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[1-(4-Hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato-κ^3N,O,S]-(1,10-phenanthroline-κ^2N,N')zinc(II)–4,4′-bipyridine (2/1)

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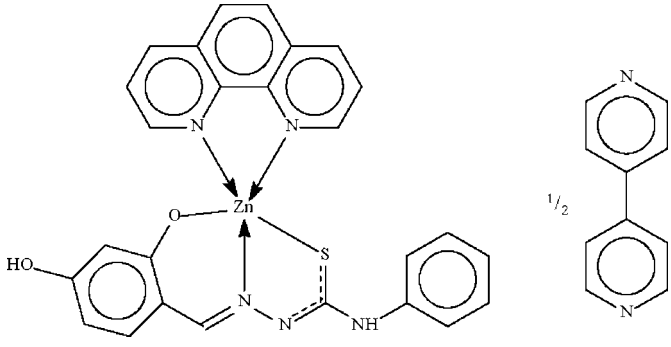
Key indicators: single-crystal X-ray study; T = 140 K; mean σ(C–C) = 0.007 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 12.4.

The Zn^{II} atom in the title compound, $[Zn(C_{14}H_{11}N_3O_2S)(C_{12}H_8N_2)]\cdot0.5C_{10}H_8N_2$, is N,N'-chelated by the N-heterocycle and N,O,S-chelated by the deprotonated Schiff base in a square-pyramidal environment. The hydroxy group of the Schiff base is a hydrogen-bond donor to 4,4′-bipyridine, which is located about a center of inversion, resulting in the formation of a supramolecular trimeric unit.

Related literature

For [1-(4-hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato](1,10-phenanthroline)zinc dimethyl sulfoxide disolvate hydrate, see: Tan *et al.* (2009). For other *N*-heterocyclic adducts of zinc 1-(2-oxidobenzylidene)-4-phenylthiosemicarbonates, see: Deng *et al.* (2007); Seena & Kurup (2008).



Experimental

Crystal data

$[Zn(C_{14}H_{11}N_3O_2S)(C_{12}H_8N_2)]\cdot0.5C_{10}H_8N_2$
M_r = 608.98
Monoclinic, $P2_1/c$
a = 11.6372 (6) Å
b = 9.8376 (5) Å
c = 23.288 (1) Å
β = 92.417 (3)°
V = 2663.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 140 K
0.10 × 0.04 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.903, T_{max} = 0.979
14867 measured reflections
4681 independent reflections
2918 reflections with $I > 2\sigma(I)$
R_{int} = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.117
S = 0.98
4681 reflections
378 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N6	0.84 (5)	2.01 (5)	2.839 (6)	168 (6)

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2484).

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supplementary materials

Acta Cryst. (2009). E**65**, m920 [**doi:10.1107/S1600536809026245**]

[1-(4-Hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato-κ^3N,O,S](1,10-phenanthroline-κ^2N,N')zinc(II)-4,4'-bipyridine (2/1)

K. W. Tan, C. H. Ng, M. J. Maah and S. W. Ng

Experimental

Zinc acetate monohydrate (0.22 g, 1 mmol), 2,4-dihydroxybenzaldehyde 4-phenylthiosemicarbazone (0.29 g, 1 mmol) and 1,10-phenanthroline (0.18 g, 1 mmol) were heated in ethanol (50 ml). The product was isolated and reacted with 4,4'-bipyridine (0.15 g, 1 mmol) in DMF to give a yellow solution. A small amount of tiny crystals were isolated when the mixture was set aside for a week.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation with U(H) set to 1.2U_{eq}(C). The amino- and hydroxy H-atoms were refined with distance restraints of O–H 0.84±0.01 Å and N–H 0.88±0.01 Å, respectively; their temperature factors were refined.

