research communications

Crystal structures of three zinc(II) halide coordination complexes with quinoline *N*-oxide

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The reaction of one equivalent of zinc(II) halide with two equivalents of quinoline *N*-oxide (QNO) in methanol yields compounds as $ZnX_2(QNO)_2$, where X = Cl (**I**), Br (**II**) and I (**III**), namely, dichloridobis(quinoline *N*-oxide-κO)zinc(II), $[ZnCl_2(C_9H_7NO)_2]$, dibromidobis(quinoline *N*-oxide-κO)-zinc(II), $[ZnBr_2(C_9H_7NO)_2]$, and diiodidobis(quinoline *N*-oxide-κO)zinc(II) $[ZnI_2(C_9H_7NO)_2]$. In all three complexes, Zn cations are coordinated by two QNO ligands bound through the oxygen atoms and two halide atoms, with X—Zn—X bond angles *ca* 20° wider than the O—Zn—O, giving rise to a distorted tetrahedral geometry. Crystals of (**II**) and (**III**) are isostructural and both show pairwise π-stacking of QNO ligands and weak C—H···X hydrogen bonds, while (**I**) packs differently, with a shorter C—H···Cl bond and without π-stacking.

1. Chemical context

N-oxide complexes have a rich history in organic transformations, including utility with transition metals in oxotransformations [see, for example, Eppenson (2003) and Moustafa *et al.* (2014)]. These transition-metal *N*-oxide complexes highlight the strong Lewis acid/Lewis base properties of the zinc(II) ion and *N*-oxides, respectively. Aromatic *N*-oxides are strong Lewis base ligands and form transition-metal complexes that are prevalent in the literature and highlight the strong transition metal interactions with the lone pair on the *N*-oxide oxygen atom. Examples of such complexes include a 4-methylpyridine *N*-oxide (MePyNO) derivative CuCl$_2$·2MePyNO (CMPYUC; Watson & Johnson, 1971) and pyridine *N*-oxide (6PyNO) derivatives Ni(BF$_4$)$_2$·6PyNO (PYNONI; van Ingen Schenau *et al.*, 1974) or Au(CF$_3$)$_3$·PyNO (NEPVOW; Pérez-Bitrián *et al.*, 2017). Previous reports of zinc(II) complexes with aromatic *N*-oxides include dibromobis(4-methoxypyridine *N*-oxide-κO)zinc(II) (GAWHIW; Shi *et al.* 2005*a*), diaquabis(picolinato *N*-oxide-$\kappa^2 O,O'$)zinc(II) (XISBOR; Li *et al.*, 2008) and dichlorobis(pyridine *N*-oxide)zinc(II) (QQQBXP01; McConnell *et al.*, 1986), all of which are mononuclear complexes.

Herein we report the crystal structures of three complexes of quinoline *N*-oxide (QNO) with zinc(II) chloride, bromide and iodide. All three were obtained by 1:2 stoichiometric reaction of the zinc(II) halide with QNO in methanol and found to be mononuclear $ZnX_2(QNO)_2$ complexes with a distorted tetrahedral environment around the zinc ion.

Figure 1
A view of compound (**I**), showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.
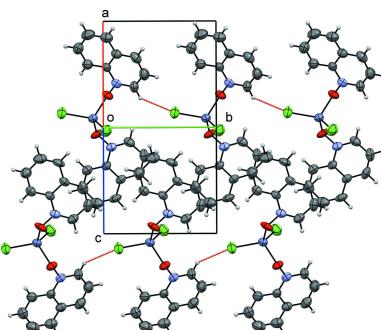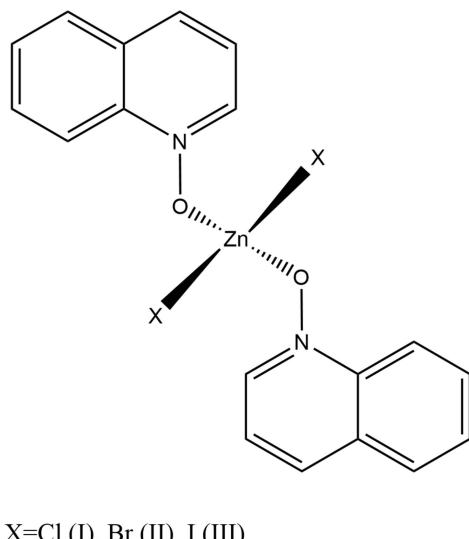
2. Structural commentary

Compound (**I**) crystallizes in the monoclinic space group $P2_1$ (Fig. 1), whereas compounds (**II**) (Fig. 2) and (**III**) (Fig. 3) both crystallize in the monoclinic space group $P2_1/c$. Each structure contains one symmetrically independent molecule, the coordination sphere around each Zn atom being a distorted tetrahedron. Selected bond lengths and angles in these complexes are shown in Table 1. Compounds (**II**) and (**III**) are isostructural in both the molecular conformation and crystal packing, while (**I**) differs in both aspects, as illustrated by an overlay of molecules (**I**) and (**II**) (Fig. 4*a*) on one hand, and molecules (**II**) and (**III**) on the other (Fig. 4*b*). Most notably, (**I**) differs in the orientation of the QNO rings relative to each other, the C2—N1—N2—C11 torsion angles being −16.9 (5)° in (**I**) *versus* −113.9 (3)° in (**II**) and −111.6 (3)° in (**III**).

Figure 2
A view of compound (**II**), showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

3. Supramolecular features

Figs. 5, 6 and 7 show the packing of compounds (**I**), (**II**) and (**III**), respectively. In the crystal structures, the packing is stabilized by van der Waals interactions and, in (**II**) and (**III**), by similar systems of pairwise π–π stacking interactions. Quinoline moieties $Cg1$–$Cg3$ and $Cg2$–$Cg4$ (see Figs. 6 and 7) are stacked each against its own inversion-related equivalent, with the separations between their (parallel) mean planes
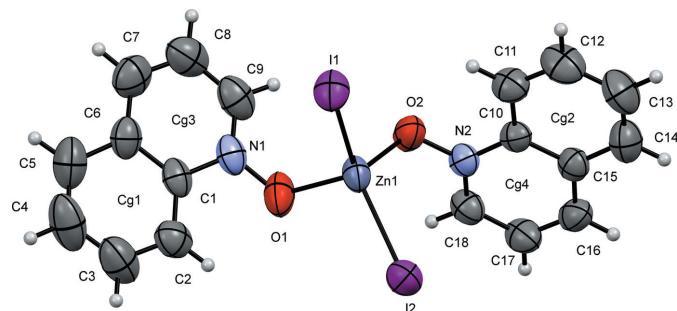

Figure 3
A view of compound (**III**), showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

equaling 3.483 (5) and 3.402 (5) Å, respectively, for (**II**), 3.466 (5) and 3.436 (5) Å for (**III**). The structure of (**I**) has no π-stacking. Besides, all three structures are characterized by C—H···X hydrogen bonds (X = halogen), see below.

Table 1
Selected bond lengths and angles (Å, °).

Compound (**I**)		Compound (**II**)		Compound (**III**)	
Zn1—Cl1	2.215 (2)	Zn1—Br1	2.3575 (9)	Zn1—I1	2.5534 (8)
Zn1—Cl2	2.211 (2)	Zn1—Br2	2.3472 (10)	Zn1—I2	2.5475 (9)
Zn1—O1	1.991 (5)	Zn1—O1	1.975 (4)	Zn1—O1	1.974 (4)
Zn1—O2	1.959 (5)	Zn1—O2	1.989 (4)	Zn1—O2	1.995 (4)
Cl1—Zn1—Cl2	117.80 (9)	Br1—Zn1—Br2	123.45 (4)	I1—Zn1—I2	122.34 (3)
O1—Zn1—O2	99.4 (2)	O1—Zn1—O2	103.10 (16)	O1—Zn1—O2	104.12 (19)
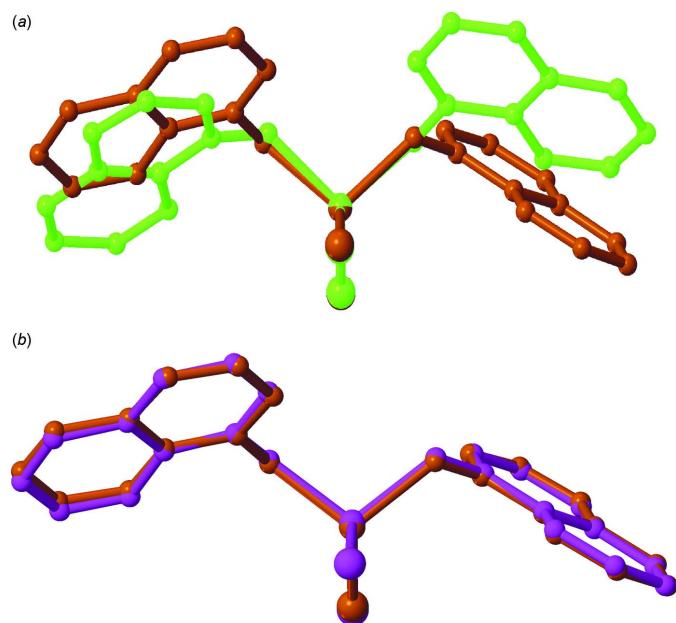
Figure 4
(a) Molecular overlay of compound (**I**) (green) and compound (**II**) (brown). (b) Molecular overlay of compound (**II**) (brown) and compound (**III**) (purple).

