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Tetraaqua(2,2′-bipyridine)zinc(II) 4,4′-(6-diethylamino-1,3,5-triazine-2,4-diyldiimino)dibenzenesulfonate

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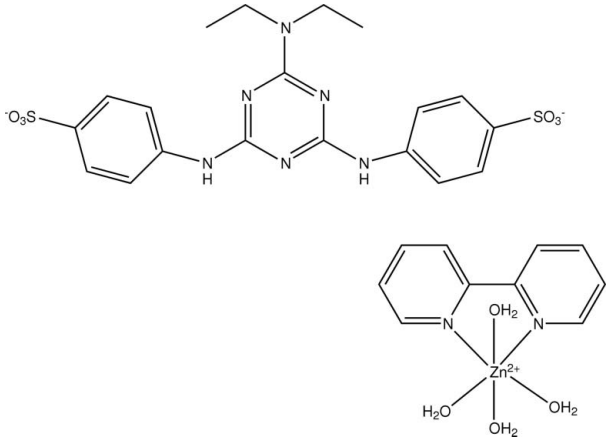
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.136; data-to-parameter ratio = 16.0.

Reaction of the newly designed ligand 2,4-bis(4-sulfophenylamino)-6-diethylamino-1,3,5-triazine (H_2DSNT) and 2,2-bipyridine (2,2′-bipy) with $ZnCl_2$ in water yields the supramolecular title compound, $[Zn(C_{10}H_8N_2)(H_2O)_4]\cdot(C_{19}H_{20}N_6O_6S_2)$. In this compound, the coordination geometry of the Zn^{II} atom is octahedral, involving two N atoms from 2,2′-bipy and four O atoms from coordinated water molecules. $DSNT^{2-}$ balances the charge of the Zn^{II} cation and builds up an intricate hydrogen-bond network with coordinated water molecules in the $[Zn(2,2'\text{-bipy})(H_2O)_4]^{2+}$ cation. Both ions lie on mirror planes.

Related literature

For related literature, see: Gunderman *et al.* (1997); Kosnic *et al.* (1992); Shubnell *et al.* (1994); Thurston *et al.* (1951).



Experimental

Crystal data

$[Zn(C_{10}H_8N_2)(H_2O)_4]\cdot(C_{19}H_{20}N_6O_6S_2)$
M_r = 786.19
Orthorhombic, *Pnma*
a = 12.758 (3) Å
b = 21.015 (6) Å
c = 12.828 (4) Å
V = 3439.3 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 293 (2) K
0.30 × 0.10 × 0.08 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*SPHERE* in *CrystalStructure*; Molecular Structure Corporation & Rigaku, 2000)
T_{min} = 0.886, T_{max} = 0.930
25765 measured reflections
4045 independent reflections
3553 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.136
S = 1.07
4045 reflections
253 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O6	0.829 (19)	1.915 (19)	2.743 (4)	177 (4)
O1—H2···O5^{i}	0.825 (19)	1.99 (2)	2.798 (4)	165 (5)
O2—H3···O5	0.840 (18)	1.898 (18)	2.734 (3)	174 (4)
O3—H4···N2^{ii}	0.841 (19)	1.91 (2)	2.753 (4)	176 (5)

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Molecular Structure Corporation & Rigaku, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2046).

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supplementary materials

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Tetraaqua(2,2'-bipyridine)zinc(II) 4,4'-(6-diethylamino-1,3,5-triazine-2,4-diyldiimino)dibenzenesulfonate

J. Chen and Y. Ruan

Comment

It is well known that chlorine atoms in cyanuric chloride are easily replaced by other organic groups (Thurston *et al.*, 1951). Using cyanuric chloride as reactant and controlling stoichiometry and reaction temperature, we have synthesized a new triazine derivative, 2,4-bis(4-sulfophenylamino) −6-diethylamino-1,3,5-triazine (H_2DSNT). Reaction of H_2DSNT and 2,2-bipy with $ZnCl_2$ in water yields a supramolecular compound [Zn(2,2'-bipy)($H_2O)_4$]DSNT.

