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(3-Carboxy-5-sulfonatobenzoato-$\kappa^2O^1,O^{1'}$)bis[2-(2-pyridyl)-1*H*-benzimidazole-κ^2N^2,N^3]zinc(II) monohydrate

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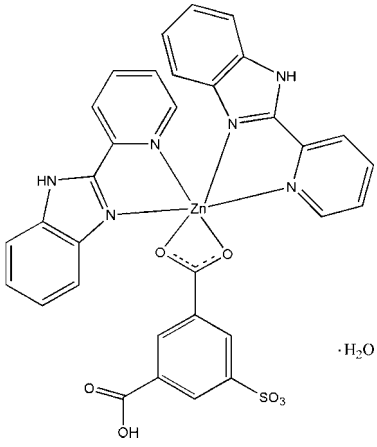
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.064; wR factor = 0.179; data-to-parameter ratio = 16.0.

In the title compound, $[Zn(C_8H_4O_7S)(C_{12}H_9N_3)_2]\cdot H_2O$, the Zn^{II} atom has a distorted octahedral coordination geometry, defined by four N atoms from two 2-(2-pyridyl)-1*H*-benzimidazole ligands and two O atoms from a deprotonated carboxylate group of the 3-carboxy-5-sulfonatobenzoate ligand. In the crystal structure, the complex molecules are linked into a three-dimensional network by intermolecular O—H···O and N—H···O hydrogen bonds, and π–π stacking interactions with centroid–centroid separations of 3.758 (2) and 3.597 (1) Å.

Related literature

For general background, see: Xia *et al.* (2005). For related structures, see: Kulynych & Shimizu (2002); Liu & Xu (2005); Sun *et al.* (2003); Xia *et al.* (2006).



Experimental

Crystal data

$[Zn(C_8H_4O_7S)(C_{12}H_9N_3)_2]\cdot H_2O$
M_r = 718.00
Triclinic, $P\overline{1}$
a = 11.086 (4) Å
b = 12.695 (5) Å
c = 13.347 (4) Å
α = 63.187 (10)°
β = 68.376 (13)°
γ = 87.122 (17)°
V = 1543.2 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 293 K
0.14 × 0.11 × 0.08 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
T_{min} = 0.843, T_{max} = 0.929
12166 measured reflections
6935 independent reflections
3857 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.179
S = 0.99
6935 reflections
434 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.080 (4)	Zn1—N6	2.210 (4)
Zn1—N3	2.257 (4)	Zn1—O1	2.216 (3)
Zn1—N4	2.067 (4)	Zn1—O2	2.193 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O1^{i}	0.86	2.15	2.884 (5)	143
N5—H5B···O3^{ii}	0.86	2.05	2.833 (5)	151
O1W—H1WA···O7^{iii}	0.82	1.87	2.678 (5)	167
O1W—H1WB···O6^{iv}	0.82	2.05	2.825 (5)	157
O4—H4B···O1W	0.82	1.78	2.575 (4)	163

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); 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: HY2185).

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supplementary materials

Acta Cryst. (2009). E**65**, m413-m414 [**doi:10.1107/S1600536809009180**]

(3-Carboxy-5-sulfonatobenzoato-$\kappa^2O^1,O^{1'}$)bis[2-(2-pyridyl)-1*H*-benzimidazole-κ^2N^2,N^3]zinc(II) monohydrate

L.-J. Chen, S. Lin, M.-X. Yang and X.-Y. Wu

Comment

Increasing interest has been focused on crystal engineering of supramolecular architectures organized by coordinating covalent bonds or supramolecular contacts such as hydrogen bonding and π–π interactions (Xia *et al.*, 2005). 5-Sulfoisophthalic acid (H_3sipa), which exhibits variation in possible binding modes of the two carboxylate groups and the soft sulfonate group, and a strong tendency to form large, tightly bound metal cluster, has been demonstrated as a useful bridge ligand for the construction of supramolecular structures (Kulynych & Shimizu *et al.*, 2002; Liu & Xu *et al.*, 2005; Sun *et al.*, 2003). On the other hand, 2-(2-pyridyl)-1*H*-benzimidazole (2-pbim) ligand presents multiple N-donor sites with the possibility of reversible protonation and deprotonation, and has the capacity to act as a donor or acceptor in the formation of multi-dimensional hydrogen bonded networks (Xia *et al.*, 2006). We report here the crystal structure of the title compound, which contains both Hsipa and 2-pbim ligands.

