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8-Hydroxy-2-methylquinolinium diiodido(2-methylquinolin-8-olato-κ^2N,O)zincate(II) methanol monosolvate

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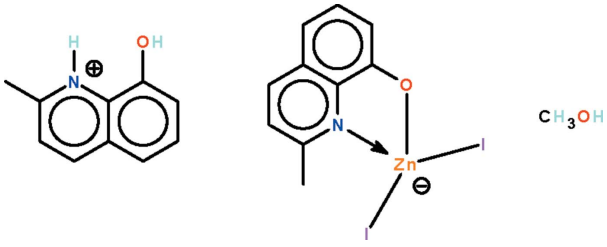
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.031; wR factor = 0.090; data-to-parameter ratio = 20.2.

The anion of the title salt, $(C_{10}H_{10}NO)[Zn(C_{10}H_8NO)I_2]\cdot CH_3OH$, has its metal atom N,O-chelated by the deprotonated 2-methyl-8-hydroxyquinoline ligand. The hydroxy unit of the cation is a hydrogen-bond donor to the alkoxide O atom of the tetrahedrally coordinated anion, whereas the ammonium cation acts as a hydrogen-bond donor to the methanolic O atom. In the crystal, adjacent ion pairs and solvent molecules are linked by a methanol–halogen O—H···I hydrogen bond, generating a chain running along the a axis.

Related literature

For the isostructural chloro analog, see: Sattarzadeh *et al.* (2009).



Experimental

Crystal data

$(C_{10}H_{10}NO)[Zn(C_{10}H_8NO)I_2]\cdot CH_4O$
M_r = 669.58
Monoclinic, $P2_1/n$
a = 10.1745 (6) Å
b = 14.6292 (9) Å
c = 16.5321 (10) Å
β = 106.356 (1)°
V = 2361.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.68 mm^{-1}
T = 295 K
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.359, T_{max} = 0.608
21863 measured reflections
5404 independent reflections
4049 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.090
S = 1.06
5404 reflections
267 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.74	2.559 (4)	172
O3—H3···I1^{i}	0.82	2.88	3.575 (4)	144
N2—H2n···O3	0.86	1.92	2.757 (5)	165

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5355).

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supporting information

Acta Cryst. (2010). E**66**, m1277 [doi:10.1107/S1600536810036718]

8-Hydroxy-2-methylquinolinium diiodido(2-methylquinolin-8-olato-κ^2N,O)zincate(II) methanol monosolvate

Ezzatollah Najafi, Mostafa M. Amini and Seik Weng Ng

S1. Comment

An earlier study reported $C_{10}H_{10}NO^{+}\cdot ZnCl_2(C_{10}H_8NO)\cdot CH_3OH$, which feature cations, tetrahedral anions and solvent molecules linked by N···O, O···O and O···Cl hydrogen bonds into a linear chain (Sattarzadeh *et al.*, 2009). The present iodide analog (Scheme I, Fig. 1) is isostructural, the two compounds displaying matching cell dimensions. The hydroxy unit of the cation is hydrogen-bond donor to the alkoxide O atom of the tetrahedrally coordinated anion whereas the ammonium unit is hydrogen-bond donor to the methanolic O atom. Adjacent ion-pairs and solvent molecules are linked by a O–$H_{methanol}$···I hydrogen bond to generate a linear chain running along the *a*-axis of the monoclinic unit cell.

S2. Experimental

Zinc iodide (0.24 g, 0.75 mmol) and 2-methyl-8-hydroxyquinoline (0.24 g, 1.5 mmol) were loaded into a convection tube; the tube was filled with dry methanol and kept at 333 K. Crystals were collected from the side arm after several days.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93–0.96, N–H 0.86 and O–H 0.82 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C,*N*,*O*).