In the title compound, as shown in Fig. 1, the coordination geometry of Zn^{II} is octahedral, with two nitrogen atoms from 2,2-bipy and four oxygen atoms from coordinated water. The Zn—N distance is 2.122 (2)Å and Zn—O distances are in the range of 2.059 (3)Å to 2.135 (3) Å. $DSNT^{2-}$ does not coordinate directly to Zn^{II} but balances the charge of the Zn^{II} cation. Previous studies revealed that the first row, divalent, transition metal ions have no tendency to coordinate to arenesulfonate (Kosnic *et al.*, 1992; Shubnell *et al.*, 1994; Gunderman *et al.*, 1997). The crystal of the title compound is stablized not only by electrostatic interactions but also by abundant hydrogen-bonding interactions between the cation $[Zn(2,2'\text{-bipy})(H_2O)_4]^{2+}$ and the anion $DSNT^{2-}$ (Fig. 2). All of the four coordinated waters build up an intricate hydrogen-bonding network with sulfonic oxygen (O5 and O6) and triazine nitrogen (N2) in the anion $DSNT^{2-}$.

Experimental

Preparation of $H_2DSNT{\cdot}4H_2O$: A solution of diethylamine (3.66 g 0.05 mol) in 20 mL acetone was added dropwise to a solution of cynanuic chloride (4.61 g, 0.025 mol) in 100 mL acetone at 0°, under stirring over a period of 45 min. The resulting white deposit $N(C_2H_5)_2{\cdot}HCl$ was filtered. To the filtrate was added dropwise a solution of 4-aminobenzenesulfonic sodium (9.81 g. 0.05 mol) in 200 mL water at 0°, under stirring over a period of 45 min, and then the mixture was heated to 45° and reacted with stirring for 12 h. After cooling to room temperature, acetone was evaporated in vacuo from the reaction solution. The white product $H_2DSNT{\cdot}4H_2O$ recrystallized in water and oven-dried at 60° in 70% yield.

Preparation of [Zn(2,2'-bipy)($H_2O)_4$]DSNT: A solution of $ZnCl_2$ (0.04 g, 0.3 mmol), 2,2'-bipy (0.07 g, 0.45 mmol), $H_2DSNT{\cdot}4H_2O$ (0.17 g, 0.3 mmol) and H_2O (27.0 g, 1.5 mol) in the mole ratio of 1:1.5:1:5000 was heated in an autoclave at 160° for 2 days and then cooled to room temperature for 3 days. The colorless crystals were collected in 62% yield.

Refinement

Anisotropic thermal parameters were applied to all non-hydrogen atoms. All H atoms were found in difference Fourier maps and all except water H atoms were subsequently placed in idealized positions with constrained distances of 0.96 Å (RCH_3),

0.97 Å (R_2CH_2), 0.95 Å ($R_2C_{ar}H$) and 0.86 Å (NH). U_{iso}(H) values were set to either 1.5U_{eq} (RCH_3) or 1.2U_{eq} of the attached atom. Water molecule hydrogen atoms were refined using restraints on bond lengths and angles.

Figures

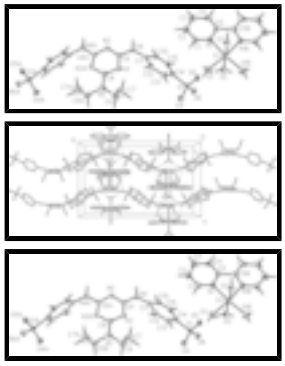


Figure 1. A view of the molecular structue of the title compound. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. Symmetry code: A x, 1/2 − y, z; B x, 3/2 − y, z.
Figure 2. Crystal structure of the title compound with hydrogen bonds indicated with dashed lines. Hydrogen atoms not taking part in hydrogen bonds were omitted for the sake of clarity.

