

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 4-Hydroxy-1-methyl-3-phenylquinolin-2(1H)-one

 Stanislav Kafka,<sup>a</sup> Andrej Pevec,<sup>b\*</sup> Karel Proisl,<sup>a</sup> Roman Kimmel<sup>a</sup> and Janez Košmrlj<sup>b</sup>
<sup>a</sup>Department of Chemistry, Faculty of Technology, Tomas Bata University in Zlin, Zlin 76272, Czech Republic, and <sup>b</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, SI-1000 Ljubljana, Slovenia

Correspondence e-mail: andrej.pevec@fktk.uni-lj.si

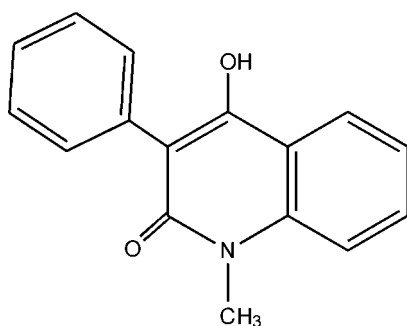
Received 16 November 2012; accepted 3 January 2013

 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.039;  $wR$  factor = 0.102; data-to-parameter ratio = 8.5.

In the title compound,  $\text{C}_{16}\text{H}_{13}\text{NO}_2$ , the quinoline system is approximately planar with a maximum deviation from the least-squares plane of 0.059 (1) Å for the N atom. The phenyl ring is rotated by 62.16 (4)° with respect to the plane of the quinoline system. In the crystal,  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds link molecules into infinite chains running along the  $b$ -axis direction.

### Related literature

For the preparation of the title compound and other 4-hydroxyquinolin-2-ones, see: Baumgarten & Kärgel (1927); Lange *et al.*, (2001); Martensson & Nilsson (1960); Bezuglyi *et al.* (1992). For synthetic utilization of the title compound, see: Kafka *et al.* (2002); Klásek *et al.* (2002).



### Experimental

#### Crystal data

 $\text{C}_{16}\text{H}_{13}\text{NO}_2$ 
 $M_r = 251.27$ 

 Monoclinic,  $P2_1$ 
 $a = 6.1787$  (2) Å

 $b = 8.2696$  (2) Å

 $c = 12.3665$  (4) Å

 $\beta = 101.632$  (2)°

 $V = 618.89$  (3) Å<sup>3</sup>
 $Z = 2$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.09$  mm<sup>-1</sup>
 $T = 293$  K

 $0.50 \times 0.25 \times 0.10$  mm

#### Data collection

Nonius KappaCCD area-detector diffractometer

Absorption correction: multi-scan (SCALEPACK; Otwinowski &amp; Minor, 1997)

 $T_{\min} = 0.957$ ,  $T_{\max} = 0.991$ 

2580 measured reflections

1479 independent reflections

 1235 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.017$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$ 
 $wR(F^2) = 0.102$ 
 $S = 1.02$ 

1479 reflections

174 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.13$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.16$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2O}\cdots\text{O1}^i$	0.82	1.89	2.655 (2)	156

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

Data collection: COLLECT (Nonius, 1998); cell refinement: DENZO and SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO and SCALEPACK; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009) and DIAMOND (Brandenburg, 1999); software used to prepare material for publication: WinGX (Farrugia, 2012).

This study was supported by the internal grant of the TBU in Zlin (No. IGA/FT/2012/043) funded from the resources of specific university research and the Slovenian Research Agency (Project P1-0230-0103 and Joint Project BI-CZ/07-08-018). This work was also partly supported through the infrastructure of the EN-FIST Centre of Excellence, Ljubljana.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2079).

### References

- Baumgarten, P. & Kärgel, W. (1927). *Ber. Dtsch. Chem. Ges. B*, **60**, 832–842.
- Bezuglyi, P. A., Ukrainets, I. V., Treskach, V. I. & Turov, A. V. (1992). *Khim. Geterotsykl. Soedin.* pp. 522–524.
- Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Kafka, S., Klásek, A., Polis, J. & Košmrlj, J. (2002). *Heterocycles*, **57**, 1659–1682.
- Klásek, A., Polis, J., Mrkvička, V. & Košmrlj, J. (2002). *J. Heterocycl. Chem.* **39**, 1315–1320.
- Lange, J. H. M., Verveer, P. C., Osnabrug, S. J. M. & Visser, G. M. (2001). *Tetrahedron Lett.* **42**, 1367–1369.
- Martensson, O. & Nilsson, E. (1960). *Acta Chem. Scand.* **14**, 1129–1150.
- Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D* **65**, 148–155.

