

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Bis[N^3 -(2-hydroxybenzoyl)pyridine-2-carboxamidrazonato- $\kappa^3 N^1, N^2, O$]zinc(II)

Yong Li

Department of Environmental Engineering, Anhui University of Technology,
Maanshan 243002, People's Republic of China
Correspondence e-mail: farnesene@gmail.com

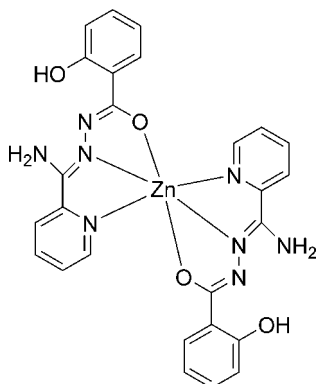
Received 18 October 2007; accepted 24 October 2007

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(C-C) = 0.003$ Å;
 R factor = 0.035; wR factor = 0.098; data-to-parameter ratio = 13.2.

In the title compound, $[Zn(C_{13}H_{11}N_4O_2)_2]$, the Zn atom is coordinated in a distorted octahedral manner by pyridyl N atoms, amidrazonate N atoms and carbamoyl O atoms from two tridentate N^3 -salicyloylpyridine-2-carboxamidrazonate ligands. N—H...O hydrogen bonds link the molecules to form a one-dimensional chain parallel to the b axis. The O—H...N hydrogen bonds are intramolecular and do not participate in the packing.

Related literature

For a related structure, see: Van Koningsbruggen *et al.* (1993, 1995).



Experimental

Crystal data

$[Zn(C_{13}H_{11}N_4O_2)_2]$
 $M_r = 575.89$
Monoclinic, $P2_1/c$

$a = 10.7704$ (9) Å
 $b = 13.1196$ (11) Å
 $c = 19.6427$ (14) Å

$\beta = 115.630$ (4)°
 $V = 2502.5$ (4) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 1.03$ mm⁻¹
 $T = 173$ (2) K
 $0.45 \times 0.42 \times 0.35$ mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2000)
 $T_{\min} = 0.636$, $T_{\max} = 0.700$

13224 measured reflections
4662 independent reflections
4269 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.098$
 $S = 1.06$
4662 reflections

354 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.85$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—N2	2.0234 (16)	Zn1—N4	2.2980 (17)
Zn1—O2	2.1611 (14)		
N2—Zn1—O2	75.46 (6)	N2—Zn1—N4	73.79 (6)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N7—H7B...O2 ⁱ	0.88	2.17	2.882 (2)	138
N7—H7A...O3 ⁱⁱ	0.88	2.49	3.100 (2)	127
N3—H3B...O4 ⁱⁱⁱ	0.88	2.18	2.837 (2)	131
N3—H3A...O1 ^{iv}	0.88	2.43	3.116 (2)	136
O3—H3C...N5	0.84	1.79	2.536 (2)	147
O1—H1...N1	0.84	1.82	2.556 (2)	146

Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $-x + 1, y, -z + \frac{3}{2}$; (iii) $-x + 1, -y + 2, -z + 2$; (iv) $-x + 1, y, -z + \frac{5}{2}$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2252).

References

- Bruker (2000). *SHELXTL* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2002). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2003). *SAINTE-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Van Koningsbruggen, P. J., Haasnoot, J. G., de Graaff, R. A. G. & Reedijk, J. (1993). *J. Chem. Soc. Dalton Trans.* pp. 483–484.
- Van Koningsbruggen, P. J., Haasnoot, J. G., de Graaff, R. A. G. & Reedijk, J. (1995). *Inorg. Chim. Acta*, **234**, 87–94.

supplementary materials

Acta Cryst. (2007). E63, m2837 [doi:10.1107/S1600536807052750]

Bis[*N*³-(2-hydroxybenzoyl)pyridine-2-carboxamidrazonato- κ^3 *N*¹,*N*²,*O*]zinc(II)

Y. Li

Comment

The *N*³-salicyloylpyridine-2-carboxamidrazonato ligand (abbreviated as Hspa) has several potential donor atoms and can occur in different chemical and structural conformations. In the Copper(II) coordination compound containing the dehydrogenated spa ligand (Van Koningsbruggen *et al.*, 1993, 1995), this spa ligand is fairly planar, whereas in the title complex it is slightly bent around the central Zn—N bonds, with a dihedral angle of 21.15 (6)° between the two aromatic rings (Fig. 1).