Tetraaqua(2,2'-bipyridine)zinc(II) 4,4'-(6-diethylamino-1,3,5-triazine-2,4-diyldiimino)dibenzenesulfonate

Crystal data

$[Zn(C_{10}H_8N_2)(H_2O)_4](C_{19}H_{20}N_6O_6S_2)$	F_{000} = 1632
M_r = 786.19	D_x = 1.518 Mg m^{-3}
Orthorhombic, *Pnma*	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2n	Cell parameters from 7071 reflections
a = 12.758 (3) Å	θ = 2.3–27.5º
b = 21.015 (6) Å	μ = 0.90 mm^{-1}
c = 12.828 (4) Å	T = 293 (2) K
V = 3439.3 (17) Å^3	Prism, colorless
Z = 4	0.30 × 0.10 × 0.08 mm

Data collection

Rigaku Mercury CCD diffractometer	4045 independent reflections
Radiation source: Rotating Anode	3553 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SPHERE in CrystalStructure; Molecular Structure Corporation & Rigaku, 2000)'	h = −15→16
T_{min} = 0.886, T_{max} = 0.930	k = −27→27
25765 measured reflections	l = −14→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 2.7737P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
4045 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
5 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\sigma(F^2)$ 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}
Zn	0.43110 (4)	0.7500	0.85366 (3)	0.03891 (16)
S1	0.19593 (6)	0.59726 (3)	0.70886 (6)	0.0424 (2)
O1	0.4501 (2)	0.67945 (15)	0.7439 (2)	0.0709 (8)
H1	0.400 (2)	0.6628 (18)	0.713 (3)	0.072 (13)*
H2	0.507 (2)	0.661 (2)	0.735 (4)	0.091 (16)*
O2	0.2694 (3)	0.7500	0.8186 (3)	0.0562 (8)
H3	0.234 (3)	0.7166 (12)	0.814 (3)	0.065 (11)*
O3	0.5969 (3)	0.7500	0.8764 (2)	0.0452 (7)
H4	0.618 (4)	0.7500	0.939 (2)	0.061 (15)*
H5	0.649 (4)	0.7500	0.838 (5)	0.12 (3)*
O4	0.1134 (2)	0.57237 (12)	0.6439 (2)	0.0667 (7)
O5	0.15724 (18)	0.64062 (9)	0.78904 (18)	0.0525 (5)
O6	0.27985 (19)	0.62531 (10)	0.64805 (16)	0.0514 (5)
N1	0.40742 (19)	0.68676 (11)	0.98049 (19)	0.0421 (5)
N2	0.3459 (3)	0.2500	0.9167 (3)	0.0407 (8)
N3	0.3690 (2)	0.30689 (11)	0.75770 (19)	0.0435 (6)

