Crystal structure of methyl (*E*)-4-[2-(8-hydroxyquinolin-2-yl)vinyl]benzoate

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The title compound, $C_{19}H_{15}NO_3$, was synthesized by a Perkin reaction of 2-methyl-8-hydroxyquinoline and 4-formyl-2-methylbenzoate in acetic anhydride under a nitrogen atmosphere. The molecule has an *E* conformation about the C=C bond, and the quinoline ring system and the benzene ring are inclined to one another by 29.22 (7)°. There is an intramolecular O—H···N hydrogen bond in the 8-hydroxyquinoline moiety. In the crystal, molecules are linked by pairs of O—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(28)$ ring motif. The dimers are linked by C—H···O hydrogen bonds and C—H···π interactions, forming sheets parallel to plane ($10\bar{1}$).

1. Chemical context

In recent years, 8-hydroxyquinoline and its derivatives have played an important role in coordination chemistry (Albrecht *et al.*, 2008; Cacciatore *et al.*, 2013), shown to exhibit biological activity (du Moulinet d'Hardemare *et al.*, 2012) and have found various applications in the fields of synthetic chemistry (Song *et al.*, 2006) and organic light-emitting diodes, which have been extensively exploited in the synthesis of luminescent metal complexes (Tang *et al.*, 1987). It is therefore highly desirable to develop new efficient 8-hydroxyquinoline derivatives for use in luminescent metal complexes. In the present work, we report on the synthesis and crystal structure of a new 8-hydroxyquinoline derivative, synthesized by the Perkin reaction of 2-methyl-8-hydroxyquinoline and 4-formyl-2-methylbenzoate.
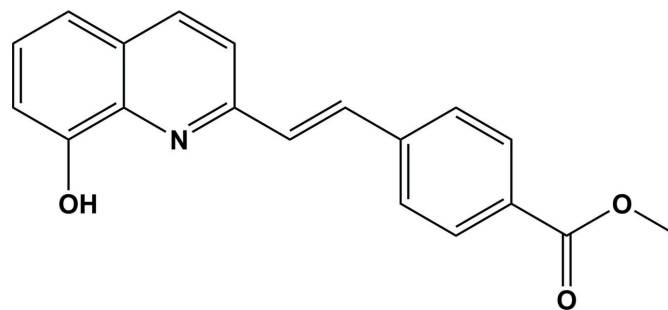
2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. It contains an 8-hydroxyquinoline moiety, with an intramolecular O—H···N hydrogen bond (Fig. 1 and Table 1),
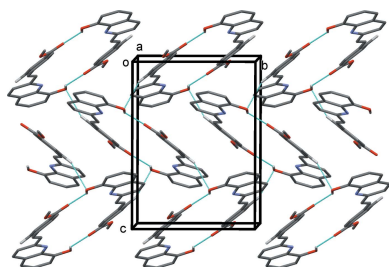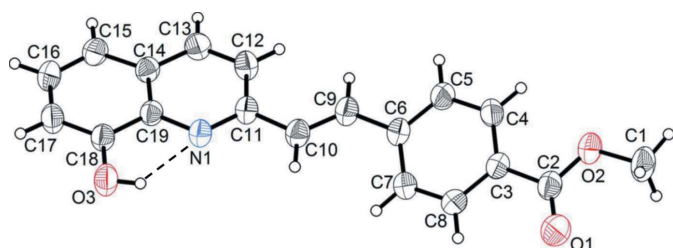
Figure 1
View of the molecular structure of the title compound, showing the atom labelling and 40% probability displacement ellipsoids. The intramolecular O—H⋯N hydrogen bond is shown as a dashed line (see Table 1).

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

$Cg1$, $Cg2$ and $Cg3$ are the centroids of rings N1/C11–C14/C19, C3–C8 and C14–C19, respectively.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H3O⋯N1	0.86 (2)	2.19 (3)	2.715 (2)	120 (2)
O3—H3O⋯O1^{i}	0.86 (2)	2.23 (2)	2.901 (2)	136 (2)
C5—H5A⋯O3^{ii}	0.93	2.57	3.437 (2)	155
C7—H7A⋯$Cg3^{iii}$	0.93	2.99	3.605 (2)	125
C8—H8A⋯$Cg1^{iii}$	0.93	2.93	3.559 (2)	126
C15—H15A⋯$Cg2^{ii}$	0.93	2.83	3.639 (2)	146

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

and a methylbenzoate unit. They are linked by the C9=C10 bond [1.321 (2) Å] with an E conformation. The C11—C10 and C6—C9 bond lengths are 1.463 (2) and 1.466 (2) Å, respectively. These distances are shorter than the standard length of a C—C single bond (ca 1.5 Å) because of the conjugate system formed by the C9=C10 bond and the aromatic systems. The quinoline ring system and the benzene ring are inclined to one another by 29.22 (7)°.

