Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aquabis(benzoato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

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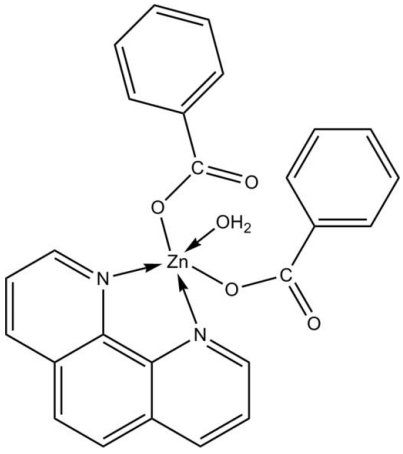
Received 20 November 2010; accepted 27 November 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.077; data-to-parameter ratio = 12.9.

The Zn atom in the title compound, $[Zn(C_7H_5O_2)_2(C_{12}H_8N_2)(H_2O)]$, is five-coordinate in a distorted trigonal–bipyramidal coordination environment involving two O atoms of two monodentate benzoates, two N atoms of a 1,10-phenanthroline molecule and one O atom of a water molecule. The axial positions are occupied by a carboxylate O atom from the benzoate ligand and an N atom from the 1,10-phenanthroline ligand [N—Zn—O = 146.90 (7)°]. The water molecule forms an intramolecular O—H···O hydrogen bond; an intermolecular O—H···O hydrogen bond gives rise to a dimer.

Related literature

For a related structure, see: Necefoglu *et al.* (2001).



Experimental

Crystal data

$[Zn(C_7H_5O_2)_2(C_{12}H_8N_2)(H_2O)]$
M_r = 505.81
Monoclinic, $P2_1/c$
a = 10.635 (5) Å
b = 21.073 (10) Å
c = 11.197 (5) Å
β = 116.647 (5)°
V = 2243.0 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.779, T_{max} = 0.815
12067 measured reflections
3992 independent reflections
3424 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.077
S = 1.03
3992 reflections
309 parameters
180 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O2	0.89	1.78	2.616 (2)	154
O5—H5B···O4^{i}	0.89	1.91	2.797 (2)	174

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5072).

References

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supporting information

Acta Cryst. (2011). E**67**, m30 [https://doi.org/10.1107/S1600536810049639]

Aquabis(benzoato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

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S1. Comment

In the present study, we report the synthesis and crystal structure of the title complex (I). The biological activity of (I) against common bacterial strains is to be investigated. Selected geometric parameters are listed in Table 1. As shown in Fig. 1, (I) is a mononuclear neutral zinc(II) complex in which the carboxylate group exhibits a monodentate coordination mode. By contrast, in the mononuclear zinc complex of diaquabis (benzoato)zinc(II), each carboxylate ligand forms a primary and a secondary Zn—O bond (Necefoglu *et al.*, 2001). The Zn ion in (I) is coordinated by two O atoms from two monodentate benzoate ligands (O1 and O3), two N atoms from the 1,10-phenanthroline ligand (N1 and N2) and one O atom from the water molecule (O5), and exhibits distorted trigonal-bipyramidal coordination. The trigonal base plane is defined by atoms N1, O1 and O5, and atoms O3 and N2 occupy the axial positions [O3—Zn—N2 =146.91 (5)°]. A strong intermolecular hydrogen bond exists, involving uncoordinated atom O4 of the carboxylate group as an acceptor and atom O5 as a donor (Table 2), resulting in the formation of a dimer (Fig. 2). There is also an intramolecular hydrogen bond between the other H atom of the water molecule and uncoordinated atom O2 of the other carboxylate group (Table 2).

S2. Experimental

$C_4H_6ZnO_4.2H_2O$(0.2195 g,1 mmol), benzoic acid(0.2442 g,2 mmol), NaOH(0.08 g;2 mmol),1,10-phenanthroline (0.1802 g,1 mmol) were added to a mixture of water (15 ml) and ethanol (10 ml). The resulting mixture was stirred at 70 for 4 h and fltered off. The filtrate was allowed to stand at room temperature and slow evaporation afforded colorless block crystals of the complex(Yield 65%).Elemental analysis: found C,61.69;H,3.98;N,5.57;calc for $C_{26}H_{20}N_2O_5Zn$:*C*,61.73; H,3.99;N,5.54(%).