N4	0.3375 (2)	0.35895 (11)	0.91325 (19)	0.0488 (6)
H4A	0.3432	0.3574	0.9800	0.059*
N5	0.3937 (3)	0.2500	0.6057 (3)	0.0537 (9)
C1	0.4098 (3)	0.62307 (15)	0.9743 (3)	0.0557 (8)
H1B	0.4235	0.6040	0.9103	0.067*
C2	0.3923 (3)	0.58491 (18)	1.0608 (4)	0.0706 (11)
H2C	0.3931	0.5408	1.0548	0.085*
C3	0.3740 (3)	0.6129 (2)	1.1541 (4)	0.0737 (12)
H3C	0.3624	0.5880	1.2128	0.088*
C4	0.3726 (3)	0.6784 (2)	1.1621 (3)	0.0625 (10)
H4C	0.3607	0.6980	1.2261	0.075*
C5	0.3892 (2)	0.71461 (15)	1.0731 (2)	0.0429 (6)
C6	0.3526 (2)	0.30361 (13)	0.8596 (2)	0.0391 (6)
C7	0.5088 (4)	0.3373 (3)	0.5446 (4)	0.1052 (18)
H7A	0.5078	0.3766	0.5064	0.158*
H7B	0.5549	0.3078	0.5106	0.158*
H7C	0.5332	0.3451	0.6142	0.158*
C8	0.3780 (3)	0.2500	0.7101 (3)	0.0417 (9)
C9	0.4006 (3)	0.31016 (19)	0.5486 (3)	0.0679 (10)
H9A	0.3543	0.3409	0.5812	0.082*
H9B	0.3760	0.3034	0.4778	0.082*
C10	0.2344 (3)	0.45445 (14)	0.9133 (2)	0.0494 (7)
H10A	0.2026	0.4406	0.9745	0.059*
C11	0.3135 (3)	0.41848 (13)	0.8685 (2)	0.0431 (7)
C12	0.3653 (3)	0.44191 (14)	0.7808 (3)	0.0510 (8)
H12A	0.4218	0.4197	0.7530	0.061*
C13	0.3325 (2)	0.49819 (14)	0.7351 (3)	0.0480 (7)
H13A	0.3667	0.5134	0.6761	0.058*
C14	0.2496 (2)	0.53166 (12)	0.7764 (2)	0.0393 (6)
C15	0.2028 (3)	0.51068 (14)	0.8677 (2)	0.0486 (7)
H15A	0.1498	0.5346	0.8983	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0438 (3)	0.0402 (3)	0.0327 (2)	0.000	−0.00015 (19)	0.000
S1	0.0499 (4)	0.0316 (3)	0.0458 (4)	0.0035 (3)	−0.0082 (3)	−0.0008 (3)
O1	0.0510 (15)	0.095 (2)	0.0670 (16)	0.0160 (15)	−0.0110 (13)	−0.0421 (16)
O2	0.0423 (17)	0.0390 (17)	0.087 (2)	0.000	−0.0084 (17)	0.000
O3	0.0445 (17)	0.0561 (18)	0.0349 (15)	0.000	0.0009 (13)	0.000
O4	0.0663 (16)	0.0561 (14)	0.0778 (18)	0.0017 (12)	−0.0350 (13)	−0.0046 (12)
O5	0.0641 (14)	0.0371 (10)	0.0563 (13)	0.0076 (10)	0.0041 (11)	−0.0052 (9)
O6	0.0677 (14)	0.0416 (11)	0.0449 (12)	−0.0003 (10)	0.0038 (10)	0.0052 (9)
N1	0.0406 (13)	0.0414 (12)	0.0442 (13)	−0.0023 (10)	0.0003 (10)	0.0057 (10)
N2	0.054 (2)	0.0332 (16)	0.0354 (16)	0.000	−0.0077 (15)	0.000
N3	0.0511 (14)	0.0411 (12)	0.0382 (12)	−0.0007 (11)	−0.0051 (11)	0.0041 (10)
N4	0.0758 (19)	0.0357 (12)	0.0349 (12)	0.0067 (12)	−0.0084 (12)	0.0020 (10)
N5	0.064 (2)	0.063 (2)	0.0337 (18)	0.000	0.0008 (18)	0.000