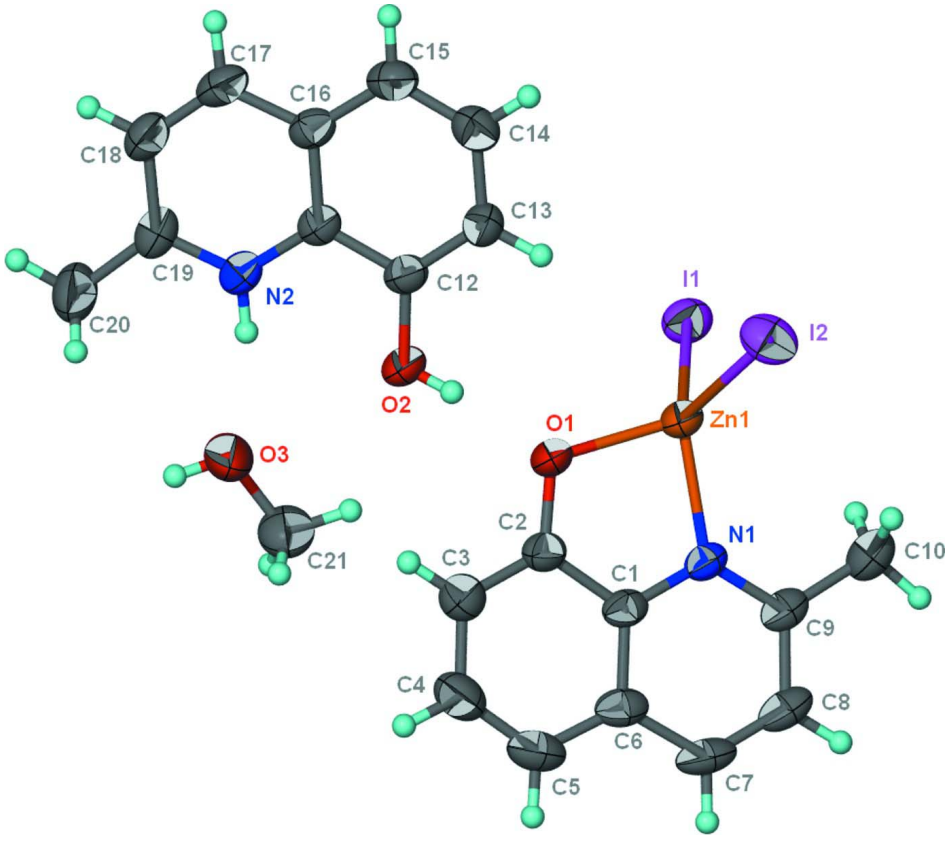

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

$(C_{10}H_{10}NO)[Zn(C_{10}H_8NO)I_2]\cdot CH_4O$
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Hall symbol: -P 2yn
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$b = 14.6292\ (9)$ Å
$c = 16.5321\ (10)$ Å
$\beta = 106.356\ (1)°$
$V = 2361.1\ (2)$ Å^3
$Z = 4$
$F(000) = 1288$
$D_x = 1.884$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6864 reflections
$\theta = 2.5–25.1°$
$\mu = 3.68$ mm^{-1}
$T = 295$ K
Triangular block, yellow
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.359$, $T_{max} = 0.608$
21863 measured reflections
5404 independent reflections
4049 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -13\rightarrow13$
$k = -19\rightarrow19$
$l = -21\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.090$
$S = 1.06$
5404 reflections
267 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 2.9232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.78$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.99864 (3)	0.22364 (2)	0.185681 (19)	0.05940 (11)
I2	1.12403 (4)	0.50224 (2)	0.22894 (2)	0.06773 (12)
Zn1	0.98601 (5)	0.37087 (4)	0.26758 (3)	0.04947 (13)
O1	0.7946 (3)	0.4058 (2)	0.25987 (17)	0.0590 (8)