S3. Refinement

H atoms on C atoms were positioned geometrically refined using a riding model with C—H=0.93–0.96ÅandU_{iso}(H) = 1.2U_{eq}(C),The water H atoms were located in difference density Fourier maps and refined using a riding model with O—H=0.82Åand U_{iso}(H) = 1.5U_{eq}(C).

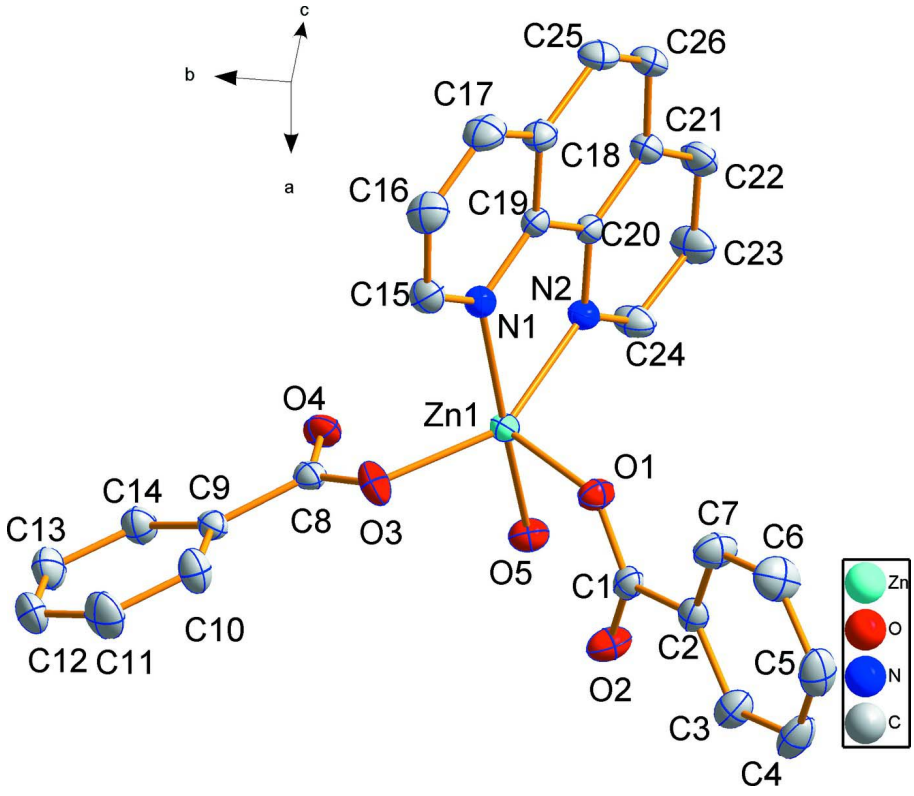

Figure 1

The structure of the title compound(I) and the atom-numbering scheme. H atoms have been omitted for clarity.

