0.0135 (18)	0.0158 (18)	0.0150 (18)	0.0028 (15)	0.0047 (14)	0.0023 (14)
C16	0.0176 (19)	0.0125 (17)	0.0134 (18)	0.0012 (15)	0.0051 (14)	−0.0008 (14)
N17	0.0162 (16)	0.0114 (15)	0.0239 (17)	−0.0034 (13)	0.0102 (13)	−0.0023 (12)
C18	0.0135 (18)	0.0132 (19)	0.0168 (19)	0.0010 (15)	0.0027 (14)	0.0008 (14)
O19	0.0187 (14)	0.0123 (13)	0.0197 (13)	−0.0020 (10)	0.0051 (10)	−0.0012 (10)
N20	0.0152 (16)	0.0118 (15)	0.0206 (16)	−0.0075 (12)	0.0069 (12)	−0.0046 (12)
C21	0.0097 (17)	0.0181 (19)	0.0159 (19)	−0.0002 (14)	0.0032 (13)	0.0028 (15)
C22	0.0135 (18)	0.0140 (18)	0.0159 (18)	0.0023 (15)	0.0063 (14)	0.0017 (15)
N23	0.0130 (15)	0.0109 (14)	0.0150 (15)	−0.0010 (12)	0.0026 (12)	−0.0008 (12)
C24	0.0160 (19)	0.0206 (19)	0.0182 (19)	−0.0010 (16)	0.0041 (15)	0.0009 (16)
C25	0.020 (2)	0.0181 (19)	0.023 (2)	−0.0019 (16)	0.0102 (16)	−0.0044 (16)
C26	0.019 (2)	0.0146 (18)	0.023 (2)	−0.0004 (16)	0.0061 (15)	−0.0043 (15)
O27	0.0123 (12)	0.0171 (12)	0.0134 (12)	−0.0012 (10)	0.0022 (9)	−0.0033 (10)
O28	0.0161 (13)	0.0223 (13)	0.0242 (14)	−0.0026 (11)	0.0076 (10)	−0.0102 (11)
O29	0.0218 (14)	0.0253 (13)	0.0132 (13)	0.0031 (11)	0.0055 (10)	−0.0013 (10)
O30	0.0283 (15)	0.0196 (14)	0.0234 (15)	−0.0081 (12)	0.0100 (11)	−0.0030 (11)
O31	0.0189 (15)	0.0168 (14)	0.0195 (14)	0.0026 (11)	0.0018 (11)	0.0012 (11)
O32	0.0122 (13)	0.0132 (12)	0.0259 (15)	−0.0036 (10)	0.0070 (10)	−0.0049 (11)
O33	0.0133 (13)	0.0229 (17)	0.0177 (13)	−0.0032 (11)	0.0073 (10)	−0.0038 (10)
O34	0.0349 (17)	0.0226 (15)	0.0268 (16)	0.0016 (13)	0.0088 (13)	−0.0024 (12)
O35	0.0384 (19)	0.0336 (17)	0.050 (2)	0.0036 (15)	0.0193 (15)	0.0041 (15)
C36	0.031 (3)	0.039 (3)	0.049 (3)	0.003 (2)	0.015 (2)	0.010 (2)

Geometric parameters (Å, º)

Zn1—N1	2.116 (3)	C14—H14	0.9300
Zn1—N23^{i}	2.126 (3)	C15—C16	1.383 (5)
Zn1—O33	2.062 (2)	C15—N17	1.416 (4)
Zn1—O31	2.149 (3)	C16—H16	0.9300
Zn1—O32	2.158 (3)	N17—C18	1.373 (4)
Zn1—O27	2.217 (2)	N17—H17	0.8600
S1—O30	1.468 (3)	C18—O19	1.227 (4)
S1—O29	1.471 (2)	C18—N20	1.379 (4)
S1—O28	1.474 (3)	N20—C21	1.406 (5)
S1—O27	1.482 (2)	N20—H20	0.8600
N1—C6	1.331 (4)	C21—C26	1.386 (5)
N1—C2	1.344 (4)	C21—C22	1.392 (5)
C2—C3	1.399 (4)	C22—N23	1.342 (4)