3. Supramolecular features

In the crystal, molecules are linked by pairs of O—H⋯O hydrogen bonds, forming inversion dimers with an $R_2^2(28)$ ring motif (Table 1 and Fig. 2). The dimers are linked by C—H⋯O hydrogen bonds and C—H⋯π interactions, forming sheets parallel to (10$\bar{1}$); see Table 1 and Fig. 3.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.37, last update May 2016; Groom et $al.$, 2016) for the substructure 2-styrylquinolin-8-ol gave 17 hits; however, certain of these involve bis(8-hydroxyquinolines) or a (9-anthryl) moiety. Three compounds are similar to the title
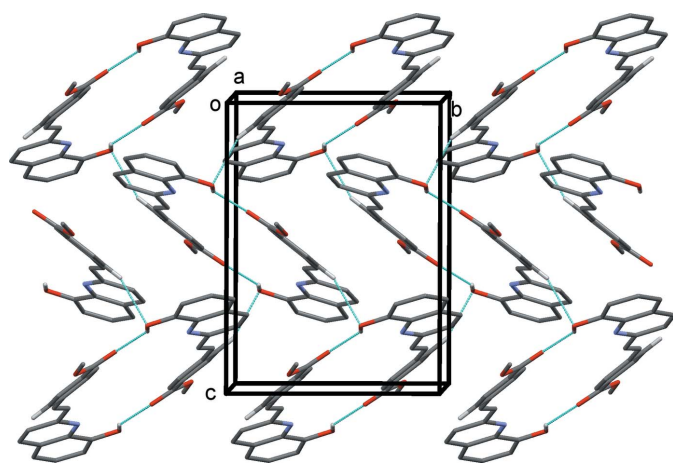
compound in the sense that they also have an E conformation about the C=C bond, and in the crystal they also form inversion dimers. They include 2-{2-[4-(trifluoromethyl)phenyl]vinyl}quinolin-8-ol (HUKTOY; Huo et $al.$, 2015), 2-[2-(4-methoxyphenyl)vinyl]quinolin-8-ol (MIMPOP; Yuan et $al.$, 2013), and 2-[2-(2,4-dinitrophenyl)vinyl]quinolin-8-ol (WELKEF; Yuan et $al.$, 2013). In these three compounds, the quinoline and benzene rings are inclined to one another by 36.72 (10) and 16.66 (10)° in HUKTOY (there are two independent molecules in the asymmetric unit), 42.59 (7)° in

Figure 3
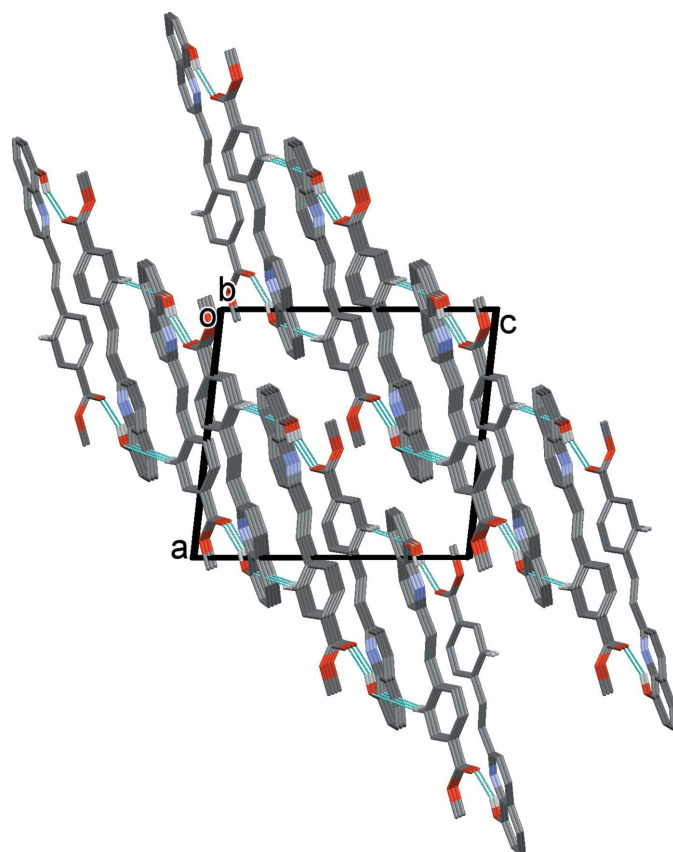A view along the b axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H3O and H5A are included.