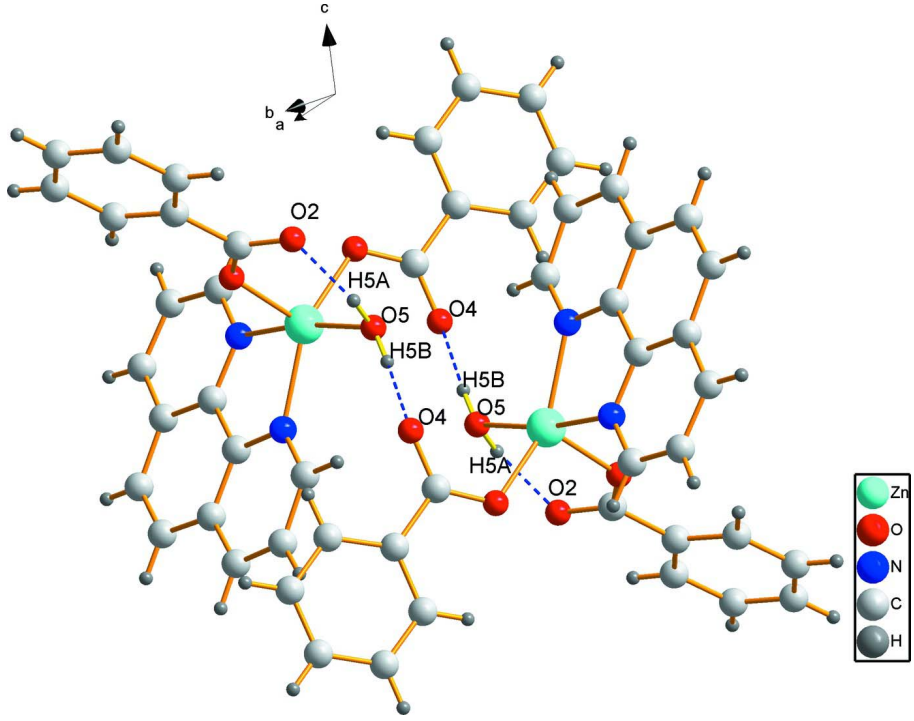

Figure 2

Part of the packing of the title compand, viewed down the direction. Dashing lines indicate hydrongen bonds.

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Crystal data

$[Zn(C_7H_5O_2)_2(C_{12}H_8N_2)(H_2O)]$
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$b = 21.073$ (10) Å
$c = 11.197$ (5) Å
$\beta = 116.647$ (5)°
$V = 2243.0$ (18) Å^3
$Z = 4$
$F(000) = 1040$
$D_x = 1.498$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3686 reflections
$\theta = 2.4$–$24.4°$
$\mu = 1.14$ mm^{-1}
$T = 293$ K
Block, colorless
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.779$, $T_{max} = 0.815$
12067 measured reflections
3992 independent reflections
3424 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.9°$
$h = -10\rightarrow12$
$k = -25\rightarrow23$
$l = -12\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.077$
$S = 1.03$
3992 reflections
309 parameters
180 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.4116P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.73455 (2)	0.468990 (10)	0.79430 (2)	0.02980 (9)
O2	0.91421 (15)	0.39030 (7)	0.67036 (15)	0.0479 (4)

O5	0.95726 (15)	0.46026 (7)	0.87826 (14)	0.0394 (3)
O1	0.70176 (15)	0.39837 (6)	0.66424 (14)	0.0382 (3)
O3	0.73550 (16)	0.54552 (7)	0.69395 (15)	0.0462 (4)
N1	0.51084 (17)	0.48044 (7)	0.73798 (16)	0.0332 (4)
O4	0.84175 (16)	0.59595 (7)	0.88755 (14)	0.0452 (4)
N2	0.71843 (17)	0.43150 (8)	0.96095 (16)	0.0329 (4)
C2	0.7328 (2)	0.32287 (9)	0.52375 (18)	0.0347 (5)
C9	0.8066 (2)	0.65093 (9)	0.68988 (18)	0.0313 (4)
C1	0.7887 (2)	0.37425 (9)	0.62746 (18)	0.0328 (4)
C8	0.79431 (19)	0.59369 (10)	0.7643 (2)	0.0337 (4)
C19	0.4736 (2)	0.45195 (9)	0.82630 (19)	0.0305 (4)
C22	0.6643 (2)	0.37283 (11)	1.1555 (2)	0.0473 (6)
H22	0.6472	0.3532	1.2212	0.057*
C20	0.5848 (2)	0.42643 (8)	0.94545 (19)	0.0298 (4)
C10	0.7484 (2)	0.65085 (10)	0.5520 (2)	0.0466 (5)
H10	0.7020	0.6150	0.5043	0.056*
C17	0.2293 (3)	0.47341 (11)	0.6873 (2)	0.0519 (6)
H17	0.1349	0.4707	0.6686	0.062*
C18	0.3338 (2)	0.44721 (10)	0.8055 (2)	0.0382 (5)
C21	0.5522 (2)	0.39749 (9)	1.0407 (2)	0.0363 (5)
C24	0.8211 (2)	0.40768 (12)	1.0706 (2)	0.0462 (5)
H24	0.9129	0.4109	1.0818	0.055*
C7	0.5945 (2)	0.30438 (11)	0.4714 (2)	0.0503 (6)
H7	0.5344	0.3244	0.4994	0.060*
C3	0.8209 (2)	0.29284 (11)	0.4798 (2)	0.0450 (5)
H3	0.9145	0.3053	0.5130	0.054*
C26	0.4092 (2)	0.39395 (11)	1.0174 (2)	0.0457 (5)
H26	0.3878	0.3751	1.0811	0.055*
C25	0.3045 (2)	0.41735 (11)	0.9048 (2)	0.0477 (6)
H25	0.2120	0.4140	0.8915	0.057*
C15	0.4098 (2)	0.50578 (11)	0.6288 (2)	0.0421 (5)
H15	0.4345	0.5263	0.5689	0.050*
C14	0.8760 (2)	0.70456 (10)	0.7581 (2)	0.0431 (5)
H14	0.9174	0.7049	0.8510	0.052*
C23	0.7978 (2)	0.37786 (13)	1.1703 (2)	0.0546 (6)
H23	0.8729	0.3616	1.2459	0.066*
C16	0.2681 (2)	0.50307 (12)	0.5999 (2)	0.0518 (6)
H16	0.2003	0.5212	0.5219	0.062*
C13	0.8849 (3)	0.75778 (11)	0.6907 (2)	0.0535 (6)
H13	0.9309	0.7938	0.7380	0.064*
C4	0.7690 (3)	0.24424 (12)	0.3863 (2)	0.0549 (6)
H4	0.8285	0.2239	0.3580	0.066*
C12	0.8259 (3)	0.75749 (11)	0.5539 (3)	0.0552 (6)
H12	0.8310	0.7934	0.5081	0.066*
C11	0.7593 (3)	0.70405 (12)	0.4849 (2)	0.0607 (7)
H11	0.7210	0.7036	0.3922	0.073*
C5	0.6316 (3)	0.22613 (12)	0.3356 (2)	0.0569 (7)
H5	0.5976	0.1936	0.2730	0.068*