C2—H2	0.9300	C22—H22	0.9300
C3—C4	1.384 (4)	N23—C24	1.346 (5)
C3—N7	1.397 (4)	N23—Zn1^{ii}	2.126 (3)
C4—C5	1.364 (5)	C24—C25	1.384 (5)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.399 (5)	C25—C26	1.373 (5)
C5—H5	0.9300	C25—H25	0.9300
C6—H6	0.9300	C26—H26	0.9300
N7—C8	1.367 (4)	O31—H31A	0.81 (4)
N7—H7	0.8600	O31—H31B	0.79 (4)
C8—O9	1.230 (4)	O32—H32A	0.85 (4)
C8—O9	1.230 (4)	O32—H32B	0.73 (4)
C8—N10	1.363 (4)	O33—H33A	0.85 (4)
N10—C11	1.409 (4)	O33—H33B	0.82 (4)
N10—H10	0.8600	O34—H34A	0.90 (5)
C11—C12	1.384 (5)	O34—H34B	0.98 (5)
C11—C16	1.394 (5)	O35—C36	1.409 (5)
C12—C13	1.375 (5)	O35—H35	0.8200
C12—H12	0.9300	C36—H36A	0.9600
C13—C14	1.389 (5)	C36—H36B	0.9600
C13—H13	0.9300	C36—H36C	0.9600
C14—C15	1.382 (5)		

O33—Zn1—N1	175.25 (12)	C12—C13—H13	118.6
O33—Zn1—N23^{i}	89.98 (10)	C14—C13—H13	118.6
N1—Zn1—N23^{i}	94.71 (12)	C15—C14—C13	118.1 (3)
O33—Zn1—O31	87.88 (10)	C15—C14—H14	121.0
N1—Zn1—O31	87.42 (12)	C13—C14—H14	121.0
N23^{i}—Zn1—O31	177.64 (11)	C16—C15—C14	120.1 (3)
O33—Zn1—O32	86.97 (10)	C16—C15—N17	116.0 (3)
N1—Zn1—O32	93.83 (10)	C14—C15—N17	123.9 (3)
N23^{i}—Zn1—O32	89.81 (10)	C15—C16—C11	120.8 (3)
O31—Zn1—O32	91.08 (10)	C15—C16—H16	119.6
O33—Zn1—O27	86.75 (9)	C11—C16—H16	119.6
N1—Zn1—O27	92.41 (10)	C18—N17—C15	128.3 (3)
N23^{i}—Zn1—O27	90.39 (10)	C18—N17—H17	115.8
O31—Zn1—O27	88.50 (10)	C15—N17—H17	115.8
O32—Zn1—O27	173.72 (9)	O19—C18—N17	124.4 (3)
O30—S1—O29	108.84 (15)	O19—C18—N20	124.0 (3)
O30—S1—O28	109.45 (14)	N17—C18—N20	111.6 (3)
O29—S1—O28	109.04 (15)	C18—N20—C21	128.1 (3)
O30—S1—O27	109.73 (14)	C18—N20—H20	115.9
O29—S1—O27	109.25 (14)	C21—N20—H20	115.9
O28—S1—O27	110.50 (14)	C26—C21—C22	118.3 (3)
C6—N1—C2	119.2 (3)	C26—C21—N20	117.1 (3)
C6—N1—Zn1	120.1 (2)	C22—C21—N20	124.6 (3)
C2—N1—Zn1	120.7 (2)	N23—C22—C21	122.0 (3)
N1—C2—C3	122.0 (3)	N23—C22—H22	119.0