4. Hirshfeld surface analysis

The intermolecular interactions were further investigated by quantitative analysis of the Hirshfeld surface, and visualized with *Crystal Explorer 21* (Spackman *et al.*, 2021) and the two-dimensional fingerprint plots (McKinnon *et al.*, 2007). Figs. 8, 9 and 10 show Hirshfeld surfaces of molecules (**I**) to (**III**) mapped with the function d_{norm}, the sum of the distances from a surface point to the nearest interior (d_i) and exterior (d_e)
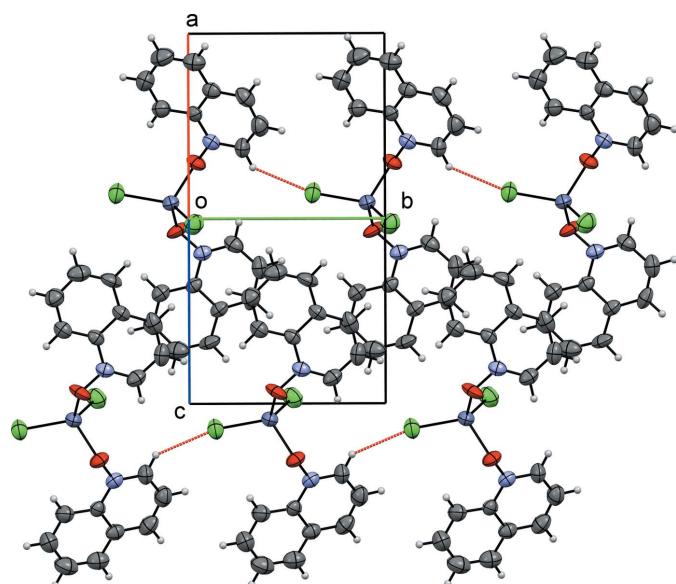
Figure 5
Crystal packing diagram of compound (**I**), viewed down the [101] direction.
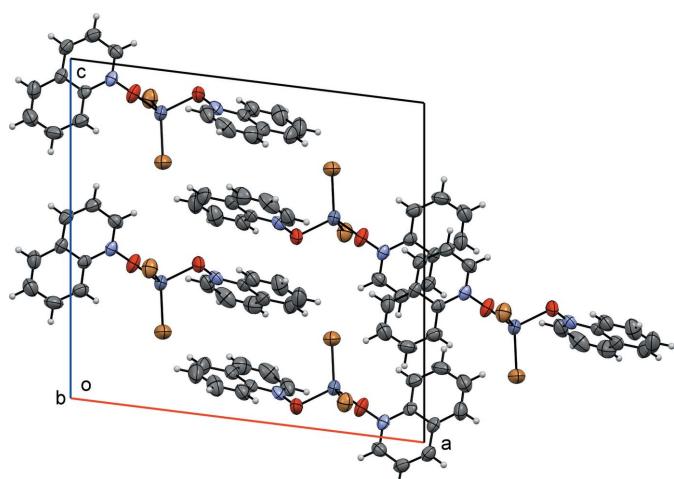
Figure 6
Crystal packing diagram of compound (**II**), viewed down the *b* axis.

atoms, normalized by the van der Waals (vdW) radii of the corresponding atoms (r_{vdW}). Contacts shorter than the sums of vdW radii are shown in red, those longer in blue, and those approximately equal to vdW as white spots.

For (**I**), the most intense red spots correspond to the intermolecular contacts O1···C9($1 - x$, $y - \frac{1}{2}$, $1 - z$) [3.048 (9) Å] and the hydrogen bond C18—H18···Cl2(x, $y + 1$, z). The latter has the distances H···Cl = 2.53 Å (for the C—H distance normalized to 1.083 Å) and C···Cl = 3.416 (9) Å within the previously observed range but shorter than the average values of 2.64 and 3.66 Å, respectively (Steiner, 1998). The other chloride ligand, Cl2, forms four H···Cl contacts of 2.83–2.98 Å, more typical for van der Waals interactions (Rowland & Taylor, 1996). For (**II**) and (**III**), the red spots correspond to C—H···X interactions, *viz.* C18—H18···X1, C5—H5···X1, C16—H16···X2, and C9—H9···X2, which can be also regarded as weak hydrogen bonds (Steiner, 1998). The H···X distances in (**II**) (X = Br) are 2.85, 2.88, 2.88 and 2.89 Å, respectively, while in (**III**) (X = I) they are 3.03, 3.12, 3.03 and 2.96 Å, respectively.
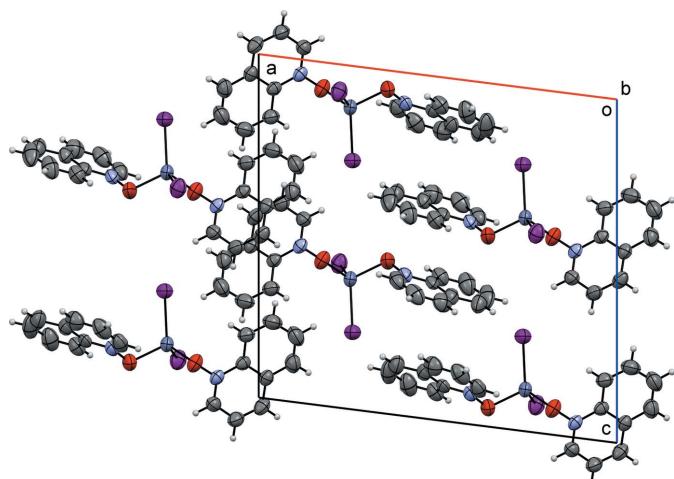
Figure 7
Crystal packing diagram of compound (**III**), viewed down the *b* axis.
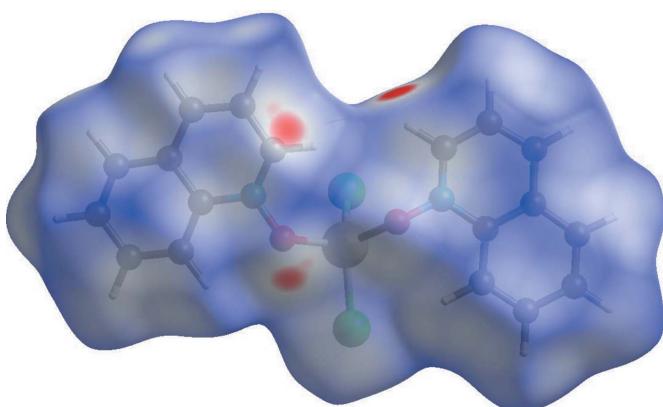
Figure 8
Hirshfeld surface for (I) mapped over d_{norm}.

Analysis of the two-dimensional fingerprint plots (Table 2) indicates that H···H contacts are the most common in all three structures. X···H contacts make the second highest contribution, which increases in the succession (I) < (II) < (III), together with the size of the halogen atoms and hence their share of the molecular surface (16.9, 18.5 and 20.6%, respectively). Interestingly, π-stacking in the structures of (II) and (III) gives only a modest increase of C···C contacts compared to (I), probably because it is counterbalanced by an overall decrease of carbon atoms' share of the surface (21.4 > 19.5 > 18.3%). No halogen···halogen contacts are observed in any of the three structures.

5. Database survey

A search in the Cambridge Structural Database (CSD, version 5.42, update of February 2021; Groom *et al.*, 2016) for aromatic *N*-oxides and halogen ligands bound to zinc returned 21 unique entries, the majority (15) of which contain pyridine *N*-oxide and its derivatives. Of these, the most closely related are pyridine *N*-oxide complexes, dichlorobis(pyridine *N*-oxide)zinc(II) (QQQBXP01; McConnell *et al.*, 1986), dibromorobis(pyridine *N*-oxide)zinc(II) (FIPVUV; Edwards *et*

Table 2
Contributions of selected intermolecular contacts (%).