Figures

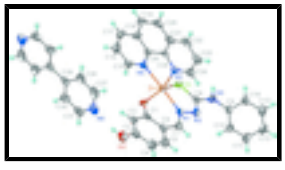


Fig. 1. Thermal ellipsoid (Barbour, 2001) plot of $Zn(C_{12}H_8N_2)(C_{14}H_{11}N_3O_2S)\cdot 0.5C_{10}H_8N_2$ at the 70% probability level. Only atoms comprising the asymmetric unit are labelled; the 4,4'-bipyridine molecule is located about a center of inversion. Hydrogen atoms are drawn as spheres of arbitrary radii.

[1-(4-Hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato- κ^3N,O,S](1,10-phenanthroline-κ^2N,N')zinc(II)–4,4'-bipyridine (2/1)

Crystal data

$[Zn(C_{14}H_{11}N_3O_2S)(C_{12}H_8N_2)]\cdot 0.5C_{10}H_8N_2$	F_{000} = 1252
M_r = 608.98	D_x = 1.519 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1335 reflections
a = 11.6372 (6) Å	θ = 2.4–20.2°
b = 9.8376 (5) Å	μ = 1.04 mm^{-1}
c = 23.288 (1) Å	T = 140 K
β = 92.417 (3)°	Prism, yellow
V = 2663.7 (2) Å^3	0.10 × 0.04 × 0.02 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	4681 independent reflections
Radiation source: fine-focus sealed tube	2918 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.089$
$T = 140$ K	$\theta_{max} = 25.0^{o}$
ω scans	$\theta_{min} = 1.8^{o}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -13 \rightarrow 13$
$T_{min} = 0.903$, $T_{max} = 0.979$	$k = -11 \rightarrow 11$
14867 measured reflections	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.117$	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} = 0.001$
4681 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
378 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.67107 (4)	0.62440 (5)	0.56348 (2)	0.02152 (16)
S1	0.82614 (10)	0.50702 (12)	0.52318 (5)	0.0236 (3)
O1	0.5106 (2)	0.6211 (3)	0.58865 (12)	0.0257 (7)
O2	0.2250 (3)	0.7085 (4)	0.72356 (16)	0.0416 (9)
H2	0.188 (5)	0.738 (6)	0.6945 (16)	0.07 (2)*
N1	0.7189 (3)	0.5107 (4)	0.63475 (15)	0.0216 (9)
N2	0.8294 (3)	0.4544 (4)	0.63924 (15)	0.0256 (9)
N3	0.9923 (3)	0.4067 (4)	0.59142 (16)	0.0263 (10)
H3	1.029 (3)	0.427 (5)	0.5604 (12)	0.036 (15)*
N4	0.6154 (3)	0.7367 (4)	0.48877 (15)	0.0218 (9)
N5	0.7320 (3)	0.8198 (4)	0.58516 (15)	0.0222 (9)
N6	0.1202 (3)	0.8459 (4)	0.62781 (18)	0.0371 (11)
C1	0.4781 (4)	0.6105 (5)	0.64195 (18)	0.0242 (10)
C2	0.3686 (4)	0.6607 (5)	0.6553 (2)	0.0272 (12)
H2A	0.3205	0.6984	0.6254	0.033*