## supplementary materials

*Acta Cryst.* (2013). E69, o231 [doi:10.1107/S1600536813000226]

## 4-Hydroxy-1-methyl-3-phenylquinolin-2(1H)-one

Stanislav Kafka, Andrej Pevec, Karel Proisl, Roman Kimmel and Janez Košmrlj

### Comment

The title compound, (I) (Fig. 1), was first prepared by the thermal condensation of diethyl phenylmalonate with *N*-methylaniline (Baumgarten & Kärgel 1927). This reaction, performed with various malonates and anilines, is still the most widely used general method for the preparation of 4-hydroxyquinolin-2-ones, including compound I. The performance of the reaction under microwave irradiation was described by Lange *et al.* (2001). Among other approaches to the preparation of compound I and other 4-hydroxyquinoline-2-diones, intramolecular condensations of 2-acylamino-benzoates could be particularly feasible (Martensson & Nilsson, 1960; Bezuglyi *et al.*, 1992). Recently, compound I was utilized for the preparation of the corresponding 3-bromo- and 3-chloro-1-methyl-3-phenylquinoline-2,4(1*H*,3*H*)-diones, from which other compounds were prepared by nucleophilic substitution of the halogen atom (Kafka *et al.*, 2002; Klásek *et al.*, 2002).

In the crystal structure of the title compound (I) (Fig. 2) 4-hydroxy-1-methyl-3-phenylquinolin-2(1*H*)-one molecules are connected by intermolecular O—H...O hydrogen bonds between the hydroxyl and carbonyl groups (Table 1). These connections form linear chains along the *b*-axis in the crystal structure.

### Experimental

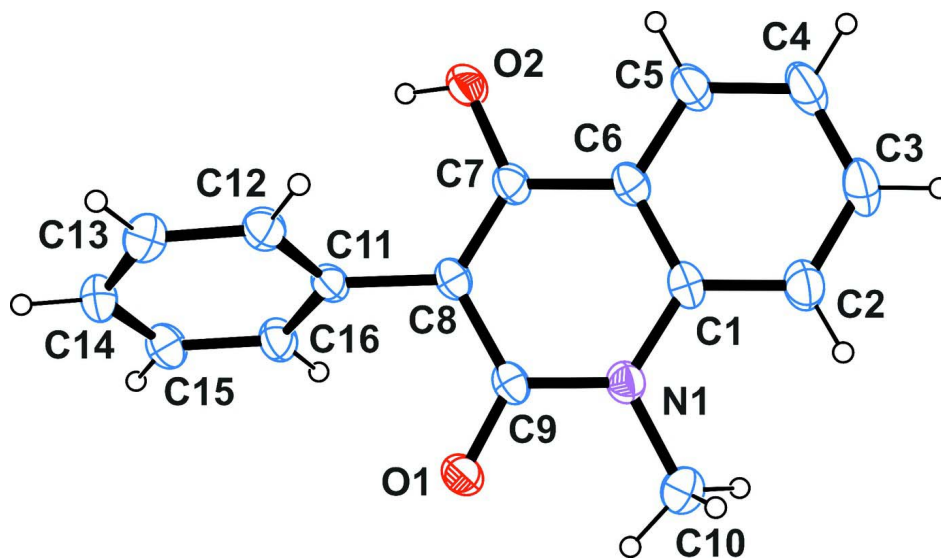
Title compound was prepared according to a modified procedure published by Baumgarten & Kärgel (1927). A mixture of *N*-methylaniline (10.7 g, 100 mmol) and diethyl phenylmalonate (24.8 g, 105 mmol) was gradually heated in a Wood's metal bath at 200–290 °C for 4.5 h (until the distillation of ethanol stopped; reached 8.57 g, *i.e.* 93% of theoretical mass of distillate). The hot reaction mixture was poured into a mortar, crushed after cooling and dissolved in the mixture of aqueous sodium hydroxide solution (0.5 *M*, 300 ml) and toluene (50 ml). The aqueous phase was separated, washed with toluene, shortly stirred with active carbon, filtered and acidified by addition of 10% hydrochloric acid to Congo red. The precipitated white solid was filtered off, washed with water and air dried affording 23.4 g (93% of theory) of crude product, m. p. 223–225 °C. Crystallization of the crude product from ethanol afforded 20.1 g (80% of theoretical yield) of the title compound (I), m. p. 222–226 °C. In the literature (Martensson & Nilsson, 1960), the same m. p. is given.