O2	0.5880 (3)	0.3620 (2)	0.13701 (17)	0.0575 (8)
H2	0.6556	0.3798	0.1736	0.086*
O3	0.3218 (4)	0.2893 (5)	0.1583 (3)	0.132 (2)
H3	0.2424	0.3008	0.1573	0.198*
N1	1.0064 (3)	0.3664 (2)	0.39435 (19)	0.0421 (7)
N2	0.3603 (3)	0.3482 (2)	0.0082 (2)	0.0464 (8)
H2N	0.3620	0.3346	0.0591	0.056*
C1	0.8857 (4)	0.3933 (3)	0.4085 (2)	0.0439 (9)
C2	0.7747 (4)	0.4140 (3)	0.3364 (2)	0.0491 (10)
C3	0.6530 (5)	0.4435 (3)	0.3495 (3)	0.0585 (11)
H3a	0.5794	0.4587	0.3036	0.070*
C4	0.6399 (5)	0.4505 (4)	0.4314 (3)	0.0675 (13)
H4	0.5568	0.4699	0.4386	0.081*
C5	0.7444 (5)	0.4301 (3)	0.5007 (3)	0.0639 (13)
H5	0.7325	0.4350	0.5543	0.077*
C6	0.8711 (5)	0.4016 (3)	0.4906 (3)	0.0507 (10)
C7	0.9878 (5)	0.3799 (3)	0.5575 (3)	0.0611 (13)
H7	0.9831	0.3834	0.6128	0.073*
C8	1.1066 (5)	0.3541 (3)	0.5424 (3)	0.0585 (12)
H8	1.1828	0.3407	0.5872	0.070*
C9	1.1151 (4)	0.3477 (3)	0.4589 (2)	0.0481 (9)
C10	1.2444 (5)	0.3205 (3)	0.4395 (3)	0.0625 (12)
H10A	1.2797	0.3717	0.4159	0.094*
H10B	1.2260	0.2710	0.3998	0.094*
H10C	1.3107	0.3014	0.4904	0.094*
C11	0.4800 (4)	0.3758 (3)	−0.0072 (2)	0.0423 (8)
C12	0.6010 (4)	0.3837 (3)	0.0609 (2)	0.0445 (9)
C13	0.7190 (4)	0.4124 (3)	0.0438 (3)	0.0487 (9)
H13	0.7998	0.4173	0.0873	0.058*
C14	0.7184 (5)	0.4343 (3)	−0.0388 (3)	0.0558 (11)