There are two intramolecular O—H···N hydrogen bonds involving the hydroxyl groups, whereas intermolecular N—H···O hydrogen bonds connect the molecules to build up a chain parallel to the *b* axis (Fig. 2).

Experimental

The ligand *N*³-salicyloylpyridine-2-carboxamidrazonato (Hspa) was synthesized according to literature (Van Koningsbruggen *et al.*, 1993, 1995). [Zn(C₁₃H₁₁N₄O₂)₂] was synthesized by adding ligand (0.0256 g, 0.10 mmol) and Et₃N (0.010 g, 0.1 mmol) in 1 ml DMSO to a solution of Zn(acac)₂ (0.0263 g, 0.10 mmol) in CH₂Cl₂ (4 ml). The compound crystallized upon evaporation of the solvent at room temperature after a few days.

Refinement

H atoms of the hydroxyls were located in a difference synthesis and refined isotropically, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Other H atoms were positioned geometrically and refined using a riding mode, with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C}, \text{N})$.

Figures

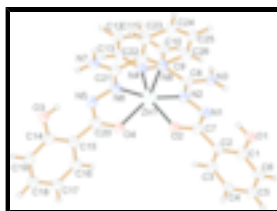


Fig. 1. A view of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

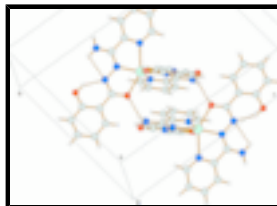


Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

supplementary materials

Bis[N^3 -(2-hydroxybenzoyl)pyridine-2-carboxamidrazonato- $\kappa^3 N^1, N^2, O$]zinc(II)

Crystal data

[Zn(C₁₃H₁₁N₄O₂)₂]

$M_r = 575.89$

Monoclinic, $P2/c$

Hall symbol: -P 2yc

$a = 10.7704$ (9) Å

$b = 13.1196$ (11) Å

$c = 19.6427$ (14) Å

$\beta = 115.630$ (4)°

$V = 2502.5$ (4) Å³

$Z = 4$

$F_{000} = 1184$

$D_x = 1.529$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 10850 reflections

$\theta = 2.4$ – 28.2 °

$\mu = 1.03$ mm⁻¹

$T = 173$ (2) K

Block, yellow

$0.45 \times 0.42 \times 0.35$ mm

Data collection

Bruker APEX CCD
diffractometer

Monochromator: graphite

$T = 173$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2000)

$T_{\min} = 0.636$, $T_{\max} = 0.700$

13224 measured reflections

4662 independent reflections

4269 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 25.5$ °

$\theta_{\min} = 1.6$ °

$h = -13$ → 11

$k = -13$ → 15

$l = -23$ → 23

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.098$

$S = 1.06$

4662 reflections

354 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

$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 1.8417P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.85$ e Å⁻³