### Refinement

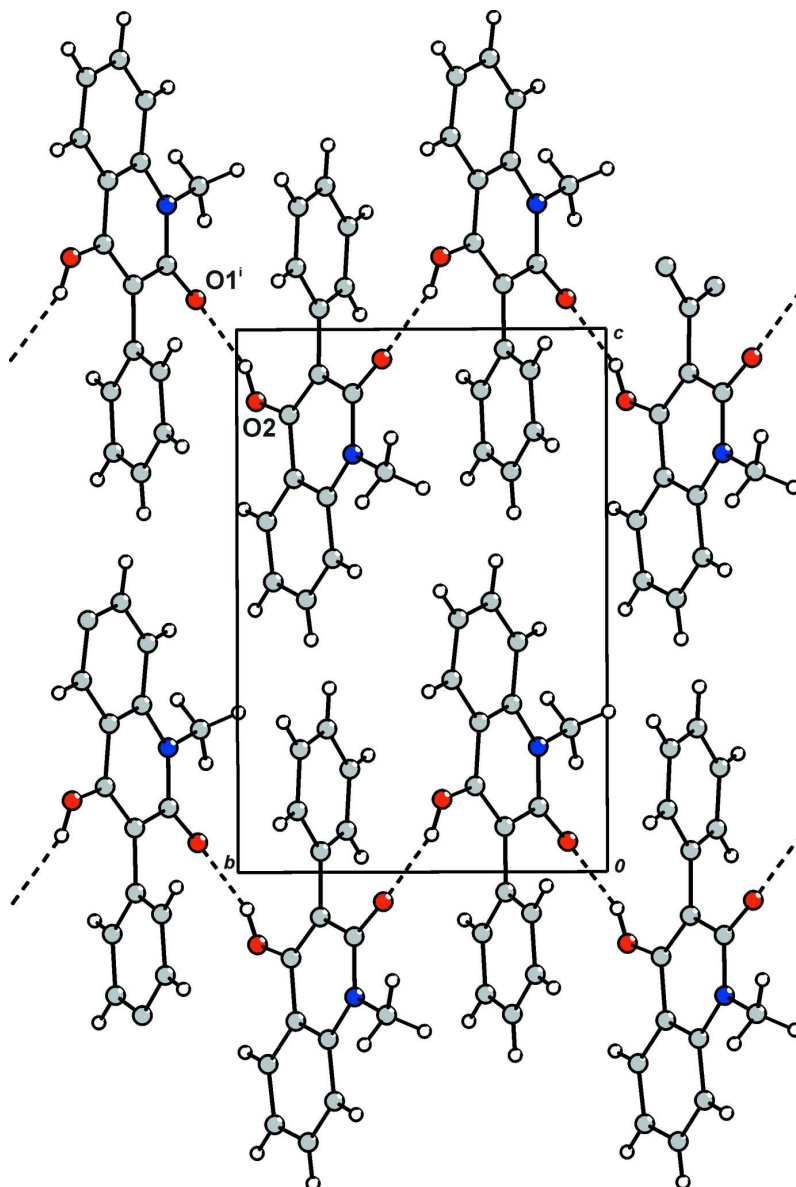
All H atoms were included in the model at geometrically calculated positions and refined using a riding model, with C—H bond lengths constrained to 0.93 Å (aromatic CH), 0.96 Å (methyl CH<sub>3</sub>), and O—H = 0.82 Å, and with  $U_{\text{iso}}(\text{H})$  values of  $1.2U_{\text{eq}}(\text{C})$  [for aromatic CH] or  $1.5U_{\text{eq}}(\text{C})$  [for OH and methyl groups]. In the absence of significant anomalous scattering, the Flack parameter could not be determined reliably. Therefore Friedel-pairs were merged prior to the final refinement cycle. 16 low angle reflections were dropped by the integration routines because of detector saturation.

**Computing details**

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

**Figure 1**

A view of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Figure 2**

The packing of (I), with the O—H···O hydrogen bonds. [Symmetry code: (i)  $-x, y + 1/2, -z + 2$ .]