C6	0.5433 (3)	0.25633 (13)	0.3777 (2)	0.0621 (7)
H6	0.4493	0.2443	0.3429	0.075*
H5B	1.0206	0.4450	0.9561	0.078 (9)*
H5A	0.9702	0.4340	0.8221	0.087 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03210 (15)	0.03006 (14)	0.03060 (14)	−0.00163 (9)	0.01704 (11)	0.00108 (9)
O2	0.0355 (9)	0.0604 (10)	0.0473 (9)	−0.0013 (7)	0.0181 (7)	−0.0157 (7)
O5	0.0324 (8)	0.0498 (9)	0.0337 (8)	0.0002 (6)	0.0128 (7)	−0.0041 (6)
O1	0.0371 (8)	0.0398 (8)	0.0400 (8)	−0.0024 (6)	0.0194 (7)	−0.0094 (6)
O3	0.0459 (9)	0.0379 (9)	0.0469 (9)	−0.0105 (7)	0.0137 (7)	0.0091 (7)
N1	0.0360 (9)	0.0313 (9)	0.0347 (9)	0.0013 (7)	0.0180 (8)	0.0012 (7)
O4	0.0547 (10)	0.0523 (9)	0.0371 (8)	0.0132 (7)	0.0282 (8)	0.0134 (7)
N2	0.0316 (9)	0.0352 (9)	0.0341 (9)	0.0006 (7)	0.0167 (7)	0.0031 (7)
C2	0.0432 (12)	0.0321 (11)	0.0279 (10)	0.0038 (9)	0.0150 (9)	0.0017 (8)
C9	0.0289 (10)	0.0326 (11)	0.0340 (10)	0.0012 (8)	0.0155 (8)	0.0048 (8)
C1	0.0360 (12)	0.0322 (11)	0.0291 (10)	0.0065 (9)	0.0135 (9)	0.0043 (8)
C8	0.0260 (10)	0.0374 (12)	0.0406 (12)	0.0052 (8)	0.0175 (9)	0.0083 (9)
C19	0.0337 (11)	0.0265 (10)	0.0358 (10)	0.0005 (8)	0.0196 (9)	−0.0026 (8)
C22	0.0525 (15)	0.0537 (14)	0.0443 (13)	0.0055 (11)	0.0294 (11)	0.0144 (10)
C20	0.0327 (11)	0.0260 (10)	0.0360 (10)	−0.0009 (8)	0.0200 (9)	−0.0026 (8)
C10	0.0559 (15)	0.0390 (13)	0.0373 (12)	−0.0062 (10)	0.0142 (11)	0.0027 (9)
C17	0.0344 (12)	0.0613 (16)	0.0593 (15)	0.0057 (11)	0.0205 (11)	0.0021 (12)
C18	0.0326 (11)	0.0383 (12)	0.0455 (12)	0.0014 (9)	0.0192 (10)	−0.0006 (9)
C21	0.0419 (12)	0.0343 (11)	0.0400 (11)	−0.0008 (9)	0.0249 (10)	0.0016 (9)
C24	0.0335 (12)	0.0637 (15)	0.0434 (13)	0.0043 (10)	0.0190 (10)	0.0112 (11)
C7	0.0502 (14)	0.0567 (15)	0.0475 (13)	−0.0043 (11)	0.0252 (11)	−0.0143 (11)
C3	0.0478 (13)	0.0474 (13)	0.0354 (11)	0.0109 (10)	0.0148 (10)	−0.0010 (10)
C26	0.0479 (13)	0.0478 (14)	0.0564 (14)	−0.0003 (10)	0.0368 (12)	0.0079 (10)
C25	0.0363 (12)	0.0556 (15)	0.0616 (15)	−0.0015 (10)	0.0311 (12)	0.0032 (11)
C15	0.0454 (13)	0.0452 (13)	0.0362 (11)	0.0059 (10)	0.0187 (10)	0.0059 (9)
C14	0.0528 (14)	0.0405 (13)	0.0375 (11)	−0.0040 (10)	0.0215 (10)	−0.0013 (9)
C23	0.0466 (14)	0.0753 (18)	0.0417 (13)	0.0133 (12)	0.0197 (11)	0.0231 (12)
C16	0.0417 (13)	0.0607 (15)	0.0447 (13)	0.0103 (11)	0.0121 (11)	0.0082 (11)
C13	0.0660 (17)	0.0355 (13)	0.0641 (16)	−0.0105 (11)	0.0338 (14)	−0.0038 (11)
C4	0.0730 (18)	0.0499 (15)	0.0419 (13)	0.0205 (13)	0.0258 (13)	−0.0031 (10)
C12	0.0735 (18)	0.0376 (13)	0.0659 (16)	0.0018 (11)	0.0415 (14)	0.0155 (11)
C11	0.0805 (19)	0.0593 (17)	0.0395 (13)	0.0022 (14)	0.0246 (13)	0.0156 (11)
C5	0.083 (2)	0.0422 (14)	0.0417 (13)	−0.0056 (13)	0.0243 (13)	−0.0106 (10)
C6	0.0618 (17)	0.0668 (18)	0.0562 (16)	−0.0205 (13)	0.0249 (13)	−0.0211 (13)