C3	0.3294 (4)	0.6565 (5)	0.7103 (2)	0.0327 (13)
C4	0.3969 (4)	0.5966 (5)	0.7542 (2)	0.0380 (14)
H4	0.3703	0.5929	0.7922	0.046*
C5	0.5007 (4)	0.5436 (6)	0.7423 (2)	0.0364 (13)
H5A	0.5445	0.5004	0.7724	0.044*
C6	0.5469 (4)	0.5492 (5)	0.68749 (19)	0.0261 (11)
C7	0.6604 (4)	0.4965 (5)	0.68069 (19)	0.0259 (11)
H7	0.6954	0.4477	0.7120	0.031*
C8	0.8810 (4)	0.4554 (4)	0.59072 (19)	0.0217 (11)
C9	1.0617 (4)	0.3594 (5)	0.63889 (19)	0.0237 (11)
C10	1.0185 (4)	0.2924 (5)	0.68556 (19)	0.0281 (12)
H10	0.9378	0.2823	0.6887	0.034*
C11	1.0937 (4)	0.2399 (5)	0.7278 (2)	0.0353 (13)
H11	1.0642	0.1921	0.7594	0.042*
C12	1.2121 (4)	0.2566 (5)	0.7242 (2)	0.0365 (13)
H12	1.2633	0.2211	0.7533	0.044*
C13	1.2540 (4)	0.3249 (5)	0.6781 (2)	0.0376 (14)
H13	1.3346	0.3377	0.6757	0.045*
C14	1.1812 (4)	0.3749 (5)	0.63541 (19)	0.0276 (11)
H14	1.2116	0.4202	0.6034	0.033*
C15	0.5563 (4)	0.6950 (5)	0.44181 (19)	0.0253 (11)
H15	0.5412	0.6006	0.4374	0.030*
C16	0.5157 (4)	0.7832 (6)	0.3990 (2)	0.0365 (14)
H16	0.4727	0.7499	0.3664	0.044*
C17	0.5390 (4)	0.9194 (6)	0.4048 (2)	0.0331 (13)
H17	0.5125	0.9813	0.3759	0.040*
C18	0.6018 (4)	0.9676 (5)	0.45336 (19)	0.0281 (12)
C19	0.6260 (4)	1.1078 (5)	0.4628 (2)	0.0367 (13)
H19	0.5970	1.1731	0.4359	0.044*
C20	0.6895 (4)	1.1493 (5)	0.5093 (2)	0.0380 (14)
H20	0.7080	1.2429	0.5136	0.046*
C21	0.7297 (4)	1.0533 (5)	0.5525 (2)	0.0307 (12)
C22	0.7924 (4)	1.0906 (5)	0.6035 (2)	0.0345 (13)
H22	0.8121	1.1830	0.6104	0.041*
C23	0.8244 (4)	0.9928 (5)	0.6427 (2)	0.0339 (13)
H23	0.8681	1.0161	0.6767	0.041*
C24	0.7919 (4)	0.8584 (5)	0.63216 (19)	0.0294 (12)
H24	0.8137	0.7912	0.6599	0.035*
C25	0.7022 (4)	0.9150 (4)	0.54532 (19)	0.0202 (10)
C26	0.6384 (4)	0.8709 (5)	0.49423 (18)	0.0212 (10)
C27	0.1329 (4)	0.9783 (5)	0.6168 (2)	0.0398 (14)
H27	0.1749	1.0319	0.6443	0.048*
C28	0.0887 (4)	1.0418 (5)	0.5679 (2)	0.0343 (13)
H28	0.1017	1.1361	0.5624	0.041*
C29	0.0256 (4)	0.9682 (5)	0.52677 (19)	0.0281 (12)
C30	0.0133 (5)	0.8298 (5)	0.5379 (2)	0.0347 (13)
H30	−0.0280	0.7736	0.5110	0.042*
C31	0.0606 (4)	0.7748 (5)	0.5876 (2)	0.0378 (13)
H31	0.0504	0.6802	0.5938	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0209 (3)	0.0191 (3)	0.0250 (3)	0.0013 (3)	0.0065 (2)	0.0033 (3)
S1	0.0228 (7)	0.0254 (7)	0.0230 (6)	0.0049 (5)	0.0050 (5)	0.0021 (5)
O1	0.0252 (18)	0.0252 (17)	0.0272 (17)	0.0055 (16)	0.0083 (14)	0.0099 (16)
O2	0.028 (2)	0.058 (3)	0.041 (2)	0.0082 (19)	0.0113 (19)	−0.001 (2)