H14	0.7991	0.4541	−0.0488	0.067*
C15	0.6026 (5)	0.4273 (3)	−0.1051 (3)	0.0548 (11)
H15	0.6049	0.4417	−0.1594	0.066*
C16	0.4804 (4)	0.3981 (3)	−0.0899 (2)	0.0461 (9)
C17	0.3539 (5)	0.3907 (3)	−0.1537 (3)	0.0564 (11)
H17	0.3501	0.4049	−0.2091	0.068*
C18	0.2383 (5)	0.3632 (3)	−0.1349 (3)	0.0571 (11)
H18	0.1564	0.3588	−0.1776	0.069*
C19	0.2415 (4)	0.3414 (3)	−0.0518 (3)	0.0542 (11)
C20	0.1160 (5)	0.3133 (4)	−0.0273 (4)	0.0782 (16)
H20A	0.1130	0.3455	0.0227	0.117*
H20B	0.1189	0.2487	−0.0168	0.117*
H20C	0.0358	0.3277	−0.0723	0.117*
C21	0.3972 (6)	0.2771 (4)	0.2385 (3)	0.0768 (15)
H21A	0.4920	0.2717	0.2404	0.115*
H21B	0.3680	0.2224	0.2605	0.115*
H21C	0.3853	0.3286	0.2718	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.06369 (19)	0.0647 (2)	0.04850 (17)	−0.01375 (14)	0.01360 (13)	−0.00404 (13)
I2	0.0790 (2)	0.0597 (2)	0.0736 (2)	−0.00371 (16)	0.03639 (18)	0.00974 (15)
Zn1	0.0457 (3)	0.0681 (3)	0.0332 (2)	−0.0018 (2)	0.00879 (19)	0.0042 (2)
O1	0.0437 (16)	0.099 (2)	0.0323 (14)	0.0011 (16)	0.0070 (12)	0.0026 (15)
O2	0.0492 (17)	0.085 (2)	0.0346 (15)	−0.0055 (16)	0.0053 (12)	0.0056 (15)
O3	0.058 (2)	0.279 (7)	0.061 (3)	0.008 (3)	0.022 (2)	0.046 (3)
N1	0.0462 (18)	0.0456 (18)	0.0308 (15)	−0.0052 (14)	0.0046 (13)	0.0035 (13)
N2	0.0467 (19)	0.0472 (19)	0.0412 (18)	0.0031 (15)	0.0057 (15)	0.0036 (15)
C1	0.052 (2)	0.045 (2)	0.0345 (19)	−0.0133 (17)	0.0110 (17)	0.0016 (16)
C2	0.048 (2)	0.061 (3)	0.039 (2)	−0.0094 (19)	0.0128 (18)	0.0015 (18)
C3	0.054 (3)	0.067 (3)	0.055 (3)	−0.003 (2)	0.016 (2)	0.003 (2)
C4	0.063 (3)	0.079 (3)	0.070 (3)	−0.005 (3)	0.034 (3)	−0.011 (3)
C5	0.083 (4)	0.067 (3)	0.051 (3)	−0.012 (3)	0.034 (3)	−0.006 (2)
C6	0.070 (3)	0.045 (2)	0.038 (2)	−0.013 (2)	0.018 (2)	0.0007 (17)
C7	0.092 (4)	0.060 (3)	0.030 (2)	−0.016 (3)	0.015 (2)	0.0013 (19)
C8	0.075 (3)	0.054 (3)	0.036 (2)	−0.005 (2)	−0.001 (2)	0.0066 (19)
C9	0.057 (2)	0.043 (2)	0.039 (2)	−0.0060 (18)	0.0048 (18)	0.0027 (17)
C10	0.060 (3)	0.065 (3)	0.052 (3)	0.003 (2)	0.000 (2)	0.003 (2)
C11	0.047 (2)	0.038 (2)	0.040 (2)	0.0055 (16)	0.0097 (17)	−0.0019 (16)
C12	0.049 (2)	0.048 (2)	0.036 (2)	0.0058 (17)	0.0106 (17)	0.0007 (16)
C13	0.042 (2)	0.057 (2)	0.044 (2)	0.0040 (18)	0.0080 (17)	−0.0008 (19)
C14	0.056 (3)	0.059 (3)	0.057 (3)	0.003 (2)	0.024 (2)	−0.001 (2)
C15	0.066 (3)	0.059 (3)	0.043 (2)	0.010 (2)	0.019 (2)	0.0031 (19)
C16	0.055 (2)	0.044 (2)	0.038 (2)	0.0074 (18)	0.0093 (18)	−0.0044 (16)
C17	0.069 (3)	0.058 (3)	0.036 (2)	0.009 (2)	0.005 (2)	−0.0038 (19)
C18	0.053 (3)	0.063 (3)	0.047 (2)	0.004 (2)	−0.001 (2)	−0.006 (2)
C19	0.049 (2)	0.051 (2)	0.054 (3)	0.0018 (19)	0.000 (2)	0.001 (2)

C20	0.050 (3)	0.098 (4)	0.079 (4)	−0.011 (3)	0.006 (3)	0.014 (3)
C21	0.078 (4)	0.085 (4)	0.069 (3)	0.002 (3)	0.022 (3)	0.023 (3)

Geometric parameters (Å, º)

