Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

8-Hydroxy-2-methylquinolinium dibromido(2-methylquinolin-8-olato-κ^2N,O)zincate acetonitrile monosolvate

Ezzatollah Najafi,[a] Mostafa M. Amini[a] and Seik Weng Ng[b,c]*

[a]Department of Chemistry, General Campus, Shahid Beheshti University, Tehran 1983963113, Iran, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

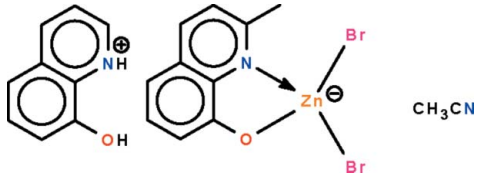
Received 4 August 2011; accepted 9 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.065; data-to-parameter ratio = 17.6.

The reaction of 2-methyl-8-hydroxyquinoline and zinc bromide in acetonitrile affords the title solvated salt, $(C_{10}H_{10}NO)[ZnBr_2(C_{10}H_8NO)]\cdot CH_3CN$, in which the Zn^{II} ion is coordinated by a N,O-chelating 2-methylquinolin-8-olate ligand and two bromide ligands in a distorted tetrahedral geometry. The cation is linked to the anion by an O—H···O hydrogen bond and the quinolinium H atom forms an intermolecular N—H···N hydrogen bond with the acetonitrile solvent molecule.

Related literature

For the crystal structure of 8-hydroxy-2-methylquinolinium dichlorido(2-methylquinolin-8-olato)zincate acetonitrile disolvate, see: Najafi *et al.* (2011). For the crystal structures of related methanol solvates, see: Najafi *et al.* (2010*a*, 2010*b*); Sattarzadeh *et al.* (2009).



Experimental

Crystal data

$(C_{10}H_{10}NO)[ZnBr_2(C_{10}H_8NO)]\cdot C_2H_3N$
M_r = 584.61
Triclinic, $P\overline{1}$
a = 7.1870 (3) Å
b = 9.7795 (5) Å
c = 16.2520 (7) Å
α = 86.159 (4)°
β = 80.775 (4)°
γ = 85.098 (4)°
V = 1121.73 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.68 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.387, T_{max} = 0.540
8710 measured reflections
4970 independent reflections
4197 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.065
S = 1.01
4970 reflections
282 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.84 (1)	1.73 (1)	2.561 (2)	173 (4)
N2—H1···N3	0.88 (1)	2.08 (1)	2.943 (3)	171 (3)

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5306).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Najafi, E., Amini, M. M. & Ng, S. W. (2010*a*). *Acta Cryst.* E**66**, m1276.
Najafi, E., Amini, M. M. & Ng, S. W. (2010*b*). *Acta Cryst.* E**66**, m1277.
Najafi, E., Amini, M. M. & Ng, S. W. (2011). *Acta Cryst.* E**67**, m1280.
Sattarzadeh, E., Mohammadnezhad, G., Amini, M. M. & Ng, S. W. (2009). *Acta Cryst.* E**65**, m553.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2011). E**67**, m1281 [**doi:10.1107/S160053681103234X**]

8-Hydroxy-2-methylquinolinium dibromido(2-methylquinolin-8-olato-κ^2N,O)zincate acetonitrile monosolvate