$\Delta\rho_{\min} = -0.47$ e Å⁻³

Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.50740 (2)	0.755008 (16)	0.997968 (12)	0.02136 (10)
O1	0.65569 (16)	0.92559 (12)	1.27605 (8)	0.0318 (3)
H1	0.5991	0.9209	1.2304	0.048*
O2	0.65510 (14)	0.71793 (11)	1.11148 (8)	0.0233 (3)
O3	0.66246 (17)	0.57460 (12)	0.79709 (9)	0.0361 (4)
H3C	0.6069	0.5801	0.8165	0.054*
O4	0.66491 (14)	0.78488 (10)	0.96013 (8)	0.0234 (3)
N1	0.55574 (16)	0.85711 (12)	1.14099 (9)	0.0225 (3)
N2	0.47785 (16)	0.86238 (12)	1.06345 (9)	0.0214 (3)
N3	0.36365 (19)	1.00564 (12)	1.07950 (10)	0.0261 (4)
H3A	0.4037	1.0007	1.1291	0.031*
H3B	0.3045	1.0551	1.0576	0.031*
N4	0.34997 (16)	0.86802 (13)	0.91667 (9)	0.0238 (4)
N5	0.56026 (17)	0.64891 (13)	0.88078 (9)	0.0243 (4)
N6	0.47942 (16)	0.64650 (13)	0.91961 (9)	0.0225 (3)
N7	0.3818 (2)	0.49273 (13)	0.85983 (11)	0.0301 (4)
H7A	0.4241	0.4949	0.8303	0.036*
H7B	0.3268	0.4414	0.8565	0.036*
N8	0.35017 (17)	0.64502 (13)	1.00461 (9)	0.0251 (4)
C1	0.7504 (2)	0.85039 (16)	1.29318 (11)	0.0268 (4)
C2	0.7468 (2)	0.77696 (16)	1.23975 (11)	0.0248 (4)
C3	0.8479 (2)	0.70121 (19)	1.26353 (13)	0.0337 (5)
H3	0.8458	0.6502	1.2287	0.040*
C4	0.9503 (2)	0.6987 (2)	1.33609 (14)	0.0416 (6)
H4	1.0176	0.6461	1.3509	0.050*
C5	0.9556 (2)	0.7724 (2)	1.38756 (13)	0.0384 (6)
H5	1.0278	0.7715	1.4373	0.046*
C6	0.8557 (2)	0.84767 (19)	1.36664 (12)	0.0342 (5)
H6	0.8588	0.8976	1.4023	0.041*
C7	0.64676 (19)	0.78135 (15)	1.15900 (11)	0.0207 (4)
C8	0.39280 (19)	0.93784 (14)	1.03738 (11)	0.0205 (4)
C9	0.31880 (18)	0.94341 (14)	0.95347 (11)	0.0202 (4)
C10	0.2237 (2)	1.01911 (16)	0.91557 (12)	0.0253 (4)

supplementary materials

H10	0.2038	1.0718	0.9426	0.030*
C11	0.1584 (2)	1.01588 (17)	0.83733 (12)	0.0297 (5)
H11	0.0932	1.0668	0.8099	0.036*
C12	0.1884 (2)	0.93879 (17)	0.79973 (12)	0.0314 (5)
H12	0.1438	0.9350	0.7462	0.038*
C13	0.2853 (2)	0.86639 (17)	0.84151 (11)	0.0287 (5)
H13	0.3065	0.8133	0.8154	0.034*
C14	0.7624 (2)	0.64543 (17)	0.82713 (12)	0.0298 (5)
C15	0.7599 (2)	0.72169 (16)	0.87768 (11)	0.0248 (4)
C16	0.8671 (2)	0.79311 (17)	0.90454 (12)	0.0299 (5)
H16	0.8650	0.8461	0.9370	0.036*
C17	0.9754 (2)	0.7883 (2)	0.88506 (14)	0.0372 (5)
H17	1.0474	0.8372	0.9042	0.045*
C18	0.9785 (3)	0.7114 (2)	0.83724 (14)	0.0414 (6)
H18	1.0543	0.7068	0.8248	0.050*
C19	0.8724 (3)	0.6415 (2)	0.80769 (13)	0.0382 (5)
H19	0.8745	0.5904	0.7739	0.046*
C20	0.6551 (2)	0.72165 (15)	0.90799 (11)	0.0214 (4)
C21	0.4011 (2)	0.56730 (15)	0.90969 (10)	0.0222 (4)
C22	0.32611 (19)	0.56442 (15)	0.95812 (10)	0.0207 (4)
C23	0.2401 (2)	0.48520 (16)	0.95648 (12)	0.0263 (4)
H23	0.2257	0.4289	0.9235	0.032*
C24	0.1753 (2)	0.48959 (17)	1.00393 (13)	0.0309 (5)
H24	0.1152	0.4365	1.0037	0.037*
C25	0.1992 (2)	0.57185 (19)	1.05130 (13)	0.0358 (5)
H25	0.1563	0.5763	1.0845	0.043*
C26	0.2868 (2)	0.64814 (18)	1.04985 (13)	0.0323 (5)
H26	0.3025	0.7051	1.0824	0.039*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02212 (15)	0.02048 (16)	0.02072 (15)	-0.00079 (8)	0.00856 (11)	-0.00534 (8)
O1	0.0361 (8)	0.0338 (8)	0.0204 (7)	0.0050 (7)	0.0075 (6)	-0.0043 (6)
O2	0.0244 (7)	0.0239 (7)	0.0199 (7)	0.0020 (6)	0.0079 (6)	-0.0023 (5)
O3	0.0447 (9)	0.0381 (9)	0.0352 (9)	-0.0083 (7)	0.0263 (8)	-0.0123 (7)
O4	0.0261 (7)	0.0216 (7)	0.0233 (7)	-0.0018 (6)	0.0115 (6)	-0.0036 (6)
N1	0.0232 (8)	0.0240 (8)	0.0166 (8)	0.0011 (7)	0.0051 (7)	-0.0021 (6)
N2	0.0208 (8)	0.0232 (8)	0.0168 (8)	0.0000 (6)	0.0050 (6)	-0.0033 (6)
N3	0.0323 (9)	0.0242 (9)	0.0196 (8)	0.0074 (7)	0.0092 (7)	0.0009 (6)
N4	0.0220 (8)	0.0261 (9)	0.0214 (8)	-0.0021 (7)	0.0077 (7)	-0.0036 (7)
N5	0.0280 (9)	0.0251 (9)	0.0230 (8)	-0.0030 (7)	0.0140 (7)	-0.0039 (7)
N6	0.0231 (8)	0.0245 (9)	0.0209 (8)	-0.0023 (7)	0.0105 (7)	-0.0047 (7)
N7	0.0438 (11)	0.0241 (10)	0.0300 (10)	-0.0115 (7)	0.0231 (9)	-0.0086 (7)
N8	0.0235 (8)	0.0266 (9)	0.0250 (8)	-0.0014 (7)	0.0101 (7)	-0.0049 (7)
C1	0.0278 (10)	0.0298 (11)	0.0224 (10)	-0.0026 (8)	0.0106 (8)	0.0018 (8)
C2	0.0229 (10)	0.0291 (10)	0.0216 (10)	-0.0018 (8)	0.0090 (8)	0.0012 (8)
C3	0.0299 (11)	0.0402 (13)	0.0282 (11)	0.0074 (10)	0.0099 (9)	0.0019 (10)