Compound	(I)	(II)	(III)
H···H	32.0	36.7	36.5
H···X/X···H	24.4	28.4	30.0
C···H/H···C	22.7	18.5	18.0
C···C	5.4	7.1	6.4
O···H/H···O	6.0	4.0	3.7

al., 1999) and diiodorobis(pyridine *N*-oxide)zinc(II) (IPNOZN01; Edwards *et al.*, 1999). Related to these are methyl derivatives of pyridine *N*-oxide complexes with ZnCl$_2$, *viz.* dichlorobis(2,6-dimethylpyridine *N*-oxide)zinc(II) (LUTOZN; Sager & Watson, 1968), three isomers of dichlorobis(methylpyridine *N*-oxide)zinc(II) (QQQBXG, QQQBXJ, QQQBXM), for which only unit-cell parameters were determined (Kidd *et al.*, 1967), and finally, diiodobis(4-methylpyridine *N*-oxide)zinc(II) (SANRUV; Shi *et al.*, 2005b). There is one known structure of a quinoline *N*-oxide derivative, dichlorobis(2-methylquinoline *N*-oxide)zinc(II) (AFUSEZ; Ivashevskaja *et al.*, 2002).

6. Synthesis and crystallization

The water content of QNO and ZnBr$_2$ have been determined by Thermal Gravimetric Analysis. The formulation for each was found to be QNO·0.28H$_2$O (M_W = 150.21 g mol^{-1}) and ZnBr$_2$·0.86H$_2$O (F_W = 240.69 g mol^{-1}).

The title compounds were all synthesized in a similar manner. Compound (I) was synthesized by dissolving 0.0986 g of QNO·0.28H$_2$O (0.656 mmol, purchased from Aldrich) in 33 mL of methanol to which 0.0440 g of ZnCl$_2$ (0.176 mmol, purchased from Strem Chemicals) were added at 295 K. The solution was covered with parafilm then allowed to sit; X-ray quality crystals were grown by slow evaporation at 295 K. Yield, 0.0822 g (60.2%). Selected IR bands (ATR–IR, cm^{-1}): 3107 (w), 3083 (w), 3057 (w), 1579 (m), 1513 (m), 1447 (m), 1402 (s), 1269 (s), 1227 (m), 1203 (s), 1179 (m), 1144 (m), 1089 (s), 1050 (m), 883 (s), 800 (s), 768 (s), 723 (m), 584 (m), 559 (m), 542 (m).
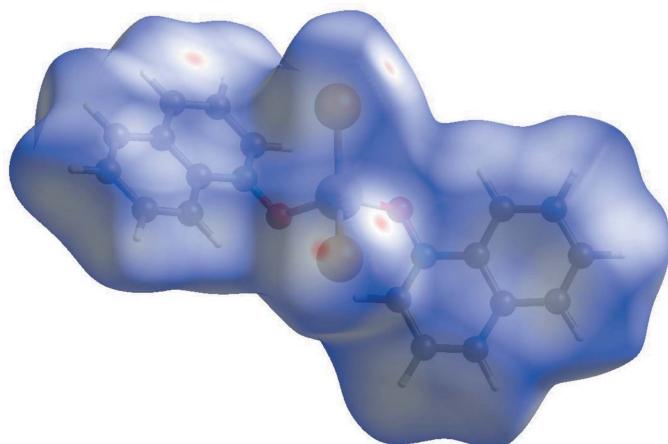
Figure 9
Hirshfeld surface for (II) mapped over d_{norm}.
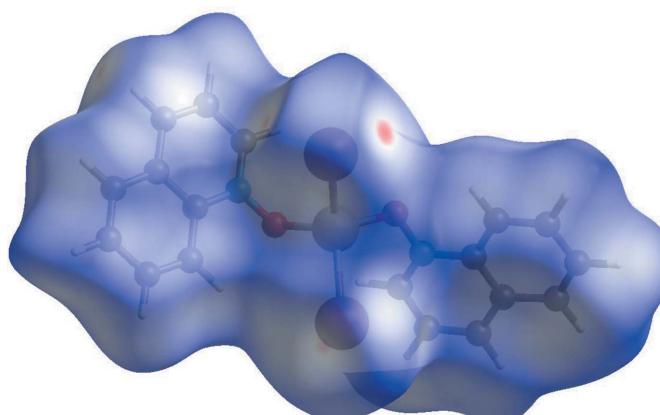
Figure 10
Hirshfeld surface for (III) mapped over d_{norm}.

Table 3
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$[ZnCl_2(C_9H_7NO)_2]$	$[ZnBr_2(C_9H_7NO)_2]$	$[ZnI_2(C_9H_7NO)_2]$
M_r	426.58	515.50	609.48
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	298	298	297
a, b, c (Å)	8.5167 (4), 7.8697 (4), 13.1617 (7)	16.3922 (11), 7.3527 (6), 15.5809 (10)	16.7231 (7), 7.6155 (4), 15.8689 (7)
β (°)	94.890 (5)	97.113 (6)	97.192 (4)
V (Å^3)	878.94 (8)	1863.5 (2)	2005.08 (16)
Z	2	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.72	5.62	4.32
Crystal size (mm)	$0.1 \times 0.1 \times 0.03$	$0.15 \times 0.08 \times 0.03$	$0.3 \times 0.3 \times 0.3$
Data collection			
Diffractometer	Rigaku XtaLAB mini	XtaLAB Mini (ROW)	Rigaku XtaLAB mini
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)
T_{min}, T_{max}	0.968, 1.000	0.833, 1.000	0.896, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5308, 3169, 2456	7207, 3415, 2095	11510, 3668, 2748
R_{int}	0.036	0.043	0.032
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602	0.602	0.602
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.077, 1.03	0.042, 0.090, 1.02	0.035, 0.085, 1.07
No. of reflections	3169	3415	3668
No. of parameters	226	226	227
No. of restraints	1	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.42, −0.35	0.55, −0.35	0.80, −0.81
Absolute structure	Flack x determined using 810 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).	–	–
Absolute structure parameter	−0.006 (15)	–	–

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), and *OLEX2* (Dolomanov *et al.*, 2009).

Compound (**II**) was synthesized by dissolving 0.0983 g of QNO·0.28H$_2$O (0.654 mmol), in 40 mL of methanol to which 0.0778 g of ZnBr$_2$·0.86H$_2$O (0.323 mmol, purchased from Alfa Aesar) were added at 295 K. The solution was covered with parafilm then allowed to sit; X-ray quality crystals were grown by slow evaporation at 295 K. Yield, 0.0866 g (46.7%). Selected IR bands (ATR–IR, cm^{-1}): 3106 (*w*), 3075 (*w*), 3061 (*w*), 3016 (*w*), 1580 (*m*), 1510 (*s*), 1455 (*m*), 1270 (*s*), 1227 (*m*), 1214 (*s*), 1204 (*s*), 1173 (*m*), 1138 (*m*), 1086 (*s*), 1048 (*m*), 877 (*m*), 800 (*s*), 767 (*s*), 720 (*s*), 581 (*m*), 563 (*m*), 500 (*m*).

Compound (**III**) was synthesized by dissolving 0.0517 g of QNO·0.28H$_2$O (0.352 mmol) in approximately 36 mL of methanol to which 0.0524 g of ZnI$_2$ (0.164 mmol, purchased from Aldrich) were added at 295 K. The solution was covered with parafilm then allowed to sit; X-ray quality crystals were grown by slow evaporation at 295 K. Yield, 0.0910 g (52.3%). Selected IR Bands (ATR–IR, cm^{-1}): 3100 (*w*), 3090 (*w*), 2076 (*w*), 3059 (*w*), 3027 (*w*),1580 (*s*), 1507 (*s*), 1382 (*s*), 1267 (*m*), 1225 (*m*), 1207 (*s*), 1169 (*m*), 1141 (*m*), 1044 (*m*), 880 (*s*), 807 (*s*), 769 (*s*), 720 (*m*), 580 (*m*), 562 (*m*), 499 (*m*).

Infrared spectroscopy confirms the presence of the QNO ligand in all three complexes. Characteristic IR bands include weak νC—H aromatic stretches observed from 3020– 3107 cm^{-1} and νN—O stretches of the bound *N*-oxide in the range 1350–1150 cm^{-1}; notably, a medium band observed in the ligand at 1311 cm^{-1}, appears at between 1225–1227 cm^{-1} in the three metal complexes. Finally, a broad absorbance in the free ligand from 3100–3500 cm^{-1} (assigned to the water νO—H stretch) is absent in all of the metal complexes (Mautner *et al.*, 2016).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All carbon-bound H atoms were positioned geometrically and refined as riding: C—H = 0.95– 0.98 Å with U_{iso}(H) = $1.2U_{eq}$(C).