E. Najafi, M. M. Amini and S. W. Ng

Comment

We have synthesized methanol-solvated 8-hydroxy-2-methylquinolinium dihalo(2-methylquinolin-8-olato)zincates(II) by the direct reaction of the zinc halide and 8-hydroxy-2-methylquinolin in methanol. The salts have the Zn^{II} atom in a tetrahedral geometry, and the ion-pairs are linked to the solvent molecules by hydrogen bonds (Najafi *et al.*, 2010*a*; Najafi *et al.*, 2010*b*; Sattarzadeh *et al.*, 2009). In this study we used acetonitrile as a solvent. In a previous study, the reaction of zinc chloride and the quinoline in acetonitrile yielded the disolvated salt (Najafi *et al.*, 2011). In the present study, zinc dibromide gave a mono-solvated salt (Fig. 1). In $(C_{10}H_{10}NO)[ZnBr_2(C_{10}H_8NO)]\cdot CH_3CN$, the metal in the anion is *N*,*O*-chelated by the deprotonated ligand and it exists in a distorted tetrahedral geometry. The cation is linked to the anion by an O–H···O hydrogen bond and the quinolinium H atom forms a hydrogen bond with the solvent molecule (Table 1).

Experimental

Zinc chloride (0.23 g, 0.75 mmol) and 2-methyl-8-hydroxyquinoline (0.24 g, 1.5 mmol) were loaded into a convection tube and the tube was filled with acetonitrile and kept at 333 K. Yellow crystals were collected from the side arm after several days.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation. The N and O bound H atoms were located in a difference Fourier map, and were refined with distance restraints of N–H 0.88±0.01, O–H 0.84±0.01 Å; their temperature factors were refined. The (2 - 2 7) and (0 1 1) were removed.

Figures

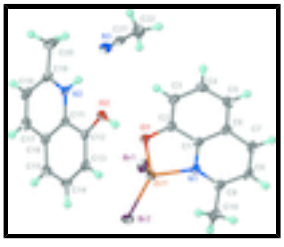


Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $(C_{10}H_{10}NO)[ZnBr_2(C_{10}H_8NO)]\cdot CH_3CN$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

8-Hydroxy-2-methylquinolinium dibromido(2-methylquinolin-8-olato-κ^2N,O)zincate acetonitrile monosolvate

Crystal data

$(C_{10}H_{10}NO)[ZnBr_2(C_{10}H_8NO)]\cdot C_2H_3N$	$Z = 2$
$M_r = 584.61$	$F(000) = 580$
Triclinic, $P\overline{1}$	$D_x = 1.731$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.1870$ (3) Å	Cell parameters from 4618 reflections
$b = 9.7795$ (5) Å	$\theta = 2.4$–$29.1°$
$c = 16.2520$ (7) Å	$\mu = 4.68$ mm^{-1}
$\alpha = 86.159$ (4)°	$T = 100$ K
$\beta = 80.775$ (4)°	Block, yellow
$\gamma = 85.098$ (4)°	0.25 × 0.20 × 0.15 mm
$V = 1121.73$ (9) Å^3	