I1—Zn1	2.5665 (6)	C8—H8	0.9300
I2—Zn1	2.5649 (6)	C9—C10	1.493 (6)
Zn1—O1	1.982 (3)	C10—H10A	0.9600
Zn1—N1	2.048 (3)	C10—H10B	0.9600
O1—C2	1.341 (5)	C10—H10C	0.9600
O2—C12	1.340 (5)	C11—C16	1.407 (5)
O2—H2	0.8200	C11—C12	1.419 (5)
O3—C21	1.343 (6)	C12—C13	1.375 (6)
O3—H3	0.8200	C13—C14	1.400 (6)
N1—C9	1.331 (5)	C13—H13	0.9300
N1—C1	1.371 (5)	C14—C15	1.369 (6)
N2—C19	1.333 (5)	C14—H14	0.9300
N2—C11	1.373 (5)	C15—C16	1.402 (6)
N2—H2N	0.8600	C15—H15	0.9300
C1—C6	1.412 (5)	C16—C17	1.420 (6)
C1—C2	1.425 (6)	C17—C18	1.359 (7)
C2—C3	1.385 (6)	C17—H17	0.9300
C3—C4	1.402 (7)	C18—C19	1.403 (6)
C3—H3a	0.9300	C18—H18	0.9300
C4—C5	1.359 (7)	C19—C20	1.502 (7)
C4—H4	0.9300	C20—H20A	0.9600
C5—C6	1.409 (7)	C20—H20B	0.9600
C5—H5	0.9300	C20—H20C	0.9600
C6—C7	1.412 (6)	C21—H21A	0.9600
C7—C8	1.354 (7)	C21—H21B	0.9600
C7—H7	0.9300	C21—H21C	0.9600
C8—C9	1.410 (6)		

O1—Zn1—N1	83.61 (12)	H10A—C10—H10B	109.5
O1—Zn1—I2	112.82 (10)	C9—C10—H10C	109.5
N1—Zn1—I2	111.95 (9)	H10A—C10—H10C	109.5
O1—Zn1—I1	112.11 (10)	H10B—C10—H10C	109.5
N1—Zn1—I1	120.50 (9)	N2—C11—C16	119.6 (4)
I2—Zn1—I1	112.65 (2)	N2—C11—C12	119.6 (3)
C2—O1—Zn1	111.6 (2)	C16—C11—C12	120.8 (4)
C12—O2—H2	109.5	O2—C12—C13	126.1 (4)
C21—O3—H3	109.5	O2—C12—C11	115.6 (4)
C9—N1—C1	120.2 (3)	C13—C12—C11	118.3 (4)
C9—N1—Zn1	130.5 (3)	C12—C13—C14	120.4 (4)
C1—N1—Zn1	109.2 (2)	C12—C13—H13	119.8
C19—N2—C11	123.4 (4)	C14—C13—H13	119.8
C19—N2—H2N	118.3	C15—C14—C13	122.0 (4)
C11—N2—H2N	118.3	C15—C14—H14	119.0

N1—C1—C6	122.1 (4)	C13—C14—H14	119.0
N1—C1—C2	117.1 (3)	C14—C15—C16	119.1 (4)
C6—C1—C2	120.9 (4)	C14—C15—H15	120.5
O1—C2—C3	123.7 (4)	C16—C15—H15	120.5
O1—C2—C1	118.4 (4)	C15—C16—C11	119.3 (4)
C3—C2—C1	117.9 (4)	C15—C16—C17	123.7 (4)
C2—C3—C4	120.5 (4)	C11—C16—C17	117.0 (4)
C2—C3—H3a	119.8	C18—C17—C16	121.0 (4)
C4—C3—H3a	119.8	C18—C17—H17	119.5
C5—C4—C3	122.2 (5)	C16—C17—H17	119.5
C5—C4—H4	118.9	C17—C18—C19	120.5 (4)
C3—C4—H4	118.9	C17—C18—H18	119.7
C4—C5—C6	119.4 (4)	C19—C18—H18	119.7
C4—C5—H5	120.3	N2—C19—C18	118.5 (4)
C6—C5—H5	120.3	N2—C19—C20	118.8 (4)
C7—C6—C5	124.7 (4)	C18—C19—C20	122.6 (4)
C7—C6—C1	116.1 (4)	C19—C20—H20A	109.5
C5—C6—C1	119.1 (4)	C19—C20—H20B	109.5
C8—C7—C6	121.0 (4)	H20A—C20—H20B	109.5
C8—C7—H7	119.5	C19—C20—H20C	109.5
C6—C7—H7	119.5	H20A—C20—H20C	109.5
C7—C8—C9	120.2 (4)	H20B—C20—H20C	109.5
C7—C8—H8	119.9	O3—C21—H21A	109.5
C9—C8—H8	119.9	O3—C21—H21B	109.5
N1—C9—C8	120.3 (4)	H21A—C21—H21B	109.5
N1—C9—C10	117.8 (4)	O3—C21—H21C	109.5
C8—C9—C10	121.9 (4)	H21A—C21—H21C	109.5
C9—C10—H10A	109.5	H21B—C21—H21C	109.5
C9—C10—H10B	109.5		