As shown in Fig. 1, the title complex consists of one Zn^{II} atom, two neutral 2-pbim ligands, one deprotonated $Hsipa^{2-}$ ligand and one uncoordinated water molecule. The Zn^{II} atom is six-coordinated by four N atoms from two 2-pbim ligands and two O atoms from one carboxylate group of the $Hsipa^{2-}$ ligand, forming a distorted octahedral geometry (Table 1). The chelate rings A (Zn1, N1, C7, C8, N3), B (Zn1, N4, C19, C20, N6) and C (Zn1, O1, C31, O2) are oriented at dihedral angles of A/B = 84.1 (1)°, A/C = 87.8 (1)° and B/C = 82.4 (1)°. The two 2-pbim ligands bonded to the same Zn atom are nearly perpendicular to each other.

In the crystal structure, the mononuclear Zn complex molecules are linked by intermolecular O—H···O and N—H···O hydrogen bonds involving the water molecule, the imino groups, the carboxyl groups and the sulfonate group, forming a three-dimensional network (Fig. 2 and Table 2). The structure is further stabilized by π–π stacking interactions between the benzene rings of neighboring benzimidazole moieties containing N4 and N5 atoms, and between the pyridyl ring containing N3 atom and benzimidazole moiety containing N1 and N2 atoms, with centroid-to-centroid distances of 3.758 (2) and 3.597 (1) Å, respectively.

Experimental

A mixture of $Zn(NO_3)_2.6H_2O$ (0.092 g, 0.3 mmol), NaH_2sipa (0.053 g, 0.2 mmol), 2-pbim (0.039 g, 0.2 mmol) and H_2O (10 ml) was placed in a 18 ml Teflon-lined Parr acid digestion bomb. The pH value of the reaction mixture was adjusted to *ca* 6.0 with 10% sodium hydroxide. The mixture was then heated for 3 d at 433 K under autogeneous pressure. Slow cooling of the reaction mixture to room temperature gave colorless prism crystals (yield: *ca* 78% based on Zn)

Refinement

The water H atoms were located in a difference Fourier map and fixed in refinement with O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed geometrically and refined as riding, with C—H = 0.93, O—H = 0.82 and N—H = 0.86 Å and with U_{iso}(H) = 1.5U_{eq}(O) or U_{iso}(H) = 1.2U_{eq}(C, N).

Figures

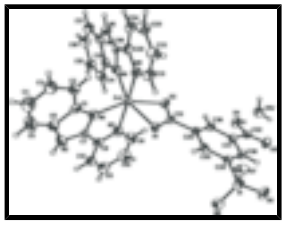

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

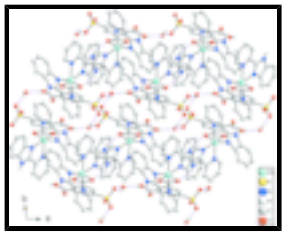

Fig. 2. A perspective view of the crystal packing down the *c* axis, showing hydrogen bonds (dashed lines). H atoms, which do not participate in hydrogen bonds, have been omitted for clarity.

(3-Carboxy-5-sulfonatobenzoato-κ^2*O*^{1},*O*$^{1'}$)bis[2-(2- pyridyl)-1*H*-benzimidazole-κ^2*N*^{2},*N*^{3}]zinc(II) monohydrate

Crystal data

$[Zn(C_8H_4O_7S)(C_{12}H_9N_3)_2]\cdot H_2O$	$Z = 2$
$M_r = 718.00$	$F_{000} = 736$
Triclinic, $P\overline{1}$	$D_x = 1.545$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.086$ (4) Å	Cell parameters from 3438 reflections
$b = 12.695$ (5) Å	$\theta = 2.4$–27.5º
$c = 13.347$ (4) Å	$\mu = 0.93$ mm^{-1}
$\alpha = 63.187$ (10)º	$T = 293$ K
$\beta = 68.376$ (13)º	Prism, colorless
$\gamma = 87.122$ (17)º	0.14 × 0.11 × 0.08 mm
$V = 1543.2$ (10) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	6935 independent reflections
Radiation source: fine-focus sealed tube	3857 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$