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	4970 independent reflections
Radiation source: SuperNova (Mo) X-ray Source	4197 reflections with $I > 2\sigma(I)$
Mirror	$R_{int} = 0.033$
Detector resolution: 10.4041 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 2.5°$
ω scans	$h = -9\rightarrow9$
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)	$k = -9\rightarrow12$
$T_{min} = 0.387$, $T_{max} = 0.540$	$l = -20\rightarrow21$
8710 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.065$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
4970 reflections	$(\Delta/\sigma)_{max} = 0.001$
282 parameters	$\Delta\rho_{max} = 0.54$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.86$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.88168 (4)	0.83050 (3)	0.860009 (16)	0.02244 (8)
Br2	0.50073 (4)	0.95447 (3)	0.711001 (16)	0.02404 (8)
Zn1	0.61597 (4)	0.77959 (3)	0.800839 (17)	0.01579 (8)
O1	0.6552 (2)	0.59396 (18)	0.75476 (10)	0.0164 (4)
O2	0.7760 (2)	0.49663 (19)	0.61189 (10)	0.0180 (4)
H2	0.735 (4)	0.535 (3)	0.6565 (12)	0.051 (11)*
N1	0.4256 (3)	0.6890 (2)	0.88999 (12)	0.0138 (5)
N2	0.8330 (3)	0.3677 (2)	0.46831 (12)	0.0137 (5)
H1	0.853 (4)	0.323 (3)	0.5148 (10)	0.026 (8)*
N3	0.9248 (3)	0.1939 (2)	0.61350 (15)	0.0268 (6)
C1	0.4381 (3)	0.5504 (3)	0.87876 (14)	0.0135 (5)
C2	0.5632 (3)	0.5020 (3)	0.80728 (14)	0.0149 (5)
C3	0.5768 (4)	0.3633 (3)	0.79535 (15)	0.0173 (6)
H3	0.6582	0.3288	0.7481	0.021*
C4	0.4733 (4)	0.2716 (3)	0.85143 (15)	0.0182 (6)
H4	0.4860	0.1765	0.8411	0.022*
C5	0.3544 (3)	0.3161 (3)	0.92073 (16)	0.0187 (6)
H5	0.2857	0.2527	0.9581	0.022*
C6	0.3357 (3)	0.4576 (3)	0.93569 (15)	0.0156 (5)
C7	0.2193 (3)	0.5165 (3)	1.00595 (15)	0.0179 (6)
H7	0.1498	0.4591	1.0471	0.022*
C8	0.2076 (3)	0.6539 (3)	1.01421 (15)	0.0181 (6)
H8	0.1275	0.6922	1.0606	0.022*
C9	0.3124 (3)	0.7408 (3)	0.95511 (15)	0.0156 (6)
C10	0.3020 (4)	0.8932 (3)	0.96312 (16)	0.0222 (6)
H10A	0.4281	0.9263	0.9462	0.033*
H10B	0.2555	0.9144	1.0213	0.033*
H10C	0.2155	0.9387	0.9271	0.033*
C11	0.7546 (3)	0.5007 (3)	0.46969 (15)	0.0134 (5)
C12	0.7190 (3)	0.5680 (3)	0.54621 (15)	0.0143 (5)
C13	0.6326 (3)	0.6992 (3)	0.54599 (16)	0.0173 (6)
H13	0.6071	0.7463	0.5963	0.021*
C14	0.5817 (3)	0.7643 (3)	0.47216 (16)	0.0190 (6)
H14	0.5201	0.8542	0.4740	0.023*
C15	0.6185 (3)	0.7019 (3)	0.39779 (16)	0.0182 (6)
H15	0.5836	0.7480	0.3486	0.022*
C16	0.7093 (3)	0.5677 (3)	0.39514 (15)	0.0159 (6)
C17	0.7563 (3)	0.4941 (3)	0.32169 (16)	0.0202 (6)
H17	0.7326	0.5375	0.2699	0.024*
C18	0.8347 (3)	0.3626 (3)	0.32364 (16)	0.0200 (6)
H18	0.8650	0.3152	0.2735	0.024*
C19	0.8711 (3)	0.2964 (3)	0.39969 (16)	0.0173 (6)
C20	0.9466 (4)	0.1505 (3)	0.40586 (17)	0.0248 (6)
H20A	0.9691	0.1260	0.4631	0.037*
H20B	1.0657	0.1380	0.3673	0.037*