N1	0.019 (2)	0.020 (2)	0.026 (2)	0.0015 (17)	0.0051 (17)	−0.0013 (17)
N2	0.022 (2)	0.029 (2)	0.026 (2)	0.0051 (18)	0.0033 (18)	0.0001 (18)
N3	0.025 (2)	0.033 (3)	0.022 (2)	0.0056 (19)	0.0056 (19)	0.0049 (19)
N4	0.024 (2)	0.020 (2)	0.022 (2)	0.0007 (17)	0.0064 (17)	−0.0015 (17)
N5	0.022 (2)	0.025 (2)	0.020 (2)	0.0028 (17)	0.0074 (18)	0.0015 (17)
N6	0.024 (2)	0.044 (3)	0.044 (3)	0.005 (2)	0.010 (2)	−0.012 (2)
C1	0.022 (3)	0.023 (3)	0.028 (3)	−0.006 (2)	0.011 (2)	−0.005 (2)
C2	0.021 (3)	0.033 (3)	0.028 (3)	−0.001 (2)	0.006 (2)	0.004 (2)
C3	0.018 (3)	0.044 (3)	0.037 (3)	−0.002 (2)	0.009 (2)	−0.005 (2)
C4	0.032 (3)	0.062 (4)	0.020 (3)	0.000 (3)	0.009 (2)	−0.003 (3)
C5	0.025 (3)	0.058 (4)	0.027 (3)	0.000 (3)	0.001 (2)	−0.001 (3)
C6	0.022 (3)	0.035 (3)	0.022 (2)	−0.003 (2)	0.002 (2)	−0.004 (2)
C7	0.029 (3)	0.029 (3)	0.020 (2)	0.001 (2)	0.004 (2)	0.004 (2)
C8	0.020 (3)	0.017 (3)	0.028 (3)	0.000 (2)	0.003 (2)	0.000 (2)
C9	0.024 (3)	0.023 (3)	0.025 (2)	0.008 (2)	0.001 (2)	−0.002 (2)
C10	0.027 (3)	0.026 (3)	0.031 (3)	0.007 (2)	−0.003 (2)	0.002 (2)
C11	0.036 (3)	0.043 (3)	0.027 (3)	0.010 (3)	0.001 (2)	0.002 (3)
C12	0.032 (3)	0.051 (4)	0.026 (3)	0.013 (3)	−0.002 (2)	−0.002 (3)
C13	0.026 (3)	0.050 (4)	0.036 (3)	0.007 (3)	−0.001 (3)	−0.009 (3)
C14	0.027 (3)	0.028 (3)	0.028 (2)	0.001 (2)	0.005 (2)	−0.003 (2)
C15	0.024 (3)	0.026 (3)	0.026 (3)	0.002 (2)	0.007 (2)	−0.007 (2)
C16	0.027 (3)	0.064 (4)	0.019 (3)	0.008 (3)	0.001 (2)	−0.006 (3)
C17	0.028 (3)	0.050 (4)	0.022 (3)	0.013 (3)	0.010 (2)	0.012 (2)
C18	0.027 (3)	0.032 (3)	0.027 (3)	0.009 (2)	0.012 (2)	0.008 (2)
C19	0.025 (3)	0.033 (3)	0.052 (3)	0.010 (3)	0.015 (3)	0.021 (3)
C20	0.028 (3)	0.021 (3)	0.067 (4)	0.005 (2)	0.022 (3)	0.009 (3)
C21	0.024 (3)	0.029 (3)	0.040 (3)	0.002 (2)	0.016 (2)	−0.005 (3)
C22	0.024 (3)	0.029 (3)	0.052 (3)	−0.007 (2)	0.015 (3)	−0.016 (3)
C23	0.028 (3)	0.037 (3)	0.037 (3)	−0.009 (3)	0.005 (2)	−0.015 (3)
C24	0.027 (3)	0.037 (3)	0.025 (3)	0.000 (2)	0.006 (2)	−0.001 (2)
C25	0.017 (2)	0.014 (2)	0.030 (3)	−0.0016 (19)	0.012 (2)	−0.001 (2)
C26	0.018 (2)	0.020 (2)	0.026 (2)	0.007 (2)	0.0075 (19)	−0.001 (2)
C27	0.028 (3)	0.038 (3)	0.053 (4)	0.002 (3)	−0.002 (3)	−0.022 (3)
C28	0.032 (3)	0.024 (3)	0.047 (3)	0.002 (2)	0.002 (3)	−0.012 (3)
C29	0.018 (3)	0.029 (3)	0.038 (3)	−0.003 (2)	0.011 (2)	−0.012 (2)
C30	0.039 (3)	0.026 (3)	0.041 (3)	−0.006 (2)	0.009 (3)	−0.007 (2)
C31	0.035 (3)	0.028 (3)	0.051 (3)	−0.007 (3)	0.011 (3)	−0.003 (3)