Detector resolution: 14.6306 pixels mm^{-1}

T = 293 K

ω scans

Absorption correction: multi-scan (CrystalClear; Rigaku, 2002)

T_{min} = 0.843, T_{max} = 0.929

12166 measured reflections

θ_{max} = 27.4°

θ_{min} = 2.4°

h = −13→14

k = −16→16

l = −14→17

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.064

$wR(F^2)$ = 0.179

S = 0.99

6935 reflections

434 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0855P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.89 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.43 e $Å^{-3}$

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.29944 (5)	0.17840 (5)	0.78119 (5)	0.0450 (2)
S1	0.04872 (11)	0.43789 (11)	1.21208 (10)	0.0462 (3)
N1	0.1432 (4)	0.0898 (4)	0.7857 (3)	0.0502 (10)
N2	0.0072 (4)	−0.0749 (4)	0.8695 (4)	0.0621 (11)
H2B	−0.0332	−0.1461	0.9201	0.075*
N3	0.2645 (4)	−0.0040 (4)	0.9412 (4)	0.0541 (10)
N4	0.4499 (3)	0.1749 (3)	0.6348 (3)	0.0498 (10)
N5	0.5526 (4)	0.2558 (3)	0.4336 (3)	0.0522 (10)
H5B	0.5771	0.3064	0.3577	0.063*
N6	0.3118 (4)	0.3556 (4)	0.6299 (4)	0.0507 (10)
C1	0.0720 (5)	0.1113 (5)	0.7172 (4)	0.0524 (12)
C2	0.0720 (5)	0.2091 (4)	0.6132 (4)	0.0537 (12)
H2A	0.1273	0.2798	0.5780	0.064*
C3	−0.0115 (6)	0.1981 (6)	0.5644 (6)	0.0768 (17)
H3A	−0.0120	0.2631	0.4942	0.092*
C4	−0.0948 (8)	0.0964 (7)	0.6132 (7)	0.107 (2)
H4A	−0.1491	0.0938	0.5751	0.128*
C5	−0.0999 (7)	−0.0010 (6)	0.7164 (6)	0.094 (2)
H5A	−0.1585	−0.0693	0.7506	0.113*
C6	−0.0172 (5)	0.0040 (5)	0.7683 (4)	0.0533 (12)
C7	0.1051 (4)	−0.0216 (4)	0.8756 (4)	0.0337 (9)
C8	0.1661 (4)	−0.0747 (4)	0.9639 (4)	0.0467 (11)
C9	0.3292 (5)	−0.0428 (5)	1.0183 (5)	0.0565 (13)