H20C	0.8548	0.0913	0.3913	0.037*
C21	0.9679 (4)	0.1787 (3)	0.67766 (18)	0.0220 (6)
C22	1.0230 (4)	0.1609 (3)	0.76012 (17)	0.0322 (7)
H22A	1.1477	0.1105	0.7564	0.048*
H22B	0.9301	0.1090	0.7976	0.048*
H22C	1.0285	0.2512	0.7820	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02081 (15)	0.02701 (17)	0.02033 (14)	−0.00692 (12)	−0.00113 (11)	−0.00586 (12)
Br2	0.03621 (17)	0.01423 (15)	0.02002 (14)	0.00516 (12)	−0.00265 (12)	−0.00189 (11)
Zn1	0.01904 (16)	0.01350 (17)	0.01443 (15)	−0.00166 (13)	−0.00014 (12)	−0.00329 (12)
O1	0.0210 (9)	0.0138 (10)	0.0130 (8)	0.0004 (8)	0.0010 (7)	−0.0027 (7)
O2	0.0249 (10)	0.0167 (10)	0.0112 (9)	0.0011 (8)	−0.0001 (8)	−0.0020 (8)
N1	0.0138 (10)	0.0161 (12)	0.0120 (10)	−0.0006 (9)	−0.0024 (8)	−0.0043 (9)
N2	0.0137 (11)	0.0139 (12)	0.0126 (11)	−0.0010 (9)	0.0015 (9)	−0.0028 (9)
N3	0.0290 (14)	0.0192 (14)	0.0296 (14)	0.0031 (11)	0.0006 (11)	−0.0007 (11)
C1	0.0136 (12)	0.0148 (14)	0.0136 (12)	−0.0001 (10)	−0.0059 (10)	−0.0046 (10)
C2	0.0157 (13)	0.0187 (15)	0.0109 (12)	−0.0003 (11)	−0.0038 (10)	−0.0030 (11)
C3	0.0197 (13)	0.0191 (15)	0.0132 (12)	0.0042 (11)	−0.0033 (11)	−0.0065 (11)
C4	0.0245 (14)	0.0115 (14)	0.0210 (13)	−0.0003 (11)	−0.0106 (11)	−0.0032 (11)
C5	0.0190 (13)	0.0187 (15)	0.0202 (13)	−0.0052 (12)	−0.0068 (11)	0.0006 (11)
C6	0.0132 (12)	0.0201 (15)	0.0147 (12)	−0.0020 (11)	−0.0051 (10)	−0.0016 (11)
C7	0.0144 (13)	0.0252 (16)	0.0146 (12)	−0.0035 (12)	−0.0025 (10)	−0.0016 (11)
C8	0.0125 (12)	0.0279 (16)	0.0139 (12)	−0.0004 (12)	0.0000 (10)	−0.0067 (12)
C9	0.0143 (13)	0.0181 (15)	0.0160 (13)	−0.0004 (11)	−0.0059 (10)	−0.0061 (11)
C10	0.0224 (14)	0.0221 (16)	0.0225 (14)	0.0008 (12)	−0.0021 (12)	−0.0095 (12)
C11	0.0081 (12)	0.0136 (13)	0.0183 (13)	−0.0027 (10)	0.0001 (10)	−0.0015 (11)
C12	0.0125 (12)	0.0157 (14)	0.0139 (12)	−0.0042 (11)	0.0025 (10)	−0.0033 (11)
C13	0.0168 (13)	0.0160 (14)	0.0185 (13)	−0.0049 (11)	0.0028 (11)	−0.0051 (11)
C14	0.0153 (13)	0.0125 (14)	0.0279 (15)	0.0013 (11)	−0.0006 (11)	−0.0009 (11)
C15	0.0175 (13)	0.0172 (15)	0.0194 (13)	−0.0026 (11)	−0.0026 (11)	0.0034 (11)
C16	0.0113 (12)	0.0204 (15)	0.0162 (13)	−0.0028 (11)	−0.0007 (10)	−0.0030 (11)
C17	0.0175 (14)	0.0276 (17)	0.0162 (13)	−0.0050 (12)	−0.0024 (11)	−0.0033 (12)
C18	0.0181 (14)	0.0263 (16)	0.0161 (13)	−0.0008 (12)	0.0003 (11)	−0.0133 (12)
C19	0.0132 (13)	0.0177 (15)	0.0211 (14)	−0.0024 (11)	0.0005 (11)	−0.0066 (11)
C20	0.0282 (15)	0.0195 (16)	0.0263 (15)	0.0037 (13)	−0.0029 (12)	−0.0086 (12)
C21	0.0205 (14)	0.0115 (14)	0.0302 (16)	0.0020 (11)	0.0054 (13)	0.0000 (12)
C22	0.0312 (17)	0.036 (2)	0.0251 (15)	0.0058 (15)	0.0005 (13)	0.0072 (14)