Figure 2
A view along the a axis of the $R_2^2(28)$ ring motifs in the crystal of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1), and for clarity only H atoms H3O and H5A are included.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{15}NO_3$
M_r	305.32
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	12.0236 (4), 9.7045 (4), 13.2607 (4)
β (°)	96.260 (2)
V (Å^3)	1538.07 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	$0.08 \times 0.06 \times 0.05$
Data collection	
Diffractometer	Bruker SMART CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2005)
T_{min}, T_{max}	0.993, 0.996
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13068, 3511, 2049
R_{int}	0.041
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.137, 1.02
No. of reflections	3511
No. of parameters	217
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.17, −0.18

Computer programs: *SMART* and *SAINT* (Bruker, 2005), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

MIMPOP and 5.63 (6)° in WELKEF, compared to 29.22 (7)° in the title compound.

5. Synthesis and crystallization

The title compound was prepared following reported procedures (Jing *et al.*, 2006; Yuan *et al.*, 2012). A mixture of 2-methy-8-hydroxyquinoline (1.59 g, 10 mmol), 4-formyl-2-methylbenzoate (1.64 g, 10 mmol) and acetic anhydride (20 ml) was stirred for 12 h at 423 K under a nitrogen atmosphere. After cooling it was poured into ice–water (150 ml) and stirred for 1–2 h. Then, the puce solid obtained was filtered and together with triethylamine (1 g, 10 mmol) was dissolved in DMF (30 ml) and the mixture stirred for 3 h at 408 K. After cooling, the reaction mixture was concentrated and purified by chromatography on silica gel (petroleum ether/EtOAc = 3/1). The product obtained was dissolved in ethanol, and on slow evaporation of the solvent yellow crystals were obtained within 2 weeks.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydroxy-H atom was located in a difference Fourier map and freely refined. The C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms: C—H = 0.93–0.96 Å with $U_{iso}(H) = 1.5U_{eq}$(C-methyl) and $1.2U_{eq}$(C) for other H atoms.

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supporting information

Crystal structure of methyl (*E*)-4-[2-(8-hydroxyquinolin-2-yl)vinyl]benzoate

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Computing details

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Methyl (*E*)-4-[2-(8-hydroxyquinolin-2-yl)vinyl]benzoate