N1—Zn1—O1—C2	3.3 (3)	C6—C7—C8—C9	−0.6 (7)
I2—Zn1—O1—C2	−107.9 (3)	C1—N1—C9—C8	0.8 (6)
I1—Zn1—O1—C2	123.7 (3)	Zn1—N1—C9—C8	176.2 (3)
O1—Zn1—N1—C9	−178.9 (4)	C1—N1—C9—C10	−178.8 (4)
I2—Zn1—N1—C9	−66.8 (4)	Zn1—N1—C9—C10	−3.4 (6)
I1—Zn1—N1—C9	69.2 (4)	C7—C8—C9—N1	−0.3 (6)
O1—Zn1—N1—C1	−3.1 (3)	C7—C8—C9—C10	179.3 (4)
I2—Zn1—N1—C1	109.0 (2)	C19—N2—C11—C16	−0.3 (6)
I1—Zn1—N1—C1	−115.0 (2)	C19—N2—C11—C12	178.1 (4)
C9—N1—C1—C6	−0.4 (6)	N2—C11—C12—O2	0.6 (5)
Zn1—N1—C1—C6	−176.7 (3)	C16—C11—C12—O2	179.0 (4)
C9—N1—C1—C2	178.7 (4)	N2—C11—C12—C13	−179.4 (4)
Zn1—N1—C1—C2	2.4 (4)	C16—C11—C12—C13	−1.0 (6)
Zn1—O1—C2—C3	175.7 (4)	O2—C12—C13—C14	−179.1 (4)
Zn1—O1—C2—C1	−2.9 (5)	C11—C12—C13—C14	0.9 (6)
N1—C1—C2—O1	0.3 (6)	C12—C13—C14—C15	−0.7 (7)
C6—C1—C2—O1	179.4 (4)	C13—C14—C15—C16	0.6 (7)
N1—C1—C2—C3	−178.4 (4)	C14—C15—C16—C11	−0.7 (6)

C6—C1—C2—C3	0.7 (6)	C14—C15—C16—C17	178.4 (4)
O1—C2—C3—C4	−179.9 (4)	N2—C11—C16—C15	179.3 (4)
C1—C2—C3—C4	−1.3 (7)	C12—C11—C16—C15	0.9 (6)
C2—C3—C4—C5	0.7 (8)	N2—C11—C16—C17	0.2 (6)
C3—C4—C5—C6	0.6 (8)	C12—C11—C16—C17	−178.2 (4)
C4—C5—C6—C7	178.9 (5)	C15—C16—C17—C18	−179.1 (4)
C4—C5—C6—C1	−1.1 (7)	C11—C16—C17—C18	0.0 (6)
N1—C1—C6—C7	−0.5 (6)	C16—C17—C18—C19	−0.1 (7)
C2—C1—C6—C7	−179.6 (4)	C11—N2—C19—C18	0.2 (6)
N1—C1—C6—C5	179.6 (4)	C11—N2—C19—C20	−178.1 (4)
C2—C1—C6—C5	0.5 (6)	C17—C18—C19—N2	0.0 (7)
C5—C6—C7—C8	−179.1 (4)	C17—C18—C19—C20	178.2 (5)
C1—C6—C7—C8	1.0 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	1.74	2.559 (4)	172
O3—H3···I1^{i}	0.82	2.88	3.575 (4)	144
N2—H2n···O3	0.86	1.92	2.757 (5)	165

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