H9A	0.3984	0.0081	1.0031	0.068*
C10	0.2964 (6)	−0.1531 (5)	1.1166 (5)	0.0701 (16)
H10A	0.3428	−0.1773	1.1670	0.084*
C11	0.1900 (6)	−0.2302 (5)	1.1404 (5)	0.0663 (15)
H11A	0.1643	−0.3067	1.2057	0.080*
C12	0.1258 (4)	−0.1844 (4)	1.0597 (4)	0.0489 (11)
H12A	0.0539	−0.2308	1.0726	0.059*
C13	0.5302 (4)	0.0978 (4)	0.6075 (5)	0.0496 (11)
C14	0.5504 (5)	−0.0146 (4)	0.6844 (4)	0.0529 (12)
H14A	0.5075	−0.0499	0.7687	0.063*
C15	0.6384 (5)	−0.0690 (4)	0.6264 (5)	0.0598 (14)
H15A	0.6554	−0.1435	0.6742	0.072*
C16	0.7031 (5)	−0.0199 (5)	0.5016 (5)	0.0694 (16)
H16A	0.7606	−0.0624	0.4684	0.083*
C17	0.6843 (5)	0.0891 (5)	0.4266 (5)	0.0623 (14)
H17A	0.7289	0.1229	0.3425	0.075*
C18	0.5970 (4)	0.1477 (4)	0.4791 (4)	0.0408 (10)
C19	0.4634 (4)	0.2702 (4)	0.5279 (3)	0.0365 (9)
C20	0.3960 (4)	0.3701 (4)	0.5214 (4)	0.0494 (11)
C21	0.2430 (4)	0.4475 (5)	0.6353 (5)	0.0545 (13)
H21A	0.1845	0.4371	0.7110	0.065*
C22	0.2562 (5)	0.5530 (5)	0.5352 (5)	0.0650 (15)
H22A	0.2092	0.6138	0.5421	0.078*
C23	0.3456 (5)	0.5667 (5)	0.4189 (5)	0.0713 (16)
H23A	0.3580	0.6363	0.3475	0.086*
C24	0.4123 (5)	0.4727 (4)	0.4171 (4)	0.0520 (12)
H24A	0.4701	0.4792	0.3427	0.062*
C25	0.3076 (4)	0.3139 (3)	0.9990 (4)	0.0342 (9)
C26	0.4187 (4)	0.3155 (4)	1.0245 (4)	0.0365 (9)
H26A	0.4935	0.2897	0.9866	0.044*
C27	0.4184 (4)	0.3552 (3)	1.1057 (3)	0.0348 (9)
C28	0.3057 (4)	0.3945 (4)	1.1619 (3)	0.0385 (10)
H28A	0.3050	0.4219	1.2160	0.046*
C29	0.1968 (4)	0.3927 (3)	1.1374 (4)	0.0374 (9)
C30	0.1967 (4)	0.3535 (3)	1.0558 (4)	0.0373 (9)
H30A	0.1223	0.3536	1.0391	0.045*
C31	0.3042 (4)	0.2663 (4)	0.9162 (4)	0.0378 (9)
C32	0.5345 (4)	0.3540 (4)	1.1378 (4)	0.0370 (9)
O1	0.1971 (3)	0.2476 (3)	0.9116 (3)	0.0423 (7)
O1W	0.8425 (3)	0.3154 (3)	1.1201 (3)	0.0623 (9)
H1WA	0.8913	0.3655	1.0516	0.093*
H1WB	0.8553	0.3320	1.1686	0.093*
O2	0.4098 (3)	0.2450 (3)	0.8526 (3)	0.0477 (8)
O3	0.5390 (3)	0.3947 (3)	1.2030 (3)	0.0506 (8)
O4	0.6277 (3)	0.3028 (3)	1.0909 (3)	0.0538 (9)
H4B	0.6863	0.2999	1.1152	0.081*
O5	0.0764 (3)	0.4722 (3)	1.2907 (3)	0.0648 (10)
O6	−0.0514 (3)	0.3350 (3)	1.2746 (3)	0.0621 (9)
O7	0.0208 (3)	0.5357 (3)	1.1155 (3)	0.0687 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0400 (3)	0.0546 (3)	0.0383 (3)	−0.0070 (2)	−0.0047 (2)	−0.0269 (3)
S1	0.0416 (6)	0.0549 (7)	0.0433 (6)	0.0136 (5)	−0.0115 (5)	−0.0285 (6)
N1	0.044 (2)	0.060 (2)	0.048 (2)	0.0038 (19)	−0.0146 (19)	−0.028 (2)
N2	0.055 (2)	0.059 (3)	0.062 (3)	−0.009 (2)	−0.020 (2)	−0.020 (2)
N3	0.045 (2)	0.064 (3)	0.062 (3)	0.011 (2)	−0.018 (2)	−0.039 (2)
N4	0.040 (2)	0.061 (2)	0.046 (2)	−0.0001 (19)	−0.0109 (18)	−0.027 (2)