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supporting information

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Computing details

For all structures, data collection: *CrysAlis PRO* (Rigaku OD, 2019); cell refinement: *CrysAlis PRO* (Rigaku OD, 2019); data reduction: *CrysAlis PRO* (Rigaku OD, 2019); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/1* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Dichloridobis(quinoline *N*-oxide-κO)zinc(II) (I)

Crystal data

[ZnCl$_2$(C$_9$H$_7$NO)$_2$]	$F(000) = 432$
$M_r = 426.58$	$D_x = 1.612$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.5167$ (4) Å	Cell parameters from 1644 reflections
$b = 7.8697$ (4) Å	$\theta = 2.4$–22.4°
$c = 13.1617$ (7) Å	$\mu = 1.72$ mm^{-1}
$\beta = 94.890$ (5)°	$T = 298$ K
$V = 878.94$ (8) Å^3	Cube, clear colourless
$Z = 2$	$0.1 \times 0.1 \times 0.03$ mm

Data collection

Rigaku XtaLAB mini diffractometer	5308 measured reflections
Radiation source: fine-focus sealed X-ray tube, Rigaku (Mo) X-ray Source	3169 independent reflections
	2456 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.036$
ω scans	$\theta_{max} = 25.4°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2019)	$h = -10 \rightarrow 10$
	$k = -9 \rightarrow 9$
$T_{min} = 0.968$, $T_{max} = 1.000$	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3169 reflections	$(\Delta/\sigma)_{max} < 0.001$
226 parameters	$\Delta\rho_{max} = 0.42$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.35$ e Å^{-3}
Primary atom site location: dual	

Absolute structure: Flack *x* determined using 810 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).

Absolute structure parameter: −0.006 (15)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.60832 (9)	0.40878 (9)	0.69325 (6)	0.0481 (2)
Cl1	0.8131 (2)	0.5260 (3)	0.78185 (18)	0.0717 (6)
Cl2	0.5724 (2)	0.1322 (2)	0.71012 (17)	0.0668 (6)
O1	0.6087 (5)	0.4435 (7)	0.5459 (4)	0.0660 (17)
O2	0.4152 (6)	0.5393 (6)	0.7184 (4)	0.0543 (13)
N1	0.6919 (7)	0.5702 (8)	0.5068 (4)	0.0472 (15)
N2	0.3927 (6)	0.6163 (7)	0.8067 (4)	0.0461 (14)
C1	0.7938 (8)	0.5254 (9)	0.4342 (5)	0.0418 (17)
C2	0.8061 (9)	0.3562 (9)	0.4045 (6)	0.052 (2)
H2	0.745778	0.272501	0.432433	0.063*
C3	0.9086 (10)	0.3150 (11)	0.3332 (6)	0.065 (2)
H3	0.916168	0.203042	0.311636	0.077*
C4	1.0011 (10)	0.4398 (14)	0.2932 (6)	0.071 (3)
H4	1.072298	0.409606	0.246598	0.085*
C5	0.9891 (9)	0.6041 (11)	0.3210 (6)	0.061 (2)
H5	1.051065	0.685676	0.292553	0.074*
C6	0.8835 (8)	0.6538 (9)	0.3931 (5)	0.0469 (18)
C7	0.8623 (9)	0.8234 (8)	0.4243 (6)	0.056 (2)
H7	0.920737	0.910057	0.397750	0.067*
C8	0.7577 (10)	0.8601 (9)	0.4927 (6)	0.063 (2)
H8	0.742052	0.972081	0.511924	0.075*
C9	0.6733 (9)	0.7293 (10)	0.5342 (6)	0.056 (2)
H9	0.602718	0.754824	0.582143	0.068*
C10	0.3113 (8)	0.5307 (9)	0.8777 (6)	0.0441 (18)
C11	0.2654 (9)	0.3621 (9)	0.8595 (6)	0.059 (2)
H11	0.289239	0.306487	0.800371	0.071*
C12	0.1846 (10)	0.2810 (12)	0.9306 (7)	0.073 (2)
H12	0.154890	0.168062	0.920740	0.087*
C13	0.1458 (11)	0.3686 (13)	1.0195 (7)	0.081 (3)
H13	0.089040	0.312853	1.066778	0.097*
C14	0.1899 (10)	0.5309 (12)	1.0360 (7)	0.069 (3)
H14	0.163818	0.585631	1.094912	0.082*
C15	0.2745 (8)	0.6187 (10)	0.9661 (5)	0.0508 (19)
C16	0.3245 (9)	0.7899 (11)	0.9803 (6)	0.065 (2)
H16	0.300458	0.850485	1.037580	0.078*

C17	0.4081 (9)	0.8637 (10)	0.9084 (6)	0.067 (2)
H17	0.443132	0.975085	0.917171	0.081*
C18	0.4411 (9)	0.7745 (11)	0.8231 (6)	0.061 (2)
H18	0.499384	0.826957	0.775384	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0494 (4)	0.0451 (5)	0.0519 (5)	−0.0013 (5)	0.0168 (4)	0.0023 (5)
Cl1	0.0656 (13)	0.0678 (14)	0.0812 (16)	−0.0173 (11)	0.0034 (12)	−0.0053 (12)
Cl2	0.0710 (14)	0.0421 (11)	0.0875 (16)	−0.0034 (10)	0.0087 (12)	0.0054 (10)
O1	0.066 (3)	0.083 (5)	0.052 (3)	−0.033 (3)	0.025 (3)	0.006 (3)
O2	0.059 (3)	0.063 (3)	0.043 (3)	0.011 (3)	0.017 (3)	−0.010 (3)
N1	0.045 (3)	0.057 (4)	0.040 (4)	−0.004 (3)	0.006 (3)	0.002 (3)
N2	0.042 (3)	0.050 (4)	0.046 (4)	0.007 (3)	0.004 (3)	−0.003 (3)
C1	0.041 (4)	0.047 (4)	0.037 (4)	−0.003 (4)	0.000 (3)	0.010 (4)
C2	0.052 (5)	0.056 (5)	0.048 (5)	−0.008 (4)	0.005 (4)	0.003 (3)
C3	0.071 (6)	0.064 (6)	0.060 (5)	0.005 (5)	0.012 (5)	−0.003 (4)
C4	0.065 (5)	0.097 (8)	0.053 (5)	0.012 (6)	0.016 (4)	0.008 (6)
C5	0.047 (5)	0.078 (6)	0.061 (6)	−0.006 (5)	0.018 (4)	0.027 (5)
C6	0.044 (4)	0.052 (5)	0.045 (4)	−0.008 (4)	0.004 (4)	0.010 (4)
C7	0.058 (5)	0.043 (5)	0.062 (5)	−0.012 (4)	−0.013 (4)	0.019 (4)
C8	0.076 (6)	0.042 (5)	0.068 (5)	0.006 (4)	−0.009 (5)	0.001 (4)
C9	0.059 (5)	0.065 (6)	0.046 (4)	0.013 (4)	0.010 (4)	−0.004 (4)
C10	0.039 (4)	0.043 (4)	0.050 (5)	0.009 (4)	0.004 (4)	0.008 (4)
C11	0.055 (5)	0.061 (6)	0.062 (5)	−0.003 (4)	0.011 (4)	−0.004 (4)
C12	0.076 (6)	0.056 (5)	0.086 (7)	−0.007 (5)	0.015 (6)	0.002 (5)
C13	0.073 (6)	0.097 (10)	0.075 (6)	−0.004 (6)	0.021 (5)	0.022 (6)
C14	0.062 (6)	0.085 (7)	0.060 (6)	0.004 (5)	0.012 (5)	0.001 (5)
C15	0.047 (4)	0.059 (5)	0.046 (5)	0.008 (4)	0.004 (4)	0.002 (4)
C16	0.066 (6)	0.065 (6)	0.063 (5)	0.010 (5)	0.001 (5)	−0.021 (5)
C17	0.070 (6)	0.053 (6)	0.078 (6)	−0.004 (4)	0.001 (5)	−0.011 (4)
C18	0.072 (6)	0.039 (4)	0.073 (6)	−0.005 (4)	0.012 (5)	−0.004 (5)

Geometric parameters (Å, º)

Zn1—Cl1	2.215 (2)	C7—H7	0.9300
Zn1—Cl2	2.211 (2)	C7—C8	1.350 (11)
Zn1—O1	1.959 (5)	C8—H8	0.9300
Zn1—O2	1.991 (4)	C8—C9	1.393 (10)
O1—N1	1.351 (7)	C9—H9	0.9300
O2—N2	1.339 (6)	C10—C11	1.398 (10)
N1—C1	1.389 (8)	C10—C15	1.412 (10)
N1—C9	1.316 (9)	C11—H11	0.9300
N2—C10	1.385 (8)	C11—C12	1.366 (10)
N2—C18	1.324 (9)	C12—H12	0.9300
C1—C2	1.395 (9)	C12—C13	1.421 (12)
C1—C6	1.403 (9)	C13—H13	0.9300