C4	0.0309 (12)	0.0556 (16)	0.0317 (12)	0.0145 (11)	0.0072 (10)	0.0094 (11)
C5	0.0278 (12)	0.0568 (15)	0.0207 (11)	-0.0018 (11)	0.0013 (9)	0.0074 (10)
C6	0.0346 (11)	0.0424 (13)	0.0216 (10)	-0.0064 (10)	0.0086 (9)	-0.0012 (9)
C7	0.0213 (9)	0.0211 (9)	0.0200 (9)	-0.0016 (7)	0.0091 (8)	-0.0003 (7)
C8	0.0196 (9)	0.0195 (9)	0.0222 (9)	-0.0040 (7)	0.0089 (8)	-0.0019 (7)
C9	0.0165 (8)	0.0211 (10)	0.0215 (9)	-0.0039 (7)	0.0068 (7)	-0.0009 (7)
C10	0.0225 (10)	0.0240 (10)	0.0260 (10)	-0.0011 (8)	0.0072 (8)	-0.0013 (8)
C11	0.0235 (10)	0.0317 (11)	0.0262 (11)	-0.0009 (8)	0.0034 (8)	0.0053 (9)
C12	0.0281 (10)	0.0404 (13)	0.0195 (10)	-0.0055 (9)	0.0043 (8)	-0.0001 (9)
C13	0.0281 (10)	0.0338 (12)	0.0227 (10)	-0.0035 (9)	0.0096 (8)	-0.0064 (8)
C14	0.0362 (11)	0.0315 (11)	0.0258 (10)	0.0013 (9)	0.0172 (9)	0.0022 (9)
C15	0.0289 (10)	0.0258 (10)	0.0219 (10)	0.0018 (8)	0.0131 (9)	0.0043 (8)
C16	0.0322 (11)	0.0308 (12)	0.0278 (11)	-0.0001 (9)	0.0139 (9)	0.0043 (9)
C17	0.0307 (12)	0.0452 (14)	0.0377 (13)	-0.0061 (10)	0.0165 (10)	0.0057 (11)
C18	0.0376 (13)	0.0578 (16)	0.0398 (13)	0.0034 (12)	0.0270 (11)	0.0063 (12)
C19	0.0443 (13)	0.0442 (14)	0.0353 (12)	0.0018 (11)	0.0259 (11)	-0.0013 (10)
C20	0.0253 (10)	0.0194 (9)	0.0191 (9)	0.0023 (8)	0.0093 (8)	0.0018 (7)
C21	0.0229 (9)	0.0224 (10)	0.0184 (9)	0.0014 (7)	0.0063 (8)	0.0003 (7)
C22	0.0166 (8)	0.0234 (10)	0.0179 (9)	0.0020 (7)	0.0036 (7)	0.0008 (7)
C23	0.0206 (10)	0.0264 (10)	0.0279 (11)	-0.0020 (8)	0.0067 (8)	-0.0019 (8)
C24	0.0229 (10)	0.0336 (12)	0.0357 (12)	-0.0032 (8)	0.0122 (9)	0.0033 (9)
C25	0.0319 (11)	0.0438 (14)	0.0388 (12)	0.0000 (10)	0.0220 (10)	-0.0005 (10)
C26	0.0307 (11)	0.0377 (12)	0.0322 (11)	-0.0018 (9)	0.0170 (9)	-0.0085 (9)