Geometric parameters (Å, °)

Zn1—O1	1.981 (3)	C11—C12	1.394 (7)

Zn1—N1	2.058 (4)	C11—H11	0.9500
Zn1—N5	2.103 (4)	C12—C13	1.373 (7)
Zn1—N4	2.138 (3)	C12—H12	0.9500
Zn1—S1	2.3692 (12)	C13—C14	1.370 (6)
S1—C8	1.748 (4)	C13—H13	0.9500
O1—C1	1.317 (5)	C14—H14	0.9500
O2—C3	1.365 (6)	C15—C16	1.389 (6)
O2—H2	0.84 (5)	C15—H15	0.9500
N1—C7	1.299 (5)	C16—C17	1.373 (7)
N1—N2	1.401 (5)	C16—H16	0.9500
N2—C8	1.302 (5)	C17—C18	1.402 (7)
N3—C8	1.380 (6)	C17—H17	0.9500
N3—C9	1.419 (6)	C18—C26	1.399 (6)
N3—H3	0.88 (3)	C18—C19	1.423 (7)
N4—C15	1.332 (5)	C19—C20	1.347 (7)
N4—C26	1.352 (6)	C19—H19	0.9500
N5—C24	1.328 (5)	C20—C21	1.445 (7)
N5—C25	1.353 (5)	C20—H20	0.9500
N6—C27	1.336 (7)	C21—C25	1.406 (6)
N6—C31	1.340 (6)	C21—C22	1.414 (7)
C1—C2	1.413 (6)	C22—C23	1.368 (7)
C1—C6	1.434 (6)	C22—H22	0.9500
C2—C3	1.379 (6)	C23—C24	1.394 (7)
C2—H2A	0.9500	C23—H23	0.9500
C3—C4	1.392 (7)	C24—H24	0.9500
C4—C5	1.356 (7)	C25—C26	1.442 (6)
C4—H4	0.9500	C27—C28	1.379 (7)
C5—C6	1.406 (6)	C27—H27	0.9500
C5—H5A	0.9500	C28—C29	1.386 (6)
C6—C7	1.435 (6)	C28—H28	0.9500
C7—H7	0.9500	C29—C30	1.394 (7)
C9—C10	1.384 (6)	C29—C29^{i}	1.495 (9)
C9—C14	1.405 (6)	C30—C31	1.371 (7)
C10—C11	1.388 (6)	C30—H30	0.9500
C10—H10	0.9500	C31—H31	0.9500
O1—Zn1—N1	88.77 (13)	C13—C12—C11	119.3 (5)
O1—Zn1—N5	104.84 (13)	C13—C12—H12	120.3
N1—Zn1—N5	103.07 (14)	C11—C12—H12	120.3
O1—Zn1—N4	89.56 (13)	C14—C13—C12	120.9 (5)
N1—Zn1—N4	177.58 (14)	C14—C13—H13	119.6
N5—Zn1—N4	79.07 (14)	C12—C13—H13	119.6
O1—Zn1—S1	148.49 (10)	C13—C14—C9	120.2 (5)
N1—Zn1—S1	82.54 (10)	C13—C14—H14	119.9
N5—Zn1—S1	106.62 (10)	C9—C14—H14	119.9
N4—Zn1—S1	98.00 (10)	N4—C15—C16	123.0 (5)
C8—S1—Zn1	92.34 (15)	N4—C15—H15	118.5
C1—O1—Zn1	126.3 (3)	C16—C15—H15	118.5
C3—O2—H2	113 (4)	C17—C16—C15	118.6 (5)