C1	0.0526 (18)	0.0438 (16)	0.071 (2)	−0.0014 (14)	−0.0004 (16)	0.0086 (16)
C2	0.056 (2)	0.056 (2)	0.100 (3)	−0.0105 (17)	−0.011 (2)	0.033 (2)
C3	0.053 (2)	0.090 (3)	0.079 (3)	−0.016 (2)	−0.0024 (19)	0.047 (2)
C4	0.0444 (17)	0.096 (3)	0.0467 (18)	−0.0018 (18)	0.0038 (14)	0.0224 (19)
C5	0.0303 (13)	0.0608 (17)	0.0376 (14)	−0.0021 (12)	−0.0008 (11)	0.0089 (13)
C6	0.0425 (15)	0.0381 (14)	0.0368 (14)	0.0009 (11)	−0.0094 (11)	0.0027 (11)
C7	0.098 (4)	0.123 (4)	0.095 (4)	−0.038 (3)	0.007 (3)	0.022 (3)
C8	0.038 (2)	0.049 (2)	0.038 (2)	0.000	−0.0039 (16)	0.000
C9	0.081 (3)	0.084 (3)	0.0393 (17)	−0.011 (2)	−0.0023 (17)	0.0125 (17)
C10	0.070 (2)	0.0414 (15)	0.0368 (14)	0.0017 (15)	0.0014 (14)	−0.0007 (12)
C11	0.0555 (18)	0.0329 (13)	0.0408 (15)	0.0004 (12)	−0.0107 (13)	0.0022 (11)
C12	0.0474 (17)	0.0424 (15)	0.063 (2)	0.0073 (13)	0.0045 (15)	0.0081 (14)
C13	0.0487 (16)	0.0417 (15)	0.0535 (17)	0.0023 (13)	0.0058 (14)	0.0092 (13)
C14	0.0439 (15)	0.0323 (13)	0.0416 (14)	−0.0005 (11)	−0.0081 (12)	−0.0022 (11)
C15	0.0619 (19)	0.0391 (15)	0.0447 (16)	0.0079 (14)	0.0044 (14)	−0.0041 (12)

Geometric parameters (Å, °)

Zn—O1	2.059 (3)	C1—C2	1.387 (5)
Zn—O1^{i}	2.059 (3)	C1—H1B	0.9300
Zn—O2	2.112 (3)	C2—C3	1.354 (6)
Zn—N1^{i}	2.122 (2)	C2—H2C	0.9300
Zn—N1	2.122 (2)	C3—C4	1.380 (6)
Zn—O3	2.135 (3)	C3—H3C	0.9300
S1—O4	1.441 (2)	C4—C5	1.388 (4)
S1—O6	1.450 (2)	C4—H4C	0.9300
S1—O5	1.460 (2)	C5—C5^{i}	1.487 (6)
S1—C14	1.766 (3)	C7—C9	1.495 (6)
O1—H1	0.829 (19)	C7—H7A	0.9600
O1—H2	0.825 (19)	C7—H7B	0.9600
O2—H3	0.840 (18)	C7—H7C	0.9600
O3—H4	0.841 (19)	C8—N3^{ii}	1.347 (3)
O3—H5	0.83 (2)	C9—H9A	0.9700
N1—C1	1.341 (4)	C9—H9B	0.9700
N1—C5	1.344 (4)	C10—C15	1.379 (4)
N2—C6	1.346 (3)	C10—C11	1.386 (4)
N2—C6^{ii}	1.346 (3)	C10—H10A	0.9300
N3—C6	1.326 (4)	C11—C12	1.394 (4)
N3—C8	1.347 (3)	C12—C13	1.385 (4)
N4—C6	1.365 (4)	C12—H12A	0.9300
N4—C11	1.410 (3)	C13—C14	1.376 (4)
N4—H4A	0.8600	C13—H13A	0.9300
N5—C8	1.355 (5)	C14—C15	1.387 (4)
N5—C9	1.464 (4)	C15—H15A	0.9300
N5—C9^{ii}	1.464 (4)		
O1—Zn—O1^{i}	92.1 (2)	C2—C3—C4	120.1 (3)
O1—Zn—O2	88.25 (11)	C2—C3—H3C	119.9