#### 4-Hydroxy-1-methyl-3-phenylquinolin-2(1H)-one

##### Crystal data

$C_{16}H_{13}NO_2$

$M_r = 251.27$

Monoclinic,  $P2_1$

Hall symbol:  $P\ 2y_b$

$a = 6.1787\ (2)\ \text{\AA}$

$b = 8.2696\ (2)\ \text{\AA}$

$c = 12.3665\ (4)\ \text{\AA}$

$\beta = 101.632\ (2)^\circ$

$V = 618.89\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 264$

$D_x = 1.348\ \text{Mg m}^{-3}$

Melting point = 495–499 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1471 reflections

$\theta = 1.0\text{--}27.5^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, colorless

$0.50 \times 0.25 \times 0.10\ \text{mm}$

Data collection

Nonius KappaCCD area-detector diffractometer	2580 measured reflections
Radiation source: fine-focus sealed tube	1479 independent reflections
Graphite monochromator	1235 reflections with $I > 2\sigma(I)$
$\varphi$ scans + $\omega$ scans	$R_{\text{int}} = 0.017$
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)	$\theta_{\text{max}} = 27.4^\circ$ , $\theta_{\text{min}} = 5.5^\circ$
$T_{\text{min}} = 0.957$ , $T_{\text{max}} = 0.991$	$h = -7 \rightarrow 7$
	$k = -10 \rightarrow 8$
	$l = -16 \rightarrow 15$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.0786P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1479 reflections	$(\Delta/\sigma)_{\text{max}} = 0.0001$
174 parameters	$\Delta\rho_{\text{max}} = 0.13 \text{ e } \text{\AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.16 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

**Experimental.** 216 frames in 4 sets of  $\varphi$  scans +  $\omega$  scans. Rotation/frame = 2.0 °. Crystal-detector distance = 31 mm. Measuring time = 200 s/°.

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	-0.3506 (3)	0.6870 (2)	0.76995 (14)	0.0421 (5)
O1	-0.3484 (2)	0.6084 (2)	0.94498 (12)	0.0461 (4)
O2	0.2230 (3)	0.9476 (3)	0.86700 (12)	0.0527 (5)
H2O	0.2433	0.9751	0.9320	0.079*
C1	-0.2491 (4)	0.7574 (3)	0.69150 (17)	0.0408 (5)
C2	-0.3367 (5)	0.7420 (4)	0.57760 (19)	0.0563 (7)
H2	-0.4659	0.6833	0.5536	0.068*
C3	-0.2321 (5)	0.8131 (4)	0.50211 (19)	0.0640 (8)
H3	-0.2903	0.8004	0.4272	0.077*
C4	-0.0430 (6)	0.9027 (4)	0.5350 (2)	0.0631 (7)
H4	0.0251	0.9512	0.4827	0.076*
C5	0.0453 (5)	0.9202 (3)	0.64626 (19)	0.0531 (6)
H5	0.1720	0.9821	0.6688	0.064*
C6	-0.0539 (4)	0.8458 (3)	0.72531 (17)	0.0408 (5)
C7	0.0393 (4)	0.8579 (3)	0.84224 (17)	0.0392 (5)