Geometric parameters (Å, °)

Zn1—N6	2.0213 (16)	C4—C5	1.383 (4)
Zn1—N2	2.0234 (16)	C4—H4	0.9500
Zn1—O2	2.1611 (14)	C5—C6	1.385 (3)
Zn1—O4	2.1622 (14)	C5—H5	0.9500
Zn1—N8	2.2711 (17)	C6—H6	0.9500
Zn1—N4	2.2980 (17)	C8—C9	1.490 (3)
O1—C1	1.352 (3)	C9—C10	1.389 (3)
O1—H1	0.8400	C10—C11	1.387 (3)
O2—C7	1.282 (2)	C10—H10	0.9500
O3—C14	1.350 (3)	C11—C12	1.371 (3)
O3—H3C	0.8400	C11—H11	0.9500
O4—C20	1.286 (2)	C12—C13	1.387 (3)
N1—C7	1.332 (2)	C12—H12	0.9500
N1—N2	1.387 (2)	C13—H13	0.9500
N2—C8	1.294 (2)	C14—C19	1.394 (3)
N3—C8	1.341 (3)	C14—C15	1.418 (3)
N3—H3A	0.8800	C15—C16	1.400 (3)
N3—H3B	0.8800	C15—C20	1.487 (3)
N4—C13	1.333 (3)	C16—C17	1.378 (3)
N4—C9	1.350 (3)	C16—H16	0.9500
N5—C20	1.329 (3)	C17—C18	1.389 (4)
N5—N6	1.384 (2)	C17—H17	0.9500
N6—C21	1.299 (3)	C18—C19	1.382 (4)