Geometric parameters (Å, °)

Br1—Zn1	2.3738 (4)	C9—C10	1.500 (4)
Br2—Zn1	2.3566 (4)	C10—H10A	0.9800
Zn1—O1	1.9907 (18)	C10—H10B	0.9800
Zn1—N1	2.0386 (19)	C10—H10C	0.9800
O1—C2	1.339 (3)	C11—C16	1.409 (3)
O2—C12	1.336 (3)	C11—C12	1.423 (3)

O2—H2	0.837 (10)	C12—C13	1.377 (4)
N1—C9	1.328 (3)	C13—C14	1.406 (4)
N1—C1	1.373 (3)	C13—H13	0.9500
N2—C19	1.334 (3)	C14—C15	1.369 (4)
N2—C11	1.373 (3)	C14—H14	0.9500
N2—H1	0.875 (10)	C15—C16	1.415 (4)
N3—C21	1.131 (3)	C15—H15	0.9500
C1—C6	1.416 (3)	C16—C17	1.415 (4)
C1—C2	1.431 (3)	C17—C18	1.360 (4)
C2—C3	1.375 (4)	C17—H17	0.9500
C3—C4	1.406 (4)	C18—C19	1.408 (4)
C3—H3	0.9500	C18—H18	0.9500
C4—C5	1.372 (3)	C19—C20	1.485 (4)
C4—H4	0.9500	C20—H20A	0.9800
C5—C6	1.412 (4)	C20—H20B	0.9800
C5—H5	0.9500	C20—H20C	0.9800
C6—C7	1.426 (3)	C21—C22	1.453 (4)
C7—C8	1.353 (4)	C22—H22A	0.9800
C7—H7	0.9500	C22—H22B	0.9800
C8—C9	1.407 (4)	C22—H22C	0.9800
C8—H8	0.9500		
O1—Zn1—N1	83.97 (8)	C9—C10—H10C	109.5
O1—Zn1—Br2	114.56 (5)	H10A—C10—H10C	109.5
N1—Zn1—Br2	117.98 (6)	H10B—C10—H10C	109.5
O1—Zn1—Br1	111.06 (5)	N2—C11—C16	119.2 (2)
N1—Zn1—Br1	109.80 (6)	N2—C11—C12	119.6 (2)
Br2—Zn1—Br1	115.446 (16)	C16—C11—C12	121.2 (2)
C2—O1—Zn1	110.82 (14)	O2—C12—C13	126.2 (2)
C12—O2—H2	112 (2)	O2—C12—C11	115.8 (2)
C9—N1—C1	120.2 (2)	C13—C12—C11	118.0 (2)
C9—N1—Zn1	130.70 (18)	C12—C13—C14	120.8 (2)
C1—N1—Zn1	108.86 (15)	C12—C13—H13	119.6
C19—N2—C11	123.8 (2)	C14—C13—H13	119.6
C19—N2—H1	116.0 (19)	C15—C14—C13	121.8 (3)
C11—N2—H1	120.1 (19)	C15—C14—H14	119.1
N1—C1—C6	122.2 (2)	C13—C14—H14	119.1
N1—C1—C2	117.1 (2)	C14—C15—C16	119.1 (2)
C6—C1—C2	120.7 (2)	C14—C15—H15	120.4
O1—C2—C3	123.9 (2)	C16—C15—H15	120.4
O1—C2—C1	118.5 (2)	C11—C16—C17	117.0 (2)
C3—C2—C1	117.6 (2)	C11—C16—C15	119.0 (2)
C2—C3—C4	121.5 (2)	C17—C16—C15	124.0 (2)
C2—C3—H3	119.2	C18—C17—C16	121.4 (3)
C4—C3—H3	119.2	C18—C17—H17	119.3
C5—C4—C3	121.6 (3)	C16—C17—H17	119.3
C5—C4—H4	119.2	C17—C18—C19	120.2 (2)
C3—C4—H4	119.2	C17—C18—H18	119.9
C4—C5—C6	119.0 (2)	C19—C18—H18	119.9
C4—C5—H5	120.5	N2—C19—C18	118.2 (2)