N5	0.063 (2)	0.047 (2)	0.043 (2)	0.0088 (19)	−0.0158 (19)	−0.0215 (19)
N6	0.045 (2)	0.065 (3)	0.052 (2)	0.0038 (19)	−0.0195 (19)	−0.035 (2)
C1	0.047 (3)	0.077 (3)	0.041 (3)	0.015 (3)	−0.018 (2)	−0.034 (3)
C2	0.056 (3)	0.056 (3)	0.043 (3)	0.001 (2)	−0.023 (2)	−0.014 (2)
C3	0.075 (4)	0.083 (4)	0.066 (4)	−0.002 (3)	−0.038 (3)	−0.021 (3)
C4	0.118 (6)	0.119 (6)	0.085 (5)	−0.011 (5)	−0.061 (5)	−0.030 (5)
C5	0.104 (5)	0.084 (5)	0.099 (5)	−0.008 (4)	−0.064 (4)	−0.025 (4)
C6	0.056 (3)	0.059 (3)	0.043 (3)	0.004 (2)	−0.027 (2)	−0.015 (2)
C7	0.031 (2)	0.039 (2)	0.033 (2)	−0.0007 (17)	−0.0100 (17)	−0.0193 (19)
C8	0.043 (3)	0.050 (3)	0.046 (3)	0.014 (2)	−0.010 (2)	−0.028 (2)
C9	0.050 (3)	0.063 (3)	0.069 (3)	0.016 (2)	−0.040 (3)	−0.027 (3)
C10	0.068 (4)	0.071 (4)	0.072 (4)	0.027 (3)	−0.043 (3)	−0.023 (3)
C11	0.081 (4)	0.051 (3)	0.058 (3)	0.022 (3)	−0.023 (3)	−0.023 (3)
C12	0.039 (2)	0.059 (3)	0.051 (3)	0.009 (2)	−0.016 (2)	−0.029 (3)
C13	0.043 (3)	0.053 (3)	0.061 (3)	0.002 (2)	−0.019 (2)	−0.033 (3)
C14	0.062 (3)	0.041 (2)	0.046 (3)	0.005 (2)	−0.022 (2)	−0.011 (2)
C15	0.066 (3)	0.048 (3)	0.054 (3)	0.009 (3)	−0.022 (3)	−0.016 (3)
C16	0.067 (3)	0.065 (3)	0.075 (4)	0.019 (3)	−0.022 (3)	−0.036 (3)
C17	0.064 (3)	0.062 (3)	0.065 (3)	0.016 (3)	−0.017 (3)	−0.040 (3)
C18	0.042 (2)	0.044 (2)	0.040 (2)	0.007 (2)	−0.017 (2)	−0.022 (2)
C19	0.036 (2)	0.045 (2)	0.029 (2)	−0.0028 (18)	−0.0073 (17)	−0.0207 (19)
C20	0.048 (3)	0.058 (3)	0.051 (3)	0.007 (2)	−0.020 (2)	−0.031 (3)
C21	0.045 (3)	0.068 (3)	0.052 (3)	0.022 (2)	−0.015 (2)	−0.034 (3)
C22	0.049 (3)	0.068 (3)	0.069 (4)	0.011 (3)	−0.019 (3)	−0.027 (3)
C23	0.072 (4)	0.060 (3)	0.072 (4)	0.011 (3)	−0.032 (3)	−0.019 (3)
C24	0.050 (3)	0.064 (3)	0.051 (3)	0.015 (2)	−0.023 (2)	−0.032 (3)
C25	0.034 (2)	0.035 (2)	0.035 (2)	0.0031 (17)	−0.0150 (18)	−0.0161 (18)
C26	0.035 (2)	0.041 (2)	0.034 (2)	0.0098 (18)	−0.0120 (18)	−0.0193 (19)
C27	0.038 (2)	0.037 (2)	0.030 (2)	0.0065 (18)	−0.0163 (18)	−0.0146 (18)
C28	0.051 (3)	0.041 (2)	0.031 (2)	0.013 (2)	−0.0198 (19)	−0.0198 (19)
C29	0.039 (2)	0.037 (2)	0.036 (2)	0.0081 (18)	−0.0145 (19)	−0.0169 (19)
C30	0.033 (2)	0.039 (2)	0.042 (2)	0.0064 (18)	−0.0157 (19)	−0.0194 (19)
C31	0.043 (2)	0.036 (2)	0.031 (2)	0.0025 (19)	−0.0127 (19)	−0.0139 (18)
C32	0.039 (2)	0.042 (2)	0.030 (2)	0.0044 (19)	−0.0171 (19)	−0.0148 (19)
O1	0.0378 (16)	0.0528 (18)	0.0429 (17)	0.0016 (14)	−0.0164 (13)	−0.0265 (15)
O1W	0.0470 (19)	0.079 (2)	0.065 (2)	0.0038 (17)	−0.0263 (17)	−0.033 (2)
O2	0.0410 (17)	0.066 (2)	0.0487 (18)	0.0060 (15)	−0.0128 (14)	−0.0399 (17)
O3	0.061 (2)	0.063 (2)	0.0505 (19)	0.0203 (17)	−0.0378 (17)	−0.0336 (17)