O1^{i}—Zn—O2	88.25 (11)	C4—C3—H3C	119.9
O1—Zn—N1^{i}	172.70 (12)	C3—C4—C5	118.9 (4)
O1^{i}—Zn—N1^{i}	95.18 (12)	C3—C4—H4C	120.6
O2—Zn—N1^{i}	91.38 (11)	C5—C4—H4C	120.6
O1—Zn—N1	95.18 (12)	N1—C5—C4	121.0 (3)
O1^{i}—Zn—N1	172.70 (12)	N1—C5—C5^{i}	115.81 (16)
O2—Zn—N1	91.38 (11)	C4—C5—C5^{i}	123.2 (2)
N1^{i}—Zn—N1	77.54 (14)	N3—C6—N2	126.1 (3)
O1—Zn—O3	88.68 (10)	N3—C6—N4	118.3 (2)
O1^{i}—Zn—O3	88.68 (10)	N2—C6—N4	115.5 (2)
O2—Zn—O3	175.57 (14)	C9—C7—H7A	109.5
N1^{i}—Zn—O3	92.07 (9)	C9—C7—H7B	109.5
N1—Zn—O3	92.07 (9)	H7A—C7—H7B	109.5
O4—S1—O6	112.06 (16)	C9—C7—H7C	109.5
O4—S1—O5	112.78 (16)	H7A—C7—H7C	109.5
O6—S1—O5	112.01 (13)	H7B—C7—H7C	109.5
O4—S1—C14	106.48 (14)	N3—C8—N3^{ii}	125.1 (4)
O6—S1—C14	107.15 (14)	N3—C8—N5	117.42 (18)
O5—S1—C14	105.83 (13)	N3^{ii}—C8—N5	117.42 (18)
Zn—O1—H1	122 (3)	N5—C9—C7	113.7 (4)
Zn—O1—H2	122 (3)	N5—C9—H9A	108.8
H1—O1—H2	115 (4)	C7—C9—H9A	108.8
Zn—O2—H3	123 (3)	N5—C9—H9B	108.8
Zn—O3—H4	116 (4)	C7—C9—H9B	108.8
Zn—O3—H5	135 (6)	H9A—C9—H9B	107.7
H4—O3—H5	108 (6)	C15—C10—C11	120.3 (3)
C1—N1—C5	119.4 (3)	C15—C10—H10A	119.9
C1—N1—Zn	125.2 (2)	C11—C10—H10A	119.9
C5—N1—Zn	115.41 (19)	C10—C11—C12	119.1 (3)
C6—N2—C6^{ii}	113.7 (3)	C10—C11—N4	118.2 (3)
C6—N3—C8	114.4 (3)	C12—C11—N4	122.6 (3)
C6—N4—C11	125.5 (2)	C13—C12—C11	120.0 (3)
C6—N4—H4A	117.2	C13—C12—H12A	120.0
C11—N4—H4A	117.2	C11—C12—H12A	120.0
C8—N5—C9	120.3 (2)	C14—C13—C12	120.3 (3)
C8—N5—C9^{ii}	120.3 (2)	C14—C13—H13A	119.8
C9—N5—C9^{ii}	119.5 (4)	C12—C13—H13A	119.8
N1—C1—C2	121.7 (4)	C13—C14—C15	119.6 (3)
N1—C1—H1B	119.1	C13—C14—S1	120.5 (2)
C2—C1—H1B	119.1	C15—C14—S1	119.7 (2)
C3—C2—C1	118.9 (4)	C10—C15—C14	120.3 (3)
C3—C2—H2C	120.6	C10—C15—H15A	119.8
C1—C2—H2C	120.6	C14—C15—H15A	119.8
O1—Zn—N1—C1	1.3 (3)	C6—N3—C8—N5	179.3 (3)
O2—Zn—N1—C1	89.7 (3)	C9—N5—C8—N3	0.2 (6)
N1^{i}—Zn—N1—C1	−179.2 (2)	C9^{ii}—N5—C8—N3	−177.9 (4)