C2—H2	0.9300	C13—C14	1.344 (12)
C2—C3	1.373 (10)	C14—H14	0.9300
C3—H3	0.9300	C14—C15	1.399 (10)
C3—C4	1.390 (11)	C15—C16	1.420 (11)
C4—H4	0.9300	C16—H16	0.9300
C4—C5	1.350 (12)	C16—C17	1.362 (11)
C5—H5	0.9300	C17—H17	0.9300
C5—C6	1.417 (10)	C17—C18	1.373 (10)
C6—C7	1.412 (10)	C18—H18	0.9300
Cl2—Zn1—Cl1	117.80 (9)	C8—C7—H7	119.9
O1—Zn1—Cl1	113.30 (15)	C7—C8—H8	120.2
O1—Zn1—Cl2	104.40 (18)	C7—C8—C9	119.7 (7)
O1—Zn1—O2	99.4 (2)	C9—C8—H8	120.2
O2—Zn1—Cl1	108.81 (16)	N1—C9—C8	121.1 (7)
O2—Zn1—Cl2	111.57 (16)	N1—C9—H9	119.4
N1—O1—Zn1	121.7 (4)	C8—C9—H9	119.4
N2—O2—Zn1	124.0 (4)	N2—C10—C11	119.6 (7)
O1—N1—C1	117.0 (6)	N2—C10—C15	118.5 (7)
C9—N1—O1	121.2 (6)	C11—C10—C15	121.9 (7)
C9—N1—C1	121.8 (6)	C10—C11—H11	120.8
O2—N2—C10	118.8 (6)	C12—C11—C10	118.4 (8)
C18—N2—O2	120.2 (6)	C12—C11—H11	120.8
C18—N2—C10	120.9 (6)	C11—C12—H12	119.9
N1—C1—C2	120.1 (7)	C11—C12—C13	120.2 (9)
N1—C1—C6	118.3 (7)	C13—C12—H12	119.9
C2—C1—C6	121.6 (7)	C12—C13—H13	119.6
C1—C2—H2	120.5	C14—C13—C12	120.9 (9)
C3—C2—C1	118.9 (7)	C14—C13—H13	119.6
C3—C2—H2	120.5	C13—C14—H14	119.5
C2—C3—H3	119.8	C13—C14—C15	121.0 (9)
C2—C3—C4	120.4 (8)	C15—C14—H14	119.5
C4—C3—H3	119.8	C10—C15—C16	119.2 (7)
C3—C4—H4	119.5	C14—C15—C10	117.6 (8)
C5—C4—C3	121.0 (8)	C14—C15—C16	123.2 (8)
C5—C4—H4	119.5	C15—C16—H16	120.6
C4—C5—H5	119.6	C17—C16—C15	118.8 (7)
C4—C5—C6	120.9 (8)	C17—C16—H16	120.6
C6—C5—H5	119.6	C16—C17—H17	119.8
C1—C6—C5	117.2 (7)	C16—C17—C18	120.3 (8)
C1—C6—C7	118.8 (7)	C18—C17—H17	119.8
C7—C6—C5	124.0 (7)	N2—C18—C17	122.1 (8)
C6—C7—H7	119.9	N2—C18—H18	118.9
C8—C7—C6	120.3 (7)	C17—C18—H18	118.9
Zn1—O1—N1—C1	127.4 (5)	C4—C5—C6—C1	0.5 (11)
Zn1—O1—N1—C9	−54.6 (8)	C4—C5—C6—C7	−178.7 (8)
Zn1—O2—N2—C10	−94.8 (6)	C5—C6—C7—C8	179.3 (7)

Zn1—O2—N2—C18	88.5 (7)	C6—C1—C2—C3	0.0 (12)
O1—N1—C1—C2	0.3 (10)	C6—C7—C8—C9	1.6 (12)
O1—N1—C1—C6	−179.2 (6)	C7—C8—C9—N1	−1.1 (12)
O1—N1—C9—C8	−179.1 (6)	C9—N1—C1—C2	−177.7 (7)
O2—N2—C10—C11	5.0 (9)	C9—N1—C1—C6	2.8 (10)
O2—N2—C10—C15	−173.8 (6)	C10—N2—C18—C17	−2.7 (11)
O2—N2—C18—C17	174.0 (6)	C10—C11—C12—C13	1.4 (12)
N1—C1—C2—C3	−179.5 (6)	C10—C15—C16—C17	−0.7 (11)
N1—C1—C6—C5	178.5 (6)	C11—C10—C15—C14	0.1 (11)
N1—C1—C6—C7	−2.2 (10)	C11—C10—C15—C16	180.0 (7)
N2—C10—C11—C12	−179.7 (7)	C11—C12—C13—C14	−1.2 (14)
N2—C10—C15—C14	179.0 (6)	C12—C13—C14—C15	0.4 (14)
N2—C10—C15—C16	−1.2 (10)	C13—C14—C15—C10	0.1 (13)
C1—N1—C9—C8	−1.1 (11)	C13—C14—C15—C16	−179.7 (8)
C1—C2—C3—C4	1.4 (12)	C14—C15—C16—C17	179.1 (8)
C1—C6—C7—C8	0.1 (11)	C15—C10—C11—C12	−0.9 (11)
C2—C1—C6—C5	−1.0 (11)	C15—C16—C17—C18	1.0 (12)
C2—C1—C6—C7	178.3 (7)	C16—C17—C18—N2	0.7 (13)
C2—C3—C4—C5	−1.9 (13)	C18—N2—C10—C11	−178.3 (7)
C3—C4—C5—C6	0.9 (13)	C18—N2—C10—C15	2.9 (10)

Dibromidobis(quinoline *N*-oxide-*κO*)zinc(II) (II)

Crystal data

[ZnBr$_2$(C$_9$H$_7$NO)$_2$]	$F(000) = 1008$
$M_r = 515.50$	$D_x = 1.837$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 16.3922$ (11) Å	Cell parameters from 1219 reflections
$b = 7.3527$ (6) Å	$\theta = 2.6$–22.0°
$c = 15.5809$ (10) Å	$\mu = 5.62$ mm^{-1}
$\beta = 97.113$ (6)°	$T = 298$ K
$V = 1863.5$ (2) Å^3	Irregular, clear colourless
$Z = 4$	$0.15 \times 0.08 \times 0.03$ mm

Data collection

XtaLAB Mini (ROW) diffractometer	7207 measured reflections
Radiation source: fine-focus sealed X-ray tube, Rigaku (Mo) X-ray Source	3415 independent reflections
	2095 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.043$
ω scans	$\theta_{max} = 25.4°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2019)	$h = -16 \rightarrow 19$
	$k = -8 \rightarrow 8$
$T_{min} = 0.833$, $T_{max} = 1.000$	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	226 parameters
Least-squares matrix: full	0 restraints
$R[F^2 > 2\sigma(F^2)] = 0.042$	Primary atom site location: dual
$wR(F^2) = 0.090$	Hydrogen site location: inferred from neighbouring sites
$S = 1.01$	
3415 reflections	H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0258P)^2]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	$U_{iso}*/U_{eq}$
Zn1	0.25508 (4)	0.26213 (9)	0.37264 (4)	0.0514 (2)
Br2	0.22409 (4)	−0.03623 (9)	0.41131 (4)	0.0695 (2)
Br1	0.26119 (4)	0.35514 (10)	0.22878 (4)	0.0698 (2)
O1	0.3616 (2)	0.3196 (6)	0.4411 (2)	0.0662 (11)
O2	0.1778 (2)	0.4332 (5)	0.4197 (2)	0.0597 (10)
N2	0.1157 (3)	0.3586 (5)	0.4557 (3)	0.0445 (11)
N1	0.4115 (3)	0.4386 (7)	0.4079 (3)	0.0543 (12)
C10	0.0394 (3)	0.3446 (7)	0.4065 (3)	0.0415 (12)
C1	0.4897 (3)	0.3784 (8)	0.3969 (3)	0.0466 (14)
C15	−0.0264 (3)	0.2713 (7)	0.4450 (3)	0.0468 (13)
C16	−0.0121 (4)	0.2148 (7)	0.5319 (3)	0.0550 (15)
H16	−0.054979	0.167100	0.558720	0.066*
C18	0.1273 (3)	0.3032 (7)	0.5371 (3)	0.0526 (15)
H18	0.179191	0.313686	0.568455	0.063*
C17	0.0635 (4)	0.2296 (8)	0.5765 (3)	0.0561 (15)
H17	0.072791	0.190483	0.633590	0.067*
C11	0.0284 (4)	0.4086 (8)	0.3210 (3)	0.0571 (16)
H11	0.071759	0.460347	0.296363	0.069*
C6	0.5437 (4)	0.5023 (9)	0.3641 (3)	0.0592 (16)
C2	0.5136 (4)	0.2028 (9)	0.4187 (3)	0.0626 (17)
H2	0.476904	0.122160	0.439392	0.075*
C14	−0.1031 (4)	0.2572 (8)	0.3940 (4)	0.0673 (17)
H14	−0.147290	0.206267	0.417522	0.081*
C13	−0.1135 (4)	0.3168 (9)	0.3113 (4)	0.0742 (19)
H13	−0.164632	0.307127	0.278474	0.089*
C12	−0.0477 (4)	0.3927 (9)	0.2752 (3)	0.0723 (19)
H12	−0.055985	0.433696	0.218351	0.087*
C9	0.3862 (4)	0.6041 (10)	0.3872 (4)	0.0730 (19)
H9	0.333060	0.639141	0.395028	0.088*
C7	0.5161 (5)	0.6777 (10)	0.3420 (4)	0.077 (2)
H7	0.550832	0.760022	0.319363	0.093*
C3	0.5912 (4)	0.1490 (10)	0.4098 (4)	0.083 (2)
H3	0.607681	0.030702	0.424267	0.099*
C8	0.4388 (5)	0.7279 (9)	0.3536 (4)	0.083 (2)
H8	0.420515	0.844968	0.339148	0.099*
C5	0.6244 (4)	0.4382 (12)	0.3568 (4)	0.085 (2)