O4	0.0399 (17)	0.081 (2)	0.069 (2)	0.0196 (17)	−0.0302 (17)	−0.052 (2)
O5	0.059 (2)	0.090 (3)	0.069 (2)	0.0218 (19)	−0.0220 (18)	−0.060 (2)
O6	0.0487 (19)	0.070 (2)	0.058 (2)	−0.0001 (17)	−0.0080 (16)	−0.0316 (19)
O7	0.064 (2)	0.073 (2)	0.055 (2)	0.0364 (19)	−0.0182 (18)	−0.0244 (19)

Geometric parameters (Å, °)

Zn1—N1	2.080 (4)	C11—C12	1.401 (7)
Zn1—N3	2.257 (4)	C11—H11A	0.9300
Zn1—N4	2.067 (4)	C12—H12A	0.9300
Zn1—N6	2.210 (4)	C13—C14	1.398 (6)
Zn1—O1	2.216 (3)	C13—C18	1.421 (6)
Zn1—O2	2.193 (3)	C14—C15	1.373 (6)
S1—O5	1.431 (4)	C14—H14A	0.9300
S1—O7	1.453 (3)	C15—C16	1.381 (7)
S1—O6	1.453 (4)	C15—H15A	0.9300
S1—C29	1.798 (4)	C16—C17	1.355 (7)
N1—C7	1.332 (5)	C16—H16A	0.9300
N1—C1	1.348 (6)	C17—C18	1.371 (6)
N2—C7	1.353 (5)	C17—H17A	0.9300
N2—C6	1.387 (6)	C19—C20	1.423 (6)
N2—H2B	0.8600	C20—C24	1.368 (7)
N3—C8	1.303 (6)	C21—C22	1.364 (7)
N3—C9	1.366 (6)	C21—H21A	0.9300
N4—C19	1.351 (5)	C22—C23	1.437 (8)
N4—C13	1.371 (6)	C22—H22A	0.9300
N5—C19	1.367 (5)	C23—C24	1.376 (7)
N5—C18	1.377 (5)	C23—H23A	0.9300
N5—H5B	0.8600	C24—H24A	0.9300
N6—C20	1.335 (6)	C25—C30	1.390 (5)
N6—C21	1.377 (6)	C25—C26	1.397 (6)
C1—C2	1.384 (6)	C25—C31	1.490 (6)
C1—C6	1.449 (7)	C26—C27	1.384 (6)
C2—C3	1.356 (7)	C26—H26A	0.9300
C2—H2A	0.9300	C27—C28	1.399 (5)
C3—C4	1.364 (9)	C27—C32	1.497 (5)
C3—H3A	0.9300	C28—C29	1.367 (6)
C4—C5	1.357 (9)	C28—H28A	0.9300
C4—H4A	0.9300	C29—C30	1.386 (6)
C5—C6	1.355 (7)	C30—H30A	0.9300
C5—H5A	0.9300	C31—O1	1.251 (5)
C7—C8	1.458 (6)	C31—O2	1.267 (5)
C8—C12	1.345 (6)	C32—O3	1.211 (5)
C9—C10	1.362 (7)	C32—O4	1.306 (5)
C9—H9A	0.9300	O1W—H1WA	0.82
C10—C11	1.418 (8)	O1W—H1WB	0.82
C10—H10A	0.9300	O4—H4B	0.82
N4—Zn1—N1	100.37 (15)	C10—C11—H11A	122.0
N4—Zn1—O2	100.82 (13)	C8—C12—C11	121.3 (5)