O3—Zn—N1—C1	−87.5 (3)	C9—N5—C8—N3^{ii}	177.9 (4)
O1—Zn—N1—C5	−178.9 (2)	C9^{ii}—N5—C8—N3^{ii}	−0.2 (6)
O2—Zn—N1—C5	−90.6 (2)	C8—N5—C9—C7	87.6 (5)
N1^{i}—Zn—N1—C5	0.5 (2)	C9^{ii}—N5—C9—C7	−94.3 (5)
O3—Zn—N1—C5	92.2 (2)	C15—C10—C11—C12	4.2 (5)
C5—N1—C1—C2	1.0 (5)	C15—C10—C11—N4	−175.1 (3)
Zn—N1—C1—C2	−179.2 (3)	C6—N4—C11—C10	134.4 (3)
N1—C1—C2—C3	−1.0 (6)	C6—N4—C11—C12	−44.9 (5)
C1—C2—C3—C4	0.2 (6)	C10—C11—C12—C13	−4.7 (5)
C2—C3—C4—C5	0.6 (6)	N4—C11—C12—C13	174.6 (3)
C1—N1—C5—C4	−0.2 (4)	C11—C12—C13—C14	0.7 (5)
Zn—N1—C5—C4	−179.9 (2)	C12—C13—C14—C15	3.7 (5)
C1—N1—C5—C5^{i}	179.3 (2)	C12—C13—C14—S1	−171.3 (2)
Zn—N1—C5—C5^{i}	−0.5 (2)	O4—S1—C14—C13	90.6 (3)
C3—C4—C5—N1	−0.6 (5)	O6—S1—C14—C13	−29.5 (3)
C3—C4—C5—C5^{i}	180.0 (2)	O5—S1—C14—C13	−149.2 (2)
C8—N3—C6—N2	0.9 (5)	O4—S1—C14—C15	−84.4 (3)
C8—N3—C6—N4	−177.0 (3)	O6—S1—C14—C15	155.6 (2)
C6^{ii}—N2—C6—N3	−3.1 (6)	O5—S1—C14—C15	35.9 (3)
C6^{ii}—N2—C6—N4	174.8 (2)	C11—C10—C15—C14	0.2 (5)
C11—N4—C6—N3	15.7 (5)	C13—C14—C15—C10	−4.2 (5)
C11—N4—C6—N2	−162.4 (3)	S1—C14—C15—C10	170.9 (2)
C6—N3—C8—N3^{ii}	1.8 (6)		

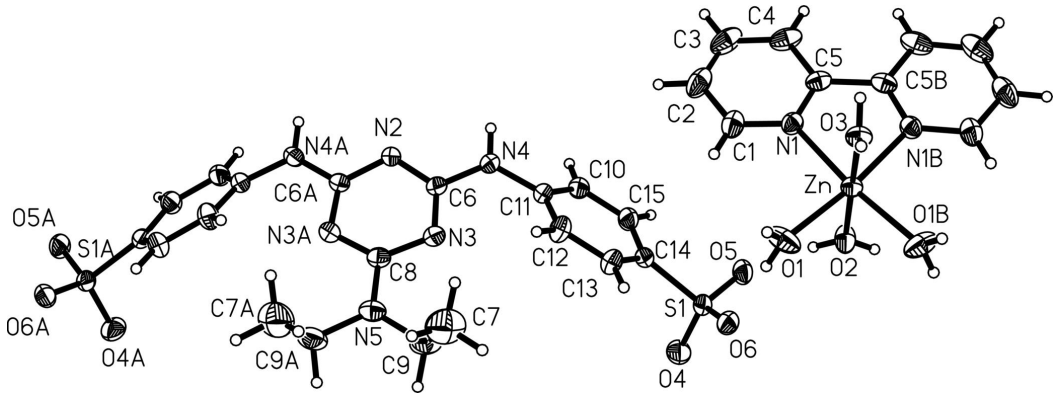
Symmetry codes: (i) *x*, −*y*+3/2, *z*; (ii) *x*, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O6	0.829 (19)	1.915 (19)	2.743 (4)	177 (4)
O1—H2···O5^{iii}	0.825 (19)	1.99 (2)	2.798 (4)	165 (5)
O2—H3···O5	0.840 (18)	1.898 (18)	2.734 (3)	174 (4)
O3—H4···N2^{iv}	0.841 (19)	1.91 (2)	2.753 (4)	176 (5)

Symmetry codes: (iii) *x*+1/2, *y*, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+2.