Crystal data

$C_{19}H_{15}NO_3$	$F(000) = 640$
$M_r = 305.32$	$D_x = 1.319$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1747 reflections
$a = 12.0236$ (4) Å	$\theta = 2.2–27.6°$
$b = 9.7045$ (4) Å	$\mu = 0.09$ mm^{-1}
$c = 13.2607$ (4) Å	$T = 296$ K
$\beta = 96.260$ (2)°	Block, yellow
$V = 1538.07$ (9) Å^3	$0.08 \times 0.06 \times 0.05$ mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	13068 measured reflections
Radiation source: fine-focus sealed tube	3511 independent reflections
Graphite monochromator	2049 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{int} = 0.041$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$\theta_{max} = 27.6°$, $\theta_{min} = 2.2°$
	$h = -15 \rightarrow 14$
	$k = -12 \rightarrow 12$
$T_{min} = 0.993$, $T_{max} = 0.996$	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	
$wR(F^2) = 0.137$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	
3511 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.1091P]$ where $P = (F_o^2 + 2F_c^2)/3$
217 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.17$ e Å^{-3}
	$\Delta\rho_{min} = -0.18$ 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.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
N1	0.87623 (11)	0.22440 (15)	0.17162 (11)	0.0507 (4)
O3	1.04463 (12)	0.41136 (15)	0.20030 (12)	0.0678 (4)
C19	0.97735 (12)	0.17971 (18)	0.21670 (12)	0.0465 (4)
C3	0.26628 (13)	0.27214 (18)	−0.01100 (13)	0.0496 (4)
C14	0.99928 (13)	0.04272 (18)	0.24806 (12)	0.0481 (4)
C11	0.79264 (13)	0.13449 (18)	0.15909 (12)	0.0491 (4)
O2	0.07181 (10)	0.24711 (14)	−0.02756 (10)	0.0691 (4)
C6	0.47912 (13)	0.17659 (19)	0.06283 (12)	0.0508 (4)
C13	0.90819 (14)	−0.04932 (19)	0.23276 (13)	0.0544 (5)
H13A	0.9178	−0.1412	0.2517	0.065*
C18	1.06399 (13)	0.27912 (19)	0.23164 (13)	0.0521 (4)
C12	0.80665 (14)	−0.0046 (2)	0.19061 (13)	0.0549 (5)
H12A	0.7464	−0.0651	0.1824	0.066*
C2	0.15483 (14)	0.3263 (2)	−0.05173 (14)	0.0574 (5)
O1	0.14069 (11)	0.42886 (17)	−0.10263 (13)	0.0939 (5)
C10	0.68606 (13)	0.18748 (19)	0.11050 (13)	0.0550 (5)
H10A	0.6873	0.2733	0.0795	0.066*
C9	0.58827 (13)	0.1246 (2)	0.10668 (13)	0.0550 (5)
H9A	0.5887	0.0370	0.1352	0.066*
C8	0.36132 (14)	0.3354 (2)	−0.03918 (13)	0.0587 (5)
H8A	0.3541	0.4107	−0.0828	0.070*
C15	1.10686 (14)	0.0073 (2)	0.29359 (13)	0.0581 (5)
H15A	1.1226	−0.0831	0.3136	0.070*
C17	1.16678 (14)	0.2423 (2)	0.27826 (15)	0.0611 (5)
H17A	1.2229	0.3081	0.2901	0.073*
C7	0.46638 (14)	0.2885 (2)	−0.00345 (14)	0.0587 (5)
H7A	0.5293	0.3318	−0.0237	0.070*
C4	0.27801 (14)	0.15980 (19)	0.05325 (14)	0.0564 (5)
H4A	0.2148	0.1156	0.0721	0.068*
C16	1.18752 (15)	0.1057 (2)	0.30817 (14)	0.0641 (5)
H16A	1.2581	0.0816	0.3387	0.077*
C5	0.38325 (14)	0.11293 (19)	0.08960 (14)	0.0589 (5)
H5A	0.3900	0.0372	0.1329	0.071*
C1	−0.04060 (15)	0.2875 (3)	−0.06672 (17)	0.0812 (7)
H1B	−0.0932	0.2228	−0.0445	0.122*