N1—Zn1—O2	156.91 (13)	C8—C12—H12A	119.4
N4—Zn1—N6	77.61 (15)	C11—C12—H12A	119.4
N1—Zn1—N6	98.96 (15)	N4—C13—C14	130.1 (5)
O2—Zn1—N6	94.45 (13)	N4—C13—C18	109.4 (4)
N4—Zn1—O1	155.82 (14)	C14—C13—C18	120.5 (4)
N1—Zn1—O1	101.58 (13)	C15—C14—C13	115.1 (4)
O2—Zn1—O1	59.76 (10)	C15—C14—H14A	122.4
N6—Zn1—O1	89.04 (13)	C13—C14—H14A	122.4
N4—Zn1—N3	106.43 (14)	C14—C15—C16	124.1 (5)
N1—Zn1—N3	76.34 (16)	C14—C15—H15A	117.9
O2—Zn1—N3	88.94 (14)	C16—C15—H15A	117.9
N6—Zn1—N3	174.19 (13)	C17—C16—C15	121.0 (5)
O1—Zn1—N3	88.58 (13)	C17—C16—H16A	119.5
O5—S1—O7	113.4 (2)	C15—C16—H16A	119.5
O5—S1—O6	114.6 (2)	C16—C17—C18	117.6 (5)
O7—S1—O6	110.6 (2)	C16—C17—H17A	121.2
O5—S1—C29	106.1 (2)	C18—C17—H17A	121.2
O7—S1—C29	105.90 (19)	C17—C18—N5	133.7 (4)
O6—S1—C29	105.4 (2)	C17—C18—C13	121.7 (4)
C7—N1—C1	108.7 (4)	N5—C18—C13	104.6 (4)
C7—N1—Zn1	113.8 (3)	N4—C19—N5	109.7 (4)
C1—N1—Zn1	137.3 (4)	N4—C19—C20	122.6 (4)
C7—N2—C6	108.8 (4)	N5—C19—C20	127.7 (4)
C7—N2—H2B	125.6	N6—C20—C24	121.2 (4)
C6—N2—H2B	125.6	N6—C20—C19	113.3 (4)
C8—N3—C9	118.6 (4)	C24—C20—C19	125.5 (4)
C8—N3—Zn1	114.3 (3)	C22—C21—N6	123.3 (4)
C9—N3—Zn1	127.0 (4)	C22—C21—H21A	118.3
C19—N4—C13	107.0 (4)	N6—C21—H21A	118.3
C19—N4—Zn1	112.3 (3)	C21—C22—C23	117.5 (5)
C13—N4—Zn1	139.7 (3)	C21—C22—H22A	121.2
C19—N5—C18	109.3 (4)	C23—C22—H22A	121.2
C19—N5—H5B	125.3	C24—C23—C22	117.5 (5)
C18—N5—H5B	125.3	C24—C23—H23A	121.3
C20—N6—C21	118.5 (4)	C22—C23—H23A	121.3
C20—N6—Zn1	113.3 (3)	C20—C24—C23	121.9 (5)
C21—N6—Zn1	128.1 (3)	C20—C24—H24A	119.0
N1—C1—C2	133.3 (5)	C23—C24—H24A	119.0
N1—C1—C6	108.1 (4)	C30—C25—C26	119.0 (4)
C2—C1—C6	118.6 (4)	C30—C25—C31	119.7 (4)
C3—C2—C1	117.6 (5)	C26—C25—C31	121.3 (3)
C3—C2—H2A	121.2	C27—C26—C25	120.6 (4)
C1—C2—H2A	121.2	C27—C26—H26A	119.7
C2—C3—C4	123.3 (6)	C25—C26—H26A	119.7
C2—C3—H3A	118.4	C26—C27—C28	119.5 (4)
C4—C3—H3A	118.4	C26—C27—C32	121.7 (3)
C5—C4—C3	121.2 (6)	C28—C27—C32	118.8 (4)
C5—C4—H4A	119.4	C29—C28—C27	120.0 (4)
C3—C4—H4A	119.4	C29—C28—H28A	120.0