C7—N1—N2	114.0 (4)	C17—C16—H16	120.7
C7—N1—Zn1	126.1 (3)	C15—C16—H16	120.7
N2—N1—Zn1	119.4 (3)	C16—C17—C18	120.2 (5)
C8—N2—N1	112.8 (4)	C16—C17—H17	119.9
C8—N3—C9	128.7 (4)	C18—C17—H17	119.9
C8—N3—H3	114 (3)	C26—C18—C17	116.9 (4)
C9—N3—H3	116 (3)	C26—C18—C19	120.0 (5)
C15—N4—C26	118.1 (4)	C17—C18—C19	123.0 (5)
C15—N4—Zn1	129.6 (3)	C20—C19—C18	121.1 (5)
C26—N4—Zn1	112.1 (3)	C20—C19—H19	119.4
C24—N5—C25	118.6 (4)	C18—C19—H19	119.4
C24—N5—Zn1	128.2 (3)	C19—C20—C21	120.8 (5)
C25—N5—Zn1	113.2 (3)	C19—C20—H20	119.6
C27—N6—C31	115.6 (5)	C21—C20—H20	119.6
O1—C1—C2	118.5 (4)	C25—C21—C22	117.3 (5)
O1—C1—C6	123.8 (4)	C25—C21—C20	118.9 (5)
C2—C1—C6	117.7 (4)	C22—C21—C20	123.8 (5)
C3—C2—C1	122.0 (4)	C23—C22—C21	119.6 (5)
C3—C2—H2A	119.0	C23—C22—H22	120.2
C1—C2—H2A	119.0	C21—C22—H22	120.2
O2—C3—C2	122.1 (4)	C22—C23—C24	119.0 (5)
O2—C3—C4	118.2 (4)	C22—C23—H23	120.5
C2—C3—C4	119.7 (4)	C24—C23—H23	120.5
C5—C4—C3	119.5 (4)	N5—C24—C23	123.0 (5)
C5—C4—H4	120.2	N5—C24—H24	118.5
C3—C4—H4	120.2	C23—C24—H24	118.5
C4—C5—C6	123.3 (5)	N5—C25—C21	122.5 (4)
C4—C5—H5A	118.4	N5—C25—C26	117.8 (4)
C6—C5—H5A	118.4	C21—C25—C26	119.8 (4)
C5—C6—C1	117.7 (4)	N4—C26—C18	123.1 (4)
C5—C6—C7	118.3 (4)	N4—C26—C25	117.6 (4)
C1—C6—C7	123.9 (4)	C18—C26—C25	119.2 (4)
N1—C7—C6	124.6 (4)	N6—C27—C28	124.0 (5)
N1—C7—H7	117.7	N6—C27—H27	118.0
C6—C7—H7	117.7	C28—C27—H27	118.0
N2—C8—N3	117.0 (4)	C27—C28—C29	120.2 (5)
N2—C8—S1	128.2 (4)	C27—C28—H28	119.9
N3—C8—S1	114.7 (3)	C29—C28—H28	119.9
C10—C9—C14	119.4 (4)	C28—C29—C30	115.9 (5)
C10—C9—N3	123.7 (4)	C28—C29—C29^{i}	122.6 (5)
C14—C9—N3	116.8 (4)	C30—C29—C29^{i}	121.5 (5)
C9—C10—C11	119.6 (5)	C31—C30—C29	120.1 (5)
C9—C10—H10	120.2	C31—C30—H30	119.9
C11—C10—H10	120.2	C29—C30—H30	119.9
C10—C11—C12	120.6 (5)	N6—C31—C30	124.1 (5)
C10—C11—H11	119.7	N6—C31—H31	117.9
C12—C11—H11	119.7	C30—C31—H31	117.9
O1—Zn1—S1—C8	−90.8 (2)	C8—N3—C9—C10	33.2 (7)