H1C	−0.0470	0.2886	−0.1395	0.122*
H1D	−0.0561	0.3777	−0.0421	0.122*
H3O	0.9748 (17)	0.414 (3)	0.178 (2)	0.101 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0405 (7)	0.0524 (9)	0.0578 (9)	0.0016 (7)	−0.0003 (6)	−0.0028 (7)
O3	0.0509 (8)	0.0541 (8)	0.0935 (10)	−0.0052 (7)	−0.0140 (8)	0.0047 (7)
C19	0.0397 (9)	0.0523 (10)	0.0470 (9)	0.0023 (8)	0.0028 (7)	−0.0005 (8)
C3	0.0447 (9)	0.0557 (11)	0.0471 (9)	0.0034 (8)	−0.0015 (7)	−0.0011 (8)
C14	0.0422 (9)	0.0528 (11)	0.0495 (9)	0.0062 (8)	0.0057 (7)	0.0010 (8)
C11	0.0412 (9)	0.0503 (10)	0.0549 (10)	0.0016 (8)	0.0005 (7)	−0.0059 (8)
O2	0.0414 (7)	0.0864 (10)	0.0774 (9)	0.0056 (7)	−0.0034 (6)	0.0080 (7)
C6	0.0445 (9)	0.0530 (10)	0.0529 (10)	0.0011 (8)	−0.0034 (7)	−0.0051 (8)
C13	0.0527 (10)	0.0471 (10)	0.0631 (11)	0.0035 (8)	0.0056 (8)	0.0009 (8)
C18	0.0430 (9)	0.0531 (11)	0.0590 (10)	0.0007 (8)	0.0007 (8)	0.0001 (9)
C12	0.0457 (9)	0.0515 (11)	0.0663 (11)	−0.0036 (8)	0.0013 (8)	−0.0061 (9)
C2	0.0447 (10)	0.0687 (13)	0.0575 (11)	0.0050 (10)	0.0003 (8)	−0.0010 (10)
O1	0.0597 (9)	0.0984 (12)	0.1208 (13)	0.0137 (8)	−0.0033 (8)	0.0450 (11)
C10	0.0468 (10)	0.0530 (11)	0.0637 (11)	0.0046 (8)	−0.0011 (8)	−0.0015 (9)
C9	0.0446 (9)	0.0549 (11)	0.0635 (11)	0.0026 (8)	−0.0032 (8)	−0.0027 (9)
C8	0.0521 (10)	0.0638 (12)	0.0586 (11)	0.0015 (9)	−0.0004 (8)	0.0133 (9)
C15	0.0456 (10)	0.0620 (12)	0.0661 (11)	0.0115 (9)	0.0034 (8)	0.0087 (9)
C17	0.0424 (10)	0.0680 (13)	0.0713 (12)	−0.0049 (9)	−0.0011 (8)	−0.0012 (10)
C7	0.0427 (9)	0.0703 (13)	0.0624 (11)	−0.0039 (9)	0.0027 (8)	0.0070 (10)
C4	0.0436 (9)	0.0584 (11)	0.0657 (11)	−0.0046 (8)	−0.0005 (8)	0.0035 (9)
C16	0.0404 (9)	0.0767 (15)	0.0731 (12)	0.0064 (9)	−0.0044 (8)	0.0075 (11)
C5	0.0495 (10)	0.0554 (11)	0.0691 (12)	−0.0004 (8)	−0.0054 (8)	0.0110 (9)
C1	0.0402 (10)	0.1128 (19)	0.0881 (15)	0.0112 (11)	−0.0039 (9)	0.0050 (13)
H3O	0.039 (13)	0.12 (2)	0.14 (2)	−0.025 (14)	−0.010 (13)	0.009 (16)

Geometric parameters (Å, º)

N1—C11	1.328 (2)	C18—C17	1.368 (2)
N1—C19	1.3657 (19)	C12—H12A	0.9300
O3—C18	1.361 (2)	C2—O1	1.204 (2)
O3—H3O	0.86 (2)	C10—C9	1.321 (2)
C19—C14	1.409 (2)	C10—H10A	0.9300
C19—C18	1.418 (2)	C9—H9A	0.9300
C3—C4	1.381 (2)	C8—C7	1.377 (2)
C3—C8	1.384 (2)	C8—H8A	0.9300
C3—C2	1.485 (2)	C15—C16	1.360 (3)
C14—C15	1.409 (2)	C15—H15A	0.9300
C14—C13	1.411 (2)	C17—C16	1.398 (3)
C11—C12	1.417 (3)	C17—H17A	0.9300
C11—C10	1.463 (2)	C7—H7A	0.9300
O2—C2	1.326 (2)	C4—C5	1.381 (2)