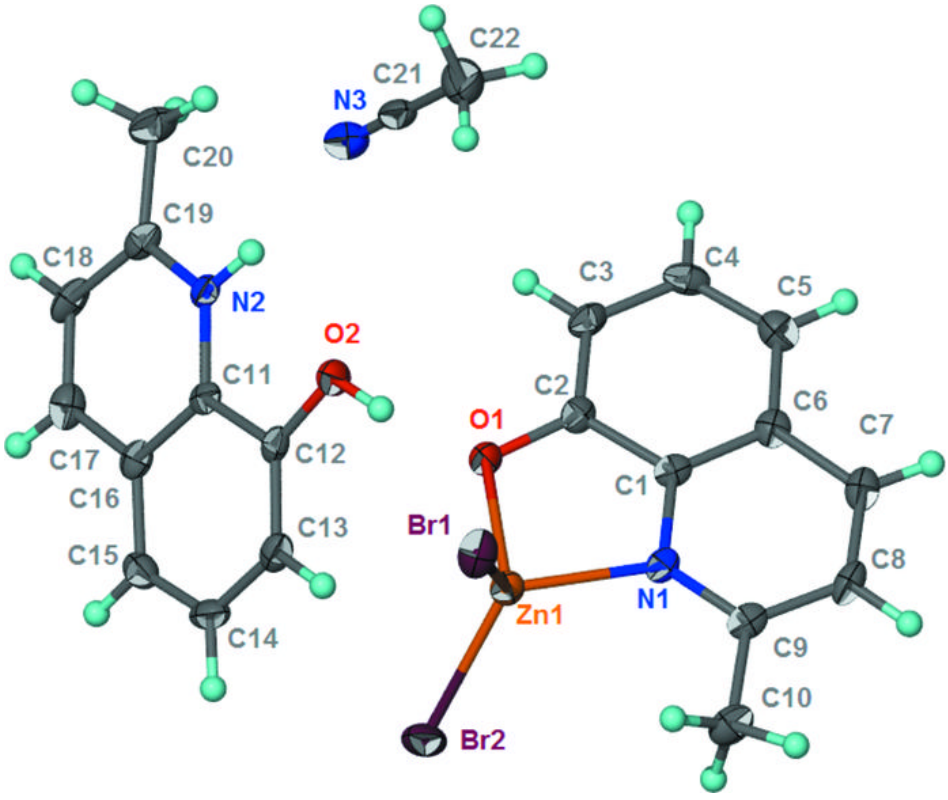
C6—C5—H5	120.5	N2—C19—C20	119.5 (2)
C1—C6—C5	119.5 (2)	C18—C19—C20	122.3 (2)
C1—C6—C7	116.0 (2)	C19—C20—H20A	109.5
C5—C6—C7	124.5 (2)	C19—C20—H20B	109.5
C8—C7—C6	120.2 (2)	H20A—C20—H20B	109.5
C8—C7—H7	119.9	C19—C20—H20C	109.5
C6—C7—H7	119.9	H20A—C20—H20C	109.5
C7—C8—C9	121.0 (2)	H20B—C20—H20C	109.5
C7—C8—H8	119.5	N3—C21—C22	179.3 (3)
C9—C8—H8	119.5	C21—C22—H22A	109.5
N1—C9—C8	120.4 (2)	C21—C22—H22B	109.5
N1—C9—C10	117.7 (2)	H22A—C22—H22B	109.5
C8—C9—C10	121.9 (2)	C21—C22—H22C	109.5
C9—C10—H10A	109.5	H22A—C22—H22C	109.5
C9—C10—H10B	109.5	H22B—C22—H22C	109.5
H10A—C10—H10B	109.5		