N1—Zn1—S1—C8	−15.58 (18)	C8—N3—C9—C14	−151.2 (5)
N5—Zn1—S1—C8	85.89 (18)	C14—C9—C10—C11	−0.9 (7)
N4—Zn1—S1—C8	166.81 (18)	N3—C9—C10—C11	174.7 (4)
N1—Zn1—O1—C1	27.9 (4)	C9—C10—C11—C12	1.4 (7)
N5—Zn1—O1—C1	−75.3 (4)	C10—C11—C12—C13	−0.5 (8)
N4—Zn1—O1—C1	−153.8 (4)	C11—C12—C13—C14	−0.9 (8)
S1—Zn1—O1—C1	101.5 (4)	C12—C13—C14—C9	1.4 (7)
O1—Zn1—N1—C7	−18.6 (4)	C10—C9—C14—C13	−0.5 (7)
N5—Zn1—N1—C7	86.4 (4)	N3—C9—C14—C13	−176.3 (4)
S1—Zn1—N1—C7	−168.2 (4)	C26—N4—C15—C16	−1.2 (7)
O1—Zn1—N1—N2	169.6 (3)	Zn1—N4—C15—C16	173.0 (3)
N5—Zn1—N1—N2	−85.5 (3)	N4—C15—C16—C17	1.1 (7)
S1—Zn1—N1—N2	19.9 (3)	C15—C16—C17—C18	−0.5 (7)
C7—N1—N2—C8	172.2 (4)	C16—C17—C18—C26	0.2 (7)
Zn1—N1—N2—C8	−14.9 (5)	C16—C17—C18—C19	−178.2 (5)
O1—Zn1—N4—C15	−73.6 (4)	C26—C18—C19—C20	3.6 (7)
N5—Zn1—N4—C15	−178.8 (4)	C17—C18—C19—C20	−178.1 (5)
S1—Zn1—N4—C15	75.7 (4)	C18—C19—C20—C21	−3.3 (7)
O1—Zn1—N4—C26	101.0 (3)	C19—C20—C21—C25	0.3 (7)
N5—Zn1—N4—C26	−4.3 (3)	C19—C20—C21—C22	−177.2 (5)
S1—Zn1—N4—C26	−109.7 (3)	C25—C21—C22—C23	0.8 (7)
O1—Zn1—N5—C24	95.4 (4)	C20—C21—C22—C23	178.3 (4)
N1—Zn1—N5—C24	3.2 (4)	C21—C22—C23—C24	−1.5 (7)
N4—Zn1—N5—C24	−178.0 (4)	C25—N5—C24—C23	0.9 (7)
S1—Zn1—N5—C24	−82.8 (4)	Zn1—N5—C24—C23	−177.7 (3)
O1—Zn1—N5—C25	−83.3 (3)	C22—C23—C24—N5	0.7 (7)
N1—Zn1—N5—C25	−175.5 (3)	C24—N5—C25—C21	−1.7 (6)
N4—Zn1—N5—C25	3.3 (3)	Zn1—N5—C25—C21	177.1 (3)
S1—Zn1—N5—C25	98.5 (3)	C24—N5—C25—C26	179.2 (4)
Zn1—O1—C1—C2	156.0 (3)	Zn1—N5—C25—C26	−2.0 (5)
Zn1—O1—C1—C6	−24.9 (6)	C22—C21—C25—N5	0.9 (7)
O1—C1—C2—C3	−178.3 (4)	C20—C21—C25—N5	−176.8 (4)
C6—C1—C2—C3	2.5 (7)	C22—C21—C25—C26	180.0 (4)
C1—C2—C3—O2	178.1 (4)	C20—C21—C25—C26	2.3 (7)
C1—C2—C3—C4	−2.6 (8)	C15—N4—C26—C18	0.9 (6)
O2—C3—C4—C5	179.7 (5)	Zn1—N4—C26—C18	−174.4 (3)
C2—C3—C4—C5	0.3 (8)	C15—N4—C26—C25	179.8 (4)
C3—C4—C5—C6	2.0 (8)	Zn1—N4—C26—C25	4.6 (5)
C4—C5—C6—C1	−2.1 (8)	C17—C18—C26—N4	−0.3 (6)
C4—C5—C6—C7	176.5 (5)	C19—C18—C26—N4	178.0 (4)
O1—C1—C6—C5	−179.3 (4)	C17—C18—C26—C25	−179.3 (4)
C2—C1—C6—C5	−0.2 (7)	C19—C18—C26—C25	−0.9 (6)
O1—C1—C6—C7	2.2 (7)	N5—C25—C26—N4	−1.8 (6)
C2—C1—C6—C7	−178.7 (4)	C21—C25—C26—N4	179.0 (4)
N2—N1—C7—C6	177.8 (4)	N5—C25—C26—C18	177.2 (4)
Zn1—N1—C7—C6	5.5 (7)	C21—C25—C26—C18	−2.0 (6)
C5—C6—C7—N1	−170.8 (5)	C31—N6—C27—C28	0.2 (7)
C1—C6—C7—N1	7.7 (8)	N6—C27—C28—C29	0.8 (8)
N1—N2—C8—N3	177.6 (4)	C27—C28—C29—C30	−1.4 (7)