O2—C1	1.448 (2)	C4—H4A	0.9300
C6—C5	1.388 (2)	C16—H16A	0.9300
C6—C7	1.395 (3)	C5—H5A	0.9300
C6—C9	1.466 (2)	C1—H1B	0.9600
C13—C12	1.357 (2)	C1—H1C	0.9600
C13—H13A	0.9300	C1—H1D	0.9600
C11—N1—C19	118.15 (15)	C11—C10—H10A	117.0
C18—O3—H3O	105.2 (17)	C10—C9—C6	127.66 (18)
N1—C19—C14	123.90 (15)	C10—C9—H9A	116.2
N1—C19—C18	116.78 (16)	C6—C9—H9A	116.2
C14—C19—C18	119.32 (14)	C7—C8—C3	120.90 (17)
C4—C3—C8	119.02 (15)	C7—C8—H8A	119.5
C4—C3—C2	122.07 (17)	C3—C8—H8A	119.5
C8—C3—C2	118.91 (17)	C16—C15—C14	119.79 (18)
C15—C14—C19	119.34 (16)	C16—C15—H15A	120.1
C15—C14—C13	124.70 (17)	C14—C15—H15A	120.1
C19—C14—C13	115.94 (14)	C18—C17—C16	120.02 (17)
N1—C11—C12	121.65 (14)	C18—C17—H17A	120.0
N1—C11—C10	116.03 (16)	C16—C17—H17A	120.0
C12—C11—C10	122.32 (15)	C8—C7—C6	120.51 (17)
C2—O2—C1	117.01 (16)	C8—C7—H7A	119.7
C5—C6—C7	118.07 (15)	C6—C7—H7A	119.7
C5—C6—C9	118.56 (17)	C5—C4—C3	120.21 (17)
C7—C6—C9	123.36 (17)	C5—C4—H4A	119.9
C12—C13—C14	120.40 (17)	C3—C4—H4A	119.9
C12—C13—H13A	119.8	C15—C16—C17	121.54 (16)
C14—C13—H13A	119.8	C15—C16—H16A	119.2
O3—C18—C17	120.02 (17)	C17—C16—H16A	119.2
O3—C18—C19	120.01 (14)	C4—C5—C6	121.28 (17)
C17—C18—C19	119.96 (17)	C4—C5—H5A	119.4
C13—C12—C11	119.92 (16)	C6—C5—H5A	119.4
C13—C12—H12A	120.0	O2—C1—H1B	109.5
C11—C12—H12A	120.0	O2—C1—H1C	109.5
O1—C2—O2	123.39 (16)	H1B—C1—H1C	109.5
O1—C2—C3	124.26 (18)	O2—C1—H1D	109.5
O2—C2—C3	112.33 (17)	H1B—C1—H1D	109.5
C9—C10—C11	126.00 (18)	H1C—C1—H1D	109.5
C9—C10—H10A	117.0		
C11—N1—C19—C14	2.0 (2)	C8—C3—C2—O2	173.08 (16)
C11—N1—C19—C18	−178.23 (15)	N1—C11—C10—C9	−167.28 (17)
N1—C19—C14—C15	179.78 (15)	C12—C11—C10—C9	13.1 (3)
C18—C19—C14—C15	0.0 (2)	C11—C10—C9—C6	177.07 (16)
N1—C19—C14—C13	−1.6 (2)	C5—C6—C9—C10	−162.92 (18)
C18—C19—C14—C13	178.58 (15)	C7—C6—C9—C10	16.0 (3)
C19—N1—C11—C12	−0.4 (2)	C4—C3—C8—C7	−0.5 (3)
C19—N1—C11—C10	179.96 (14)	C2—C3—C8—C7	−179.86 (16)

C15—C14—C13—C12	178.19 (17)	C19—C14—C15—C16	1.0 (3)
C19—C14—C13—C12	−0.3 (2)	C13—C14—C15—C16	−177.45 (18)
N1—C19—C18—O3	−0.9 (2)	O3—C18—C17—C16	−178.39 (18)
C14—C19—C18—O3	178.95 (16)	C19—C18—C17—C16	2.1 (3)
N1—C19—C18—C17	178.64 (16)	C3—C8—C7—C6	−0.6 (3)
C14—C19—C18—C17	−1.6 (2)	C5—C6—C7—C8	1.3 (3)
C14—C13—C12—C11	1.8 (3)	C9—C6—C7—C8	−177.65 (17)
N1—C11—C12—C13	−1.5 (3)	C8—C3—C4—C5	0.8 (3)
C10—C11—C12—C13	178.16 (16)	C2—C3—C4—C5	−179.85 (16)
C1—O2—C2—O1	0.9 (3)	C14—C15—C16—C17	−0.5 (3)
C1—O2—C2—C3	−177.71 (15)	C18—C17—C16—C15	−1.1 (3)
C4—C3—C2—O1	175.11 (19)	C3—C4—C5—C6	−0.1 (3)
C8—C3—C2—O1	−5.6 (3)	C7—C6—C5—C4	−1.0 (3)
C4—C3—C2—O2	−6.3 (3)	C9—C6—C5—C4	178.01 (16)

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings N1/C11–C14/C19, C3–C8 and C14–C19, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*O*···N1	0.86 (2)	2.19 (3)	2.715 (2)	120 (2)
O3—H3*O*···O1[i]	0.86 (2)	2.23 (2)	2.901 (2)	136 (2)
C5—H5*A*···O3[ii]	0.93	2.57	3.437 (2)	155
C7—H7*A*···*Cg*3[iii]	0.93	2.99	3.605 (2)	125
C8—H8*A*···*Cg*1[iii]	0.93	2.93	3.559 (2)	126
C15—H15*A*···*Cg*2[ii]	0.93	2.83	3.639 (2)	146

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) *x*−1/2, −*y*+1/2, *z*−1/2.