H5	0.662411	0.515411	0.336046	0.102*
C4	0.6460 (5)	0.2678 (14)	0.3794 (5)	0.095 (3)
H4	0.699190	0.228696	0.374594	0.114*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0345 (4)	0.0688 (5)	0.0519 (4)	−0.0003 (3)	0.0089 (3)	−0.0017 (3)
Br2	0.0598 (4)	0.0637 (4)	0.0855 (5)	0.0040 (3)	0.0113 (3)	0.0048 (4)
Br1	0.0663 (4)	0.0960 (5)	0.0476 (3)	−0.0052 (4)	0.0090 (3)	−0.0030 (4)
O1	0.037 (2)	0.102 (3)	0.059 (2)	−0.016 (2)	0.0020 (18)	0.010 (2)
O2	0.046 (2)	0.055 (2)	0.083 (3)	−0.005 (2)	0.0278 (19)	0.002 (2)
N2	0.040 (3)	0.042 (3)	0.054 (3)	0.007 (2)	0.014 (2)	−0.005 (2)
N1	0.043 (3)	0.072 (4)	0.045 (3)	−0.005 (3)	−0.007 (2)	−0.012 (3)
C10	0.043 (3)	0.039 (3)	0.043 (3)	0.007 (3)	0.011 (2)	−0.006 (3)
C1	0.039 (3)	0.062 (4)	0.037 (3)	−0.005 (3)	−0.002 (2)	−0.011 (3)
C15	0.041 (3)	0.048 (3)	0.054 (3)	0.003 (3)	0.015 (3)	−0.003 (3)
C16	0.051 (4)	0.060 (4)	0.057 (4)	−0.001 (3)	0.020 (3)	0.006 (3)
C18	0.053 (4)	0.056 (4)	0.047 (3)	0.009 (3)	−0.003 (3)	−0.004 (3)
C17	0.063 (4)	0.062 (4)	0.046 (3)	0.007 (3)	0.017 (3)	0.008 (3)
C11	0.064 (4)	0.063 (4)	0.046 (3)	0.008 (3)	0.015 (3)	−0.003 (3)
C6	0.051 (4)	0.076 (5)	0.049 (3)	−0.016 (4)	0.001 (3)	−0.015 (3)
C2	0.053 (4)	0.072 (5)	0.059 (4)	−0.003 (3)	−0.007 (3)	−0.003 (3)
C14	0.042 (4)	0.079 (5)	0.081 (5)	−0.008 (3)	0.008 (3)	0.000 (4)
C13	0.055 (4)	0.092 (5)	0.072 (4)	0.002 (4)	−0.007 (3)	−0.006 (4)
C12	0.085 (5)	0.094 (5)	0.037 (3)	0.016 (4)	0.002 (3)	−0.002 (3)
C9	0.052 (4)	0.088 (5)	0.075 (4)	0.009 (4)	−0.010 (3)	−0.028 (4)
C7	0.086 (6)	0.074 (5)	0.071 (4)	−0.029 (4)	0.002 (4)	−0.003 (4)
C3	0.064 (5)	0.079 (5)	0.101 (5)	0.010 (4)	−0.007 (4)	−0.016 (4)
C8	0.098 (6)	0.053 (4)	0.087 (5)	−0.003 (5)	−0.028 (5)	0.000 (4)
C5	0.056 (5)	0.122 (7)	0.079 (5)	−0.035 (5)	0.022 (4)	−0.023 (5)
C4	0.050 (5)	0.130 (7)	0.104 (6)	0.006 (5)	0.008 (4)	−0.029 (6)

Geometric parameters (Å, º)

Zn1—Br2	2.3472 (10)	C11—H11	0.9300
Zn1—Br1	2.3575 (8)	C11—C12	1.364 (8)
Zn1—O1	1.975 (3)	C6—C7	1.395 (8)
Zn1—O2	1.989 (4)	C6—C5	1.422 (9)
O1—N1	1.345 (5)	C2—H2	0.9300
O2—N2	1.339 (5)	C2—C3	1.356 (8)
N2—C10	1.388 (6)	C14—H14	0.9300
N2—C18	1.323 (6)	C14—C13	1.352 (8)
N1—C1	1.386 (6)	C13—H13	0.9300
N1—C9	1.313 (7)	C13—C12	1.392 (8)
C10—C15	1.406 (7)	C12—H12	0.9300
C10—C11	1.402 (7)	C9—H9	0.9300
C1—C6	1.410 (7)	C9—C8	1.400 (9)

C1—C2	1.380 (7)	C7—H7	0.9300
C15—C16	1.408 (7)	C7—C8	1.354 (9)
C15—C14	1.405 (7)	C3—H3	0.9300
C16—H16	0.9300	C3—C4	1.378 (10)
C16—C17	1.346 (7)	C8—H8	0.9300
C18—H18	0.9300	C5—H5	0.9300
C18—C17	1.387 (7)	C5—C4	1.338 (9)
C17—H17	0.9300	C4—H4	0.9300
Br2—Zn1—Br1	123.45 (4)	C12—C11—H11	121.0
O1—Zn1—Br2	105.44 (12)	C1—C6—C5	116.5 (6)
O1—Zn1—Br1	108.21 (11)	C7—C6—C1	119.2 (6)
O1—Zn1—O2	103.10 (16)	C7—C6—C5	124.2 (7)
O2—Zn1—Br2	109.17 (11)	C1—C2—H2	120.4
O2—Zn1—Br1	105.72 (11)	C3—C2—C1	119.3 (6)
N1—O1—Zn1	118.1 (3)	C3—C2—H2	120.4
N2—O2—Zn1	116.6 (3)	C15—C14—H14	119.6
O2—N2—C10	118.5 (4)	C13—C14—C15	120.8 (6)
C18—N2—O2	120.1 (4)	C13—C14—H14	119.6
C18—N2—C10	121.4 (5)	C14—C13—H13	119.9
O1—N1—C1	117.1 (5)	C14—C13—C12	120.2 (6)
C9—N1—O1	120.5 (5)	C12—C13—H13	119.9
C9—N1—C1	122.4 (6)	C11—C12—C13	121.8 (6)
N2—C10—C15	118.6 (5)	C11—C12—H12	119.1
N2—C10—C11	120.1 (5)	C13—C12—H12	119.1
C11—C10—C15	121.3 (5)	N1—C9—H9	119.9
N1—C1—C6	118.0 (6)	N1—C9—C8	120.2 (6)
C2—C1—N1	120.5 (5)	C8—C9—H9	119.9
C2—C1—C6	121.5 (6)	C6—C7—H7	120.0
C10—C15—C16	118.6 (5)	C8—C7—C6	119.9 (7)
C14—C15—C10	117.9 (5)	C8—C7—H7	120.0
C14—C15—C16	123.6 (5)	C2—C3—H3	119.7
C15—C16—H16	119.8	C2—C3—C4	120.7 (7)
C17—C16—C15	120.3 (5)	C4—C3—H3	119.7
C17—C16—H16	119.8	C9—C8—H8	119.9
N2—C18—H18	119.4	C7—C8—C9	120.2 (7)
N2—C18—C17	121.1 (5)	C7—C8—H8	119.9
C17—C18—H18	119.4	C6—C5—H5	119.7
C16—C17—C18	120.0 (5)	C4—C5—C6	120.5 (7)
C16—C17—H17	120.0	C4—C5—H5	119.7
C18—C17—H17	120.0	C3—C4—H4	119.3
C10—C11—H11	121.0	C5—C4—C3	121.5 (7)
C12—C11—C10	118.0 (6)	C5—C4—H4	119.3
Zn1—O1—N1—C1	−122.3 (4)	C1—C6—C7—C8	1.1 (9)
Zn1—O1—N1—C9	57.8 (6)	C1—C6—C5—C4	0.7 (9)
Zn1—O2—N2—C10	−97.8 (4)	C1—C2—C3—C4	0.2 (9)
Zn1—O2—N2—C18	83.4 (5)	C15—C10—C11—C12	−2.0 (8)