supplementary materials

N7—C21	1.336 (3)	C18—H18	0.9500
N7—H7A	0.8800	C19—H19	0.9500
N7—H7B	0.8800	C21—C22	1.491 (3)
N8—C26	1.335 (3)	C22—C23	1.383 (3)
N8—C22	1.347 (3)	C23—C24	1.386 (3)
C1—C6	1.398 (3)	C23—H23	0.9500
C1—C2	1.413 (3)	C24—C25	1.375 (3)
C2—C3	1.397 (3)	C24—H24	0.9500
C2—C7	1.484 (3)	C25—C26	1.384 (3)
C3—C4	1.374 (3)	C25—H25	0.9500
C3—H3	0.9500	C26—H26	0.9500
N6—Zn1—N2	164.11 (7)	N1—C7—C2	115.06 (17)
N6—Zn1—O2	115.33 (6)	N2—C8—N3	125.28 (18)
N2—Zn1—O2	75.46 (6)	N2—C8—C9	115.05 (16)
N6—Zn1—O4	75.32 (6)	N3—C8—C9	119.59 (17)
N2—Zn1—O4	117.06 (6)	N4—C9—C10	122.22 (18)
O2—Zn1—O4	93.36 (5)	N4—C9—C8	114.73 (17)
N6—Zn1—N8	74.16 (6)	C10—C9—C8	123.05 (18)
N2—Zn1—N8	94.57 (6)	C11—C10—C9	118.35 (19)
O2—Zn1—N8	91.84 (6)	C11—C10—H10	120.8
O4—Zn1—N8	148.25 (6)	C9—C10—H10	120.8
N6—Zn1—N4	95.92 (6)	C12—C11—C10	119.7 (2)
N2—Zn1—N4	73.79 (6)	C12—C11—H11	120.2
O2—Zn1—N4	148.73 (6)	C10—C11—H11	120.2
O4—Zn1—N4	95.56 (6)	C11—C12—C13	118.61 (19)
N8—Zn1—N4	96.06 (6)	C11—C12—H12	120.7
C1—O1—H1	109.5	C13—C12—H12	120.7
C7—O2—Zn1	110.66 (12)	N4—C13—C12	122.9 (2)
C14—O3—H3C	109.5	N4—C13—H13	118.5
C20—O4—Zn1	110.50 (12)	C12—C13—H13	118.5
C7—N1—N2	110.80 (15)	O3—C14—C19	117.8 (2)
C8—N2—N1	117.46 (16)	O3—C14—C15	122.60 (19)
C8—N2—Zn1	124.05 (13)	C19—C14—C15	119.6 (2)
N1—N2—Zn1	118.47 (12)	C16—C15—C14	118.28 (19)
C8—N3—H3A	120.0	C16—C15—C20	119.61 (19)
C8—N3—H3B	120.0	C14—C15—C20	121.86 (19)
H3A—N3—H3B	120.0	C17—C16—C15	121.6 (2)
C13—N4—C9	118.23 (18)	C17—C16—H16	119.2
C13—N4—Zn1	129.38 (14)	C15—C16—H16	119.2
C9—N4—Zn1	112.34 (12)	C16—C17—C18	119.5 (2)
C20—N5—N6	110.61 (16)	C16—C17—H17	120.3
C21—N6—N5	117.30 (16)	C18—C17—H17	120.3
C21—N6—Zn1	123.41 (13)	C19—C18—C17	120.6 (2)
N5—N6—Zn1	118.78 (12)	C19—C18—H18	119.7
C21—N7—H7A	120.0	C17—C18—H18	119.7
C21—N7—H7B	120.0	C18—C19—C14	120.4 (2)
H7A—N7—H7B	120.0	C18—C19—H19	119.8
C26—N8—C22	118.13 (18)	C14—C19—H19	119.8
C26—N8—Zn1	128.85 (14)	O4—C20—N5	124.56 (18)

C22—N8—Zn1	112.92 (13)	O4—C20—C15	120.22 (18)
O1—C1—C6	117.60 (19)	N5—C20—C15	115.08 (17)
O1—C1—C2	122.49 (18)	N6—C21—N7	125.48 (18)
C6—C1—C2	119.9 (2)	N6—C21—C22	114.88 (17)
C3—C2—C1	118.02 (19)	N7—C21—C22	119.63 (17)
C3—C2—C7	119.05 (19)	N8—C22—C23	122.43 (18)
C1—C2—C7	122.79 (19)	N8—C22—C21	114.46 (17)
C4—C3—C2	121.6 (2)	C23—C22—C21	123.10 (18)
C4—C3—H3	119.2	C22—C23—C24	118.7 (2)
C2—C3—H3	119.2	C22—C23—H23	120.7
C3—C4—C5	120.1 (2)	C24—C23—H23	120.7
C3—C4—H4	119.9	C25—C24—C23	119.1 (2)
C5—C4—H4	119.9	C25—C24—H24	120.4
C4—C5—C6	120.1 (2)	C23—C24—H24	120.4
C4—C5—H5	120.0	C24—C25—C26	118.9 (2)
C6—C5—H5	120.0	C24—C25—H25	120.6
C5—C6—C1	120.3 (2)	C26—C25—H25	120.6
C5—C6—H6	119.9	N8—C26—C25	122.7 (2)
C1—C6—H6	119.9	N8—C26—H26	118.6
O2—C7—N1	124.48 (17)	C25—C26—H26	118.6
O2—C7—C2	120.39 (18)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N7—H7B \cdots O2 ⁱ	0.88	2.17	2.882 (2)	138
N7—H7A \cdots O3 ⁱⁱ	0.88	2.49	3.100 (2)	127
N3—H3B \cdots O4 ⁱⁱⁱ	0.88	2.18	2.837 (2)	131
N3—H3A \cdots O1 ^{iv}	0.88	2.43	3.116 (2)	136
O3—H3C \cdots N5	0.84	1.79	2.536 (2)	147
O1—H1 \cdots N1	0.84	1.82	2.556 (2)	146

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, y, -z+3/2$; (iii) $-x+1, -y+2, -z+2$; (iv) $-x+1, y, -z+5/2$.

Fig. 2