Geometric parameters (Å, º)

Zn1—O3	1.9681 (16)	C17—C18	1.405 (3)
Zn1—O1	2.0003 (15)	C17—H17	0.9300
Zn1—N2	2.1030 (17)	C18—C25	1.428 (3)

Zn1—O5	2.1285 (17)	C21—C26	1.425 (3)
Zn1—N1	2.184 (2)	C24—C23	1.396 (3)
O2—C1	1.246 (2)	C24—H24	0.9300
O5—H5B	0.8887	C7—C6	1.383 (3)
O5—H5A	0.8928	C7—H7	0.9300
O1—C1	1.274 (2)	C3—C4	1.390 (3)
O3—C8	1.265 (3)	C3—H3	0.9300
N1—C15	1.325 (3)	C26—C25	1.346 (3)
N1—C19	1.359 (2)	C26—H26	0.9300
O4—C8	1.239 (2)	C25—H25	0.9300
N2—C24	1.322 (3)	C15—C16	1.393 (3)
N2—C20	1.357 (2)	C15—H15	0.9300
C2—C7	1.373 (3)	C14—C13	1.378 (3)
C2—C3	1.391 (3)	C14—H14	0.9300
C2—C1	1.502 (3)	C23—H23	0.9300
C9—C14	1.378 (3)	C16—H16	0.9300
C9—C10	1.382 (3)	C13—C12	1.370 (3)
C9—C8	1.505 (3)	C13—H13	0.9300
C19—C18	1.401 (3)	C4—C5	1.363 (4)
C19—C20	1.433 (3)	C4—H4	0.9300
C22—C23	1.358 (3)	C12—C11	1.370 (4)
C22—C21	1.404 (3)	C12—H12	0.9300
C22—H22	0.9300	C11—H11	0.9300
C20—C21	1.400 (3)	C5—C6	1.381 (3)
C10—C11	1.383 (3)	C5—H5	0.9300
C10—H10	0.9300	C6—H6	0.9300
C17—C16	1.372 (3)		