O1—N1—C1—C6	−178.5 (4)	C15—C16—C17—C18	0.9 (9)
O1—N1—C1—C2	0.7 (7)	C15—C14—C13—C12	0.3 (10)
O1—N1—C9—C8	179.3 (5)	C16—C15—C14—C13	178.8 (6)
O2—N2—C10—C15	−178.1 (4)	C18—N2—C10—C15	0.6 (7)
O2—N2—C10—C11	−0.3 (7)	C18—N2—C10—C11	178.4 (5)
O2—N2—C18—C17	178.4 (5)	C11—C10—C15—C16	−177.9 (5)
N2—C10—C15—C16	−0.2 (7)	C11—C10—C15—C14	2.6 (8)
N2—C10—C15—C14	−179.7 (5)	C6—C1—C2—C3	1.1 (8)
N2—C10—C11—C12	−179.7 (5)	C6—C7—C8—C9	−0.3 (10)
N2—C18—C17—C16	−0.5 (8)	C6—C5—C4—C3	0.5 (11)
N1—C1—C6—C7	−1.6 (7)	C2—C1—C6—C7	179.2 (5)
N1—C1—C6—C5	177.7 (5)	C2—C1—C6—C5	−1.5 (8)
N1—C1—C2—C3	−178.1 (5)	C2—C3—C4—C5	−1.0 (11)
N1—C9—C8—C7	0.1 (10)	C14—C15—C16—C17	178.9 (6)
C10—N2—C18—C17	−0.3 (8)	C14—C13—C12—C11	0.4 (10)
C10—C15—C16—C17	−0.6 (8)	C9—N1—C1—C6	1.4 (7)
C10—C15—C14—C13	−1.7 (9)	C9—N1—C1—C2	−179.4 (5)
C10—C11—C12—C13	0.5 (9)	C7—C6—C5—C4	179.9 (6)
C1—N1—C9—C8	−0.6 (8)	C5—C6—C7—C8	−178.1 (6)

Diiodidodobis(quinoline *N*-oxide-*κO*)zinc(II) (III)

Crystal data

[ZnI$_2$(C$_9$H$_7$NO)$_2$]	*F*(000) = 1152
M$_r$ = 609.48	*D$_x$* = 2.019 Mg m^{-3}
Monoclinic, *P*2$_1$/*c*	Mo *Kα* radiation, λ = 0.71073 Å
a = 16.7231 (7) Å	Cell parameters from 3422 reflections
b = 7.6155 (4) Å	θ = 2.6–24.1°
c = 15.8689 (7) Å	µ = 4.32 mm^{-1}
β = 97.192 (4)°	*T* = 297 K
V = 2005.08 (16) Å^3	Block, clear colourless
Z = 4	0.3 × 0.3 × 0.3 mm

Data collection

Rigaku XtaLAB mini diffractometer	3668 independent reflections
ω scans	2748 reflections with *I* > 2σ(*I*)
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2019)	*R*$_{int}$ = 0.032
T$_{min}$ = 0.896, *T*$_{max}$ = 1.000	θ$_{max}$ = 25.4°, θ$_{min}$ = 2.5°
11510 measured reflections	*h* = −20→20
	k = −8→9
	l = −19→19

Refinement

Refinement on *F*^{2}	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
R[*F*^{2} > 2σ(*F*^{2})] = 0.035	*w* = 1/[σ^2(*F$_o$*^{2}) + (0.0249*P*)^2 + 3.8317*P*]
wR(*F*^{2}) = 0.085	where *P* = (*F$_o$*^{2} + 2*F$_c$*^{2})/3
S = 1.07	(Δ/σ)$_{max}$ < 0.001
3668 reflections	Δρ$_{max}$ = 0.80 e Å^{-3}
227 parameters	Δρ$_{min}$ = −0.81 e Å^{-3}
0 restraints	

Extinction correction: SHELXL-2018/1
(Sheldrick 2015a),
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00071 (11)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
I1	0.26214 (2)	0.37499 (6)	0.22453 (2)	0.07021 (17)
I2	0.22463 (3)	−0.02923 (6)	0.41988 (3)	0.07442 (17)
Zn1	0.25578 (3)	0.28426 (10)	0.37845 (4)	0.0553 (2)
O1	0.3601 (2)	0.3426 (7)	0.4449 (3)	0.0780 (13)
O2	0.1777 (2)	0.4466 (5)	0.4234 (3)	0.0627 (10)
N1	0.4094 (3)	0.4544 (7)	0.4109 (3)	0.0592 (12)
N2	0.1160 (3)	0.3728 (6)	0.4566 (3)	0.0509 (11)
C1	0.4847 (3)	0.3925 (8)	0.3984 (3)	0.0545 (14)
C2	0.5069 (4)	0.2175 (9)	0.4180 (4)	0.0707 (17)
H2	0.470599	0.140389	0.438341	0.085*
C3	0.5817 (5)	0.1635 (11)	0.4068 (5)	0.095 (2)
H3	0.596812	0.048098	0.419687	0.114*
C4	0.6360 (5)	0.2760 (13)	0.3768 (6)	0.105 (3)
H4	0.687500	0.235837	0.370683	0.126*
C5	0.6159 (4)	0.4433 (12)	0.3560 (5)	0.088 (2)
H5	0.653406	0.516920	0.335438	0.106*
C6	0.5378 (4)	0.5077 (9)	0.3652 (4)	0.0641 (16)
C7	0.5127 (5)	0.6797 (10)	0.3444 (5)	0.082 (2)
H7	0.547198	0.757244	0.321637	0.099*
C8	0.4374 (5)	0.7327 (10)	0.3576 (5)	0.085 (2)
H8	0.419938	0.846144	0.343511	0.102*
C9	0.3871 (4)	0.6157 (10)	0.3923 (4)	0.0758 (19)
H9	0.336222	0.652818	0.402601	0.091*
C10	0.0431 (3)	0.3575 (7)	0.4054 (3)	0.0487 (12)
C11	0.0343 (4)	0.4227 (8)	0.3219 (4)	0.0638 (16)
H11	0.077050	0.475911	0.299604	0.077*
C12	−0.0388 (5)	0.4051 (10)	0.2751 (4)	0.081 (2)
H12	−0.046101	0.448351	0.219880	0.098*
C13	−0.1039 (4)	0.3237 (11)	0.3073 (5)	0.088 (2)
H13	−0.153042	0.311918	0.273148	0.106*
C14	−0.0955 (4)	0.2624 (9)	0.3879 (5)	0.0755 (19)
H14	−0.138783	0.208570	0.408920	0.091*
C15	−0.0218 (3)	0.2796 (7)	0.4398 (4)	0.0534 (13)
C16	−0.0094 (4)	0.2205 (8)	0.5249 (4)	0.0632 (16)
H16	−0.051513	0.168071	0.548760	0.076*