C6—C5—C4	118.3 (6)	C27—C28—H28A	120.0
C6—C5—H5A	120.9	C28—C29—C30	120.8 (4)
C4—C5—H5A	120.9	C28—C29—S1	121.1 (3)
C5—C6—N2	134.9 (5)	C30—C29—S1	118.2 (3)
C5—C6—C1	121.1 (5)	C29—C30—C25	120.2 (4)
N2—C6—C1	104.0 (4)	C29—C30—H30A	119.9
N1—C7—N2	110.4 (4)	C25—C30—H30A	119.9
N1—C7—C8	122.6 (4)	O1—C31—O2	121.4 (4)
N2—C7—C8	127.0 (4)	O1—C31—C25	119.3 (4)
N3—C8—C12	122.8 (5)	O2—C31—C25	119.3 (4)
N3—C8—C7	112.8 (4)	O1—C31—Zn1	61.3 (2)
C12—C8—C7	124.4 (5)	O2—C31—Zn1	60.2 (2)
C10—C9—N3	122.7 (5)	C25—C31—Zn1	178.0 (3)
C10—C9—H9A	118.7	O3—C32—O4	124.1 (4)
N3—C9—H9A	118.7	O3—C32—C27	122.6 (4)
C9—C10—C11	118.6 (5)	O4—C32—C27	113.3 (4)
C9—C10—H10A	120.7	C31—O1—Zn1	89.1 (2)
C11—C10—H10A	120.7	H1WA—O1W—H1WB	106.3
C12—C11—C10	116.1 (5)	C31—O2—Zn1	89.7 (3)
C12—C11—H11A	122.0	C32—O4—H4B	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O1^{i}	0.86	2.15	2.884 (5)	143
N5—H5B···O3^{ii}	0.86	2.05	2.833 (5)	151
O1W—H1WA···O7^{iii}	0.82	1.87	2.678 (5)	167
O1W—H1WB···O6^{iv}	0.82	2.05	2.825 (5)	157
O4—H4B···O1W	0.82	1.78	2.575 (4)	163

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

Fig. 1

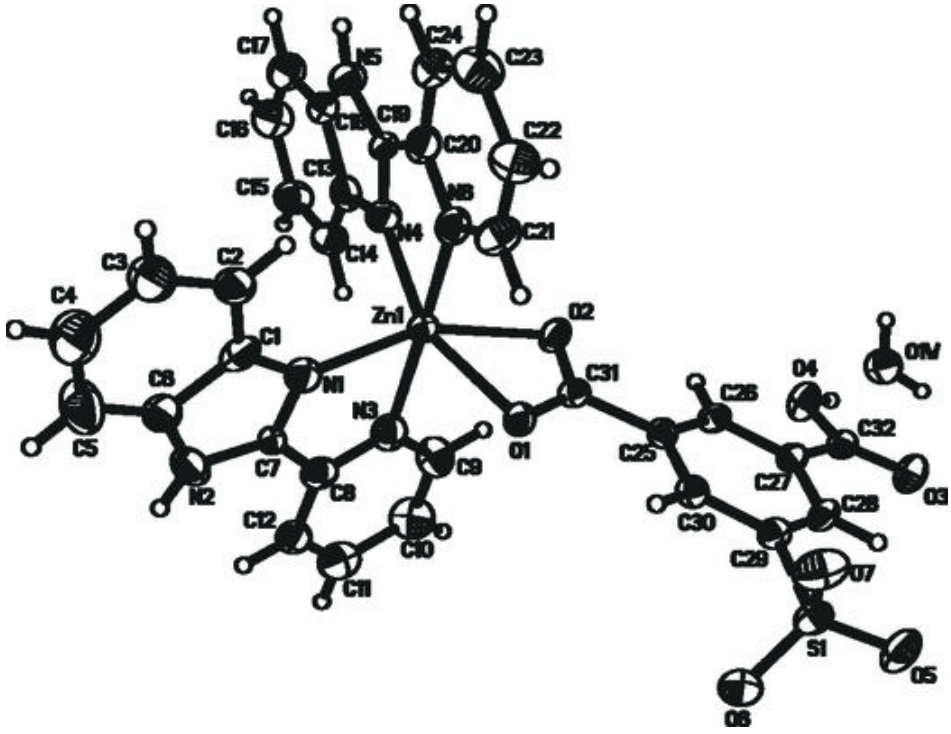
C17
N5
C24
C23
C18
C19
C22
C20
C13
C15
N6
N4
C21
C14
C3
C2
C4
Zn1
O2
C1
O1W
O4
C31
N1
C26
C8
N3
C32
C5
C7
C9
O1
C25
C27
O3
N2
C6
C28
C12
C30
C10
C29
O7
C11
S1
O5
O6

Fig. 2