Fig. 1


C4
C3
C5
C5B
C2
C1
N1
O3
N1B
Zn
O1B
O1
O2
O5
C14
C15
C10
C11
C12
C13
S1
O6
O4
N4A
N2
N4
C6A
C6
N3A
N3
C8
O5A
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O6A
O4A
C7A
N5
C7
C9A
C9

Fig. 2

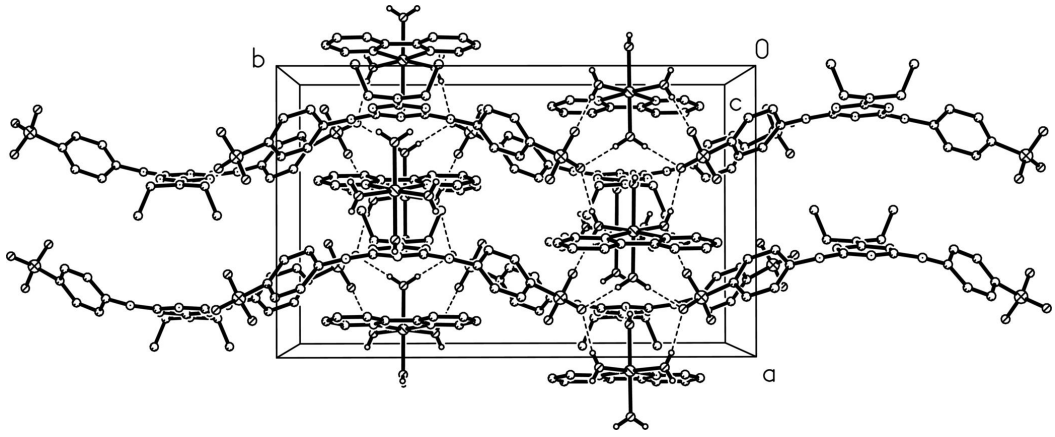
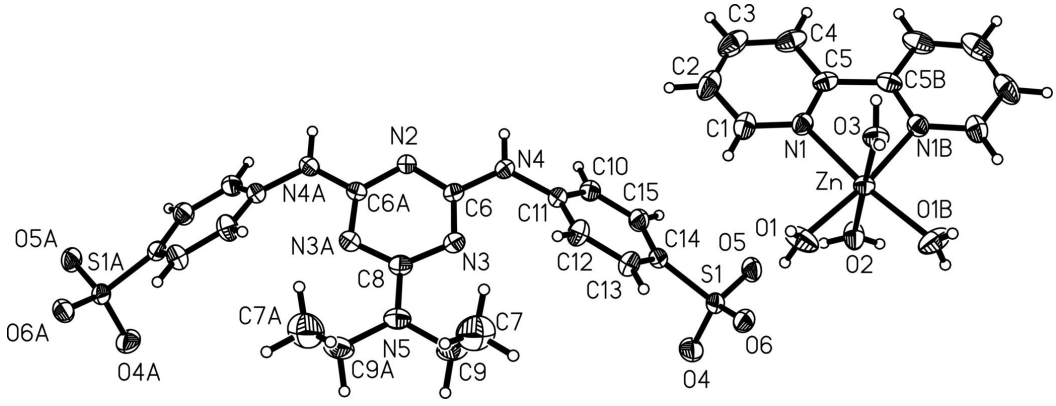


Fig. 3


C3
C4
C2
C5
C5B
C1
N1
O3
N1B
Zn
N2
N4
C10
C15
N4A
C6A
C6
C11
O1B
O5A
S1A
N3A
N3
C14
O5
O1
C12
C8
C13
S1
O2
C7A
C7
O6
O6A
N5
O4A
C9A
C9
O4