C17	0.0633 (4)	0.2398 (9)	0.5717 (4)	0.0666 (17)
H17	0.071247	0.201324	0.627730	0.080*
C18	0.1257 (4)	0.3171 (8)	0.5358 (4)	0.0589 (15)
H18	0.175593	0.330122	0.568251	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0640 (3)	0.0961 (4)	0.0508 (2)	−0.0078 (2)	0.00801 (19)	−0.0018 (2)
I2	0.0652 (3)	0.0668 (3)	0.0928 (3)	0.0106 (2)	0.0157 (2)	0.0090 (2)
Zn1	0.0377 (3)	0.0742 (5)	0.0542 (4)	−0.0006 (3)	0.0070 (3)	−0.0005 (3)
O1	0.048 (2)	0.122 (4)	0.063 (3)	−0.014 (2)	0.002 (2)	0.006 (3)
O2	0.055 (2)	0.059 (3)	0.078 (3)	−0.0007 (19)	0.024 (2)	0.003 (2)
N1	0.043 (3)	0.079 (4)	0.052 (3)	−0.001 (3)	−0.003 (2)	−0.012 (3)
N2	0.047 (2)	0.052 (3)	0.057 (3)	0.007 (2)	0.016 (2)	−0.001 (2)
C1	0.042 (3)	0.075 (4)	0.044 (3)	−0.001 (3)	−0.005 (2)	−0.014 (3)
C2	0.066 (4)	0.069 (5)	0.073 (4)	−0.001 (3)	−0.007 (3)	−0.004 (3)
C3	0.073 (5)	0.086 (6)	0.120 (7)	0.013 (4)	−0.009 (5)	−0.026 (5)
C4	0.064 (5)	0.114 (7)	0.136 (8)	0.012 (5)	0.011 (5)	−0.054 (6)
C5	0.061 (4)	0.110 (7)	0.097 (6)	−0.016 (4)	0.021 (4)	−0.026 (5)
C6	0.053 (3)	0.073 (5)	0.066 (4)	−0.011 (3)	0.006 (3)	−0.017 (3)
C7	0.083 (5)	0.076 (5)	0.086 (5)	−0.022 (4)	0.001 (4)	−0.008 (4)
C8	0.087 (5)	0.065 (5)	0.095 (5)	0.004 (4)	−0.018 (4)	−0.013 (4)
C9	0.063 (4)	0.084 (5)	0.076 (4)	0.008 (4)	−0.011 (4)	−0.024 (4)
C10	0.051 (3)	0.047 (3)	0.049 (3)	0.007 (2)	0.013 (3)	0.000 (2)
C11	0.070 (4)	0.071 (4)	0.051 (3)	0.005 (3)	0.012 (3)	0.003 (3)
C12	0.092 (5)	0.099 (6)	0.052 (4)	0.014 (4)	0.002 (4)	−0.001 (4)
C13	0.065 (4)	0.110 (6)	0.085 (5)	0.005 (4)	−0.015 (4)	−0.006 (5)
C14	0.056 (4)	0.083 (5)	0.086 (5)	−0.008 (3)	0.004 (4)	−0.010 (4)
C15	0.050 (3)	0.053 (3)	0.058 (3)	0.004 (3)	0.011 (3)	−0.003 (3)
C16	0.062 (4)	0.060 (4)	0.071 (4)	0.005 (3)	0.025 (3)	0.013 (3)
C17	0.067 (4)	0.080 (5)	0.056 (4)	0.014 (3)	0.016 (3)	0.011 (3)
C18	0.056 (3)	0.069 (4)	0.051 (3)	0.009 (3)	0.005 (3)	0.000 (3)

Geometric parameters (Å, º)

I1—Zn1	2.5534 (8)	C7—H7	0.9300
I2—Zn1	2.5473 (9)	C7—C8	1.363 (10)
Zn1—O1	1.973 (4)	C8—H8	0.9300
Zn1—O2	1.994 (4)	C8—C9	1.386 (10)
O1—N1	1.345 (6)	C9—H9	0.9300
O2—N2	1.339 (5)	C10—C11	1.405 (8)
N1—C1	1.381 (7)	C10—C15	1.405 (7)
N1—C9	1.307 (8)	C11—H11	0.9300
N2—C10	1.383 (7)	C11—C12	1.356 (9)
N2—C18	1.317 (7)	C12—H12	0.9300
C1—C2	1.408 (9)	C12—C13	1.404 (10)
C1—C6	1.397 (8)	C13—H13	0.9300

C2—H2	0.9300	C13—C14	1.352 (10)
C2—C3	1.350 (9)	C14—H14	0.9300
C3—H3	0.9300	C14—C15	1.400 (8)
C3—C4	1.377 (12)	C15—C16	1.414 (8)
C4—H4	0.9300	C16—H16	0.9300
C4—C5	1.348 (12)	C16—C17	1.350 (8)
C5—H5	0.9300	C17—H17	0.9300
C5—C6	1.420 (9)	C17—C18	1.382 (8)
C6—C7	1.402 (10)	C18—H18	0.9300
I2—Zn1—I1	122.33 (3)	C8—C7—H7	120.2
O1—Zn1—I1	108.10 (13)	C7—C8—H8	120.4
O1—Zn1—I2	105.60 (15)	C7—C8—C9	119.3 (7)
O1—Zn1—O2	104.13 (19)	C9—C8—H8	120.4
O2—Zn1—I1	106.36 (12)	N1—C9—C8	121.6 (7)
O2—Zn1—I2	108.93 (12)	N1—C9—H9	119.2
N1—O1—Zn1	118.3 (3)	C8—C9—H9	119.2
N2—O2—Zn1	116.9 (3)	N2—C10—C11	120.3 (5)
O1—N1—C1	117.2 (5)	N2—C10—C15	118.3 (5)
C9—N1—O1	120.9 (5)	C15—C10—C11	121.4 (5)
C9—N1—C1	121.9 (6)	C10—C11—H11	121.2
O2—N2—C10	118.0 (4)	C12—C11—C10	117.6 (6)
C18—N2—O2	120.2 (5)	C12—C11—H11	121.2
C18—N2—C10	121.8 (5)	C11—C12—H12	118.9
N1—C1—C2	120.7 (6)	C11—C12—C13	122.1 (6)
N1—C1—C6	118.3 (6)	C13—C12—H12	118.9
C6—C1—C2	121.0 (6)	C12—C13—H13	119.9
C1—C2—H2	120.6	C14—C13—C12	120.2 (7)
C3—C2—C1	118.8 (7)	C14—C13—H13	119.9
C3—C2—H2	120.6	C13—C14—H14	119.8
C2—C3—H3	119.4	C13—C14—C15	120.3 (7)
C2—C3—C4	121.3 (8)	C15—C14—H14	119.8
C4—C3—H3	119.4	C10—C15—C16	118.5 (5)
C3—C4—H4	119.4	C14—C15—C10	118.4 (5)
C5—C4—C3	121.2 (8)	C14—C15—C16	123.0 (6)
C5—C4—H4	119.4	C15—C16—H16	119.9
C4—C5—H5	119.8	C17—C16—C15	120.3 (6)
C4—C5—C6	120.4 (8)	C17—C16—H16	119.9
C6—C5—H5	119.8	C16—C17—H17	120.2
C1—C6—C5	117.3 (7)	C16—C17—C18	119.6 (6)
C1—C6—C7	119.3 (6)	C18—C17—H17	120.2
C7—C6—C5	123.4 (7)	N2—C18—C17	121.5 (6)
C6—C7—H7	120.2	N2—C18—H18	119.3
C8—C7—C6	119.7 (7)	C17—C18—H18	119.3
Zn1—O1—N1—C1	−119.9 (4)	C4—C5—C6—C1	1.6 (10)
Zn1—O1—N1—C9	61.5 (6)	C4—C5—C6—C7	−179.6 (7)
Zn1—O2—N2—C10	−96.9 (5)	C5—C6—C7—C8	−178.0 (7)

Zn1—O2—N2—C18	83.1 (5)	C6—C1—C2—C3	2.1 (9)
O1—N1—C1—C2	2.2 (7)	C6—C7—C8—C9	0.6 (11)
O1—N1—C1—C6	−178.3 (5)	C7—C8—C9—N1	−1.6 (11)
O1—N1—C9—C8	179.7 (5)	C9—N1—C1—C2	−179.2 (6)
O2—N2—C10—C11	−1.7 (7)	C9—N1—C1—C6	0.3 (8)
O2—N2—C10—C15	179.7 (5)	C10—N2—C18—C17	0.3 (9)
O2—N2—C18—C17	−179.7 (5)	C10—C11—C12—C13	−0.6 (11)
N1—C1—C2—C3	−178.4 (6)	C10—C15—C16—C17	0.3 (9)
N1—C1—C6—C5	177.6 (5)	C11—C10—C15—C14	2.1 (9)
N1—C1—C6—C7	−1.2 (8)	C11—C10—C15—C16	−178.5 (5)
N2—C10—C11—C12	−179.5 (6)	C11—C12—C13—C14	1.2 (12)
N2—C10—C15—C14	−179.4 (5)	C12—C13—C14—C15	0.0 (12)
N2—C10—C15—C16	0.0 (8)	C13—C14—C15—C10	−1.6 (10)
C1—N1—C9—C8	1.1 (9)	C13—C14—C15—C16	179.1 (7)
C1—C2—C3—C4	−0.1 (11)	C14—C15—C16—C17	179.6 (6)
C1—C6—C7—C8	0.7 (10)	C15—C10—C11—C12	−1.0 (9)
C2—C1—C6—C5	−2.9 (9)	C15—C16—C17—C18	−0.3 (10)
C2—C1—C6—C7	178.3 (6)	C16—C17—C18—N2	0.0 (10)
C2—C3—C4—C5	−1.2 (13)	C18—N2—C10—C11	178.3 (5)
C3—C4—C5—C6	0.4 (13)	C18—N2—C10—C15	−0.2 (8)