O3—Zn1—O1	103.76 (7)	C17—C18—C25	123.3 (2)
O3—Zn1—N2	146.90 (7)	C20—C21—C22	117.41 (19)
O1—Zn1—N2	108.03 (7)	C20—C21—C26	119.46 (19)
O3—Zn1—O5	91.91 (6)	C22—C21—C26	123.13 (18)
O1—Zn1—O5	93.06 (6)	N2—C24—C23	123.0 (2)
N2—Zn1—O5	95.34 (6)	N2—C24—H24	118.5
O3—Zn1—N1	91.63 (6)	C23—C24—H24	118.5
O1—Zn1—N1	93.46 (6)	C2—C7—C6	120.9 (2)
N2—Zn1—N1	77.64 (6)	C2—C7—H7	119.6
O5—Zn1—N1	171.63 (6)	C6—C7—H7	119.6
Zn1—O5—H5B	131.9	C4—C3—C2	119.9 (2)
Zn1—O5—H5A	103.6	C4—C3—H3	120.0
H5B—O5—H5A	100.3	C2—C3—H3	120.0
C1—O1—Zn1	128.11 (13)	C25—C26—C21	121.24 (19)
C8—O3—Zn1	115.44 (13)	C25—C26—H26	119.4
C15—N1—C19	117.96 (18)	C21—C26—H26	119.4
C15—N1—Zn1	129.69 (14)	C26—C25—C18	120.9 (2)
C19—N1—Zn1	112.11 (13)	C26—C25—H25	119.6
C24—N2—C20	118.04 (17)	C18—C25—H25	119.6
C24—N2—Zn1	127.20 (14)	N1—C15—C16	122.9 (2)

C20—N2—Zn1	114.44 (12)	N1—C15—H15	118.6
C7—C2—C3	118.9 (2)	C16—C15—H15	118.6
C7—C2—C1	120.76 (18)	C9—C14—C13	121.0 (2)
C3—C2—C1	120.37 (19)	C9—C14—H14	119.5
C14—C9—C10	118.68 (19)	C13—C14—H14	119.5
C14—C9—C8	120.55 (18)	C22—C23—C24	119.2 (2)
C10—C9—C8	120.76 (18)	C22—C23—H23	120.4
O2—C1—O1	125.05 (18)	C24—C23—H23	120.4
O2—C1—C2	118.57 (17)	C17—C16—C15	119.6 (2)
O1—C1—C2	116.39 (18)	C17—C16—H16	120.2
O4—C8—O3	124.40 (19)	C15—C16—H16	120.2
O4—C8—C9	119.53 (19)	C12—C13—C14	119.9 (2)
O3—C8—C9	116.07 (17)	C12—C13—H13	120.0
N1—C19—C18	122.98 (18)	C14—C13—H13	120.0
N1—C19—C20	117.09 (17)	C5—C4—C3	120.6 (2)
C18—C19—C20	119.93 (17)	C5—C4—H4	119.7
C23—C22—C21	119.64 (19)	C3—C4—H4	119.7
C23—C22—H22	120.2	C11—C12—C13	119.7 (2)
C21—C22—H22	120.2	C11—C12—H12	120.1
N2—C20—C21	122.68 (18)	C13—C12—H12	120.1
N2—C20—C19	117.99 (16)	C12—C11—C10	120.5 (2)
C21—C20—C19	119.32 (17)	C12—C11—H11	119.7
C9—C10—C11	120.1 (2)	C10—C11—H11	119.7
C9—C10—H10	120.0	C4—C5—C6	119.7 (2)
C11—C10—H10	120.0	C4—C5—H5	120.2
C16—C17—C18	119.1 (2)	C6—C5—H5	120.2
C16—C17—H17	120.4	C5—C6—C7	120.0 (2)
C18—C17—H17	120.4	C5—C6—H6	120.0
C19—C18—C17	117.46 (19)	C7—C6—H6	120.0
C19—C18—C25	119.19 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O2	0.89	1.78	2.616 (2)	154
O5—H5*B*···O4^{i}	0.89	1.91	2.797 (2)	174

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