N1—Zn1—O1—C2	−7.93 (16)	C6—C7—C8—C9	−1.4 (4)
Br2—Zn1—O1—C2	−125.99 (14)	C1—N1—C9—C8	1.5 (3)
Br1—Zn1—O1—C2	101.00 (15)	Zn1—N1—C9—C8	−172.56 (17)
O1—Zn1—N1—C9	−178.6 (2)	C1—N1—C9—C10	−178.9 (2)
Br2—Zn1—N1—C9	−64.0 (2)	Zn1—N1—C9—C10	7.1 (3)
Br1—Zn1—N1—C9	71.1 (2)	C7—C8—C9—N1	−0.2 (4)
O1—Zn1—N1—C1	6.82 (15)	C7—C8—C9—C10	−179.8 (2)
Br2—Zn1—N1—C1	121.47 (14)	C19—N2—C11—C16	0.4 (4)
Br1—Zn1—N1—C1	−103.42 (15)	C19—N2—C11—C12	179.9 (2)
C9—N1—C1—C6	−1.1 (4)	N2—C11—C12—O2	3.6 (3)
Zn1—N1—C1—C6	174.10 (19)	C16—C11—C12—O2	−176.9 (2)
C9—N1—C1—C2	−179.9 (2)	N2—C11—C12—C13	−177.2 (2)
Zn1—N1—C1—C2	−4.7 (3)	C16—C11—C12—C13	2.2 (3)
Zn1—O1—C2—C3	−174.4 (2)	O2—C12—C13—C14	179.0 (2)
Zn1—O1—C2—C1	7.7 (3)	C11—C12—C13—C14	−0.1 (4)
N1—C1—C2—O1	−2.0 (3)	C12—C13—C14—C15	−1.2 (4)
C6—C1—C2—O1	179.2 (2)	C13—C14—C15—C16	0.4 (4)
N1—C1—C2—C3	−180.0 (2)	N2—C11—C16—C17	−2.8 (3)
C6—C1—C2—C3	1.2 (4)	C12—C11—C16—C17	177.8 (2)
O1—C2—C3—C4	−178.4 (2)	N2—C11—C16—C15	176.4 (2)
C1—C2—C3—C4	−0.5 (4)	C12—C11—C16—C15	−3.1 (3)
C2—C3—C4—C5	−0.2 (4)	C14—C15—C16—C11	1.7 (4)
C3—C4—C5—C6	0.2 (4)	C14—C15—C16—C17	−179.2 (2)
N1—C1—C6—C5	180.0 (2)	C11—C16—C17—C18	2.6 (4)
C2—C1—C6—C5	−1.3 (4)	C15—C16—C17—C18	−176.5 (2)
N1—C1—C6—C7	−0.5 (3)	C16—C17—C18—C19	0.0 (4)
C2—C1—C6—C7	178.3 (2)	C11—N2—C19—C18	2.2 (4)
C4—C5—C6—C1	0.6 (4)	C11—N2—C19—C20	−176.8 (2)
C4—C5—C6—C7	−179.0 (2)	C17—C18—C19—N2	−2.3 (4)
C1—C6—C7—C8	1.7 (4)	C17—C18—C19—C20	176.6 (2)
C5—C6—C7—C8	−178.7 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.84 (1)	1.73 (1)	2.561 (2)	173 (4)
N2—H1···N3	0.88 (1)	2.08 (1)	2.943 (3)	171 (3)

Fig. 1


C22
C21
N3
C20
C19
C18
N2
O2
C11
C12
C17
C16
C13
C15
C14
C3
C4
C5
C2
C6
C7
O1
C1
Br1
C8
N1
Zn1
C9
C10
Br2