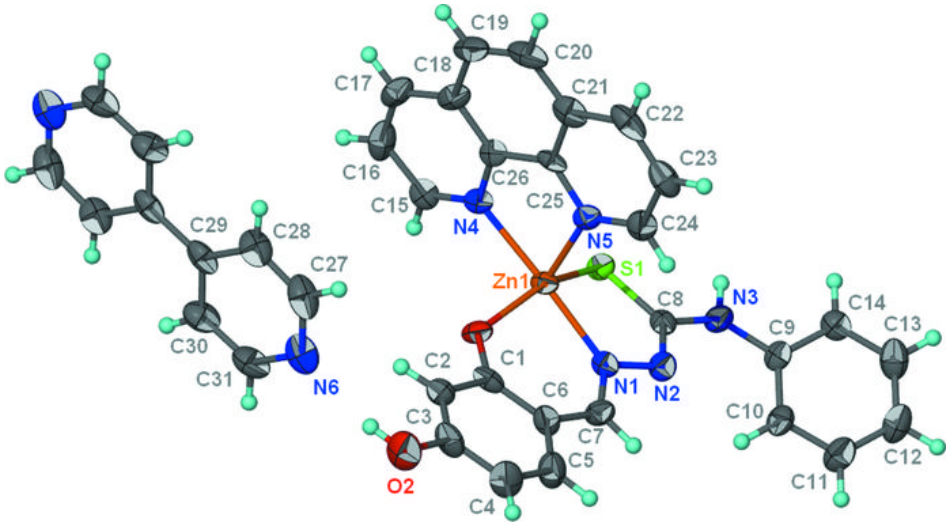
N1—N2—C8—S1	−4.2 (6)	C27—C28—C29—C29^{i}	179.3 (5)
C9—N3—C8—N2	−2.7 (7)	C28—C29—C30—C31	1.1 (7)
C9—N3—C8—S1	178.8 (4)	C29^{i}—C29—C30—C31	−179.6 (5)
Zn1—S1—C8—N2	16.5 (4)	C27—N6—C31—C30	−0.5 (7)
Zn1—S1—C8—N3	−165.2 (3)	C29—C30—C31—N6	−0.1 (8)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N6	0.84 (5)	2.01 (5)	2.839 (6)	168 (6)

Fig. 1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C27
C30
C31
N6