N1—C2—H2	119.0	C21—C22—H22	119.0
C3—C2—H2	119.0	C22—N23—C24	119.4 (3)
C4—C3—N7	118.1 (3)	C22—N23—Zn1^{ii}	121.4 (2)
C4—C3—C2	117.6 (3)	C24—N23—Zn1^{ii}	119.0 (2)
N7—C3—C2	124.3 (3)	N23—C24—C25	121.1 (3)
C5—C4—C3	120.8 (3)	N23—C24—H24	119.4
C5—C4—H4	119.6	C25—C24—H24	119.4
C3—C4—H4	119.6	C26—C25—C24	119.7 (3)
C4—C5—C6	118.2 (3)	C26—C25—H25	120.1
C4—C5—H5	120.9	C24—C25—H25	120.1
C6—C5—H5	120.9	C25—C26—C21	119.4 (3)
N1—C6—C5	122.1 (3)	C25—C26—H26	120.3
N1—C6—H6	118.9	C21—C26—H26	120.3
C5—C6—H6	118.9	S1—O27—Zn1	132.11 (14)
C8—N7—C3	127.4 (3)	Zn1—O31—H31A	113 (3)
C8—N7—H7	116.3	Zn1—O31—H31B	117 (3)
C3—N7—H7	116.3	H31A—O31—H31B	108 (4)
O9—C8—N10	123.7 (3)	Zn1—O32—H32A	127 (3)
O9—C8—N10	123.7 (3)	Zn1—O32—H32B	126 (3)
O9—C8—N7	123.8 (3)	H32A—O32—H32B	95 (4)
O9—C8—N7	123.8 (3)	Zn1—O33—H33A	121 (2)
N10—C8—N7	112.4 (3)	Zn1—O33—H33B	97 (3)
C8—N10—C11	127.6 (3)	H33A—O33—H33B	118 (4)
C8—N10—H10	116.2	H34A—O34—H34B	113 (4)
C11—N10—H10	116.2	C36—O35—H35	109.5
C12—C11—C16	119.5 (3)	O35—C36—H36A	109.5
C12—C11—N10	123.4 (3)	O35—C36—H36B	109.5
C16—C11—N10	117.0 (3)	H36A—C36—H36B	109.5
C13—C12—C11	118.6 (3)	O35—C36—H36C	109.5
C13—C12—H12	120.7	H36A—C36—H36C	109.5
C11—C12—H12	120.7	H36B—C36—H36C	109.5
C12—C13—C14	122.8 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7···O29^{iii}	0.86	2.14	2.954 (4)	157
N10—H10···O29^{iii}	0.86	2.25	3.044 (4)	154
N17—H17···O28^{iv}	0.86	2.05	2.875 (4)	160
N20—H20···O30^{iv}	0.86	2.08	2.922 (4)	164
O35—H35···O34	0.82	2.09	2.893 (4)	168
O32—H32*A*···O27^{v}	0.85 (4)	2.09 (4)	2.942 (3)	179 (4)
O31—H31*A*···O9^{v}	0.81 (4)	2.09 (4)	2.899 (4)	173 (4)
O33—H33*A*···O29^{v}	0.85 (4)	1.87 (4)	2.714 (4)	170 (4)
O34—H34*A*···O9	0.90 (5)	2.08 (5)	2.861 (4)	146 (4)
O32—H32*B*···O19^{vi}	0.73 (4)	2.08 (4)	2.774 (3)	158 (5)

O31—H31*B*···O34	0.79 (4)	2.11 (4)	2.887 (4)	168 (4)
O33—H33*B*···O28	0.82 (4)	1.84 (4)	2.633 (3)	162 (4)
O34—H34*B*···O30	0.98 (5)	1.90 (5)	2.748 (4)	144 (4)

Symmetry codes: (iii) $x, y, z+1$; (iv) $x-1, y, z+1$; (v) $x+1, y, z$; (vi) $-x+1, y+1/2, -z+1$.