C8	-0.0553 (4)	0.7782 (3)	0.91735 (16)	0.0374 (5)
C9	-0.2559 (3)	0.6871 (3)	0.88098 (16)	0.0374 (5)
C10	-0.5599 (4)	0.6003 (4)	0.7363 (2)	0.0558 (6)
H10A	-0.5330	0.4973	0.7057	0.084*
H10B	-0.6579	0.6625	0.6817	0.084*
H10C	-0.6261	0.5843	0.7994	0.084*
C11	0.0412 (3)	0.7767 (3)	1.03788 (15)	0.0374 (5)
C12	0.2473 (4)	0.7070 (3)	1.07702 (19)	0.0456 (5)
H12	0.3288	0.6669	1.0274	0.055*
C13	0.3319 (4)	0.6971 (4)	1.1895 (2)	0.0537 (6)
H13	0.4682	0.6483	1.2151	0.064*
C14	0.2142 (5)	0.7594 (4)	1.26318 (19)	0.0568 (7)
H14	0.2709	0.7523	1.3386	0.068*
C15	0.0133 (4)	0.8321 (4)	1.22571 (19)	0.0535 (6)
H15	-0.0640	0.8764	1.2758	0.064*
C16	-0.0749 (4)	0.8396 (3)	1.11342 (18)	0.0460 (6)
H16	-0.2124	0.8871	1.0886	0.055*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0427 (10)	0.0467 (10)	0.0362 (9)	0.0025 (9)	0.0062 (7)	0.0040 (9)
O1	0.0438 (8)	0.0554 (10)	0.0408 (8)	0.0007 (8)	0.0124 (6)	0.0101 (7)
O2	0.0653 (10)	0.0598 (10)	0.0366 (8)	-0.0198 (9)	0.0191 (8)	-0.0084 (8)
C1	0.0524 (12)	0.0392 (11)	0.0311 (10)	0.0092 (10)	0.0095 (9)	0.0020 (9)
C2	0.0630 (15)	0.0639 (17)	0.0397 (12)	0.0002 (13)	0.0047 (11)	0.0030 (12)
C3	0.087 (2)	0.0729 (19)	0.0299 (11)	0.0020 (17)	0.0058 (12)	0.0045 (12)
C4	0.0925 (19)	0.0656 (17)	0.0352 (11)	-0.0053 (16)	0.0220 (12)	0.0065 (12)
C5	0.0719 (15)	0.0535 (15)	0.0376 (11)	-0.0069 (13)	0.0201 (11)	-0.0013 (12)
C6	0.0531 (13)	0.0377 (11)	0.0339 (10)	0.0027 (10)	0.0143 (9)	-0.0009 (9)
C7	0.0472 (12)	0.0402 (12)	0.0325 (10)	-0.0009 (9)	0.0136 (9)	-0.0039 (9)
C8	0.0448 (11)	0.0383 (11)	0.0312 (10)	0.0041 (9)	0.0128 (8)	-0.0010 (9)
C9	0.0418 (11)	0.0392 (11)	0.0327 (10)	0.0083 (10)	0.0115 (8)	0.0030 (9)
C10	0.0476 (12)	0.0669 (16)	0.0497 (13)	-0.0029 (13)	0.0022 (10)	0.0035 (13)
C11	0.0432 (11)	0.0398 (11)	0.0315 (10)	-0.0029 (10)	0.0127 (9)	0.0005 (9)
C12	0.0439 (12)	0.0535 (14)	0.0410 (11)	0.0019 (11)	0.0126 (9)	-0.0017 (11)
C13	0.0470 (13)	0.0618 (15)	0.0492 (13)	0.0024 (12)	0.0019 (10)	0.0052 (13)
C14	0.0621 (15)	0.0732 (17)	0.0317 (11)	-0.0115 (14)	0.0017 (10)	0.0033 (11)
C15	0.0594 (15)	0.0693 (16)	0.0353 (11)	-0.0037 (13)	0.0177 (10)	-0.0062 (12)
C16	0.0483 (12)	0.0557 (14)	0.0354 (11)	0.0045 (11)	0.0118 (9)	-0.0011 (11)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

N1—C9	1.380 (3)	C7—C8	1.363 (3)
N1—C1	1.385 (3)	C8—C9	1.443 (3)
N1—C10	1.464 (3)	C8—C11	1.490 (3)
O1—C9	1.248 (3)	C10—H10A	0.9600
O2—C7	1.339 (3)	C10—H10B	0.9600
O2—H2O	0.8200	C10—H10C	0.9600
C1—C6	1.400 (3)	C11—C16	1.389 (3)

C1—C2	1.409 (3)	C11—C12	1.393 (3)
C2—C3	1.370 (4)	C12—C13	1.386 (3)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.374 (4)	C13—C14	1.376 (4)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.382 (3)	C14—C15	1.373 (4)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.397 (3)	C15—C16	1.387 (3)
C5—H5	0.9300	C15—H15	0.9300
C6—C7	1.448 (3)	C16—H16	0.9300
C9—N1—C1	122.40 (19)	O1—C9—N1	118.3 (2)
C9—N1—C10	117.14 (19)	O1—C9—C8	123.29 (18)
C1—N1—C10	120.37 (18)	N1—C9—C8	118.40 (18)
C7—O2—H2O	109.5	N1—C10—H10A	109.5
N1—C1—C6	119.64 (18)	N1—C10—H10B	109.5
N1—C1—C2	121.7 (2)	H10A—C10—H10B	109.5
C6—C1—C2	118.7 (2)	N1—C10—H10C	109.5
C3—C2—C1	120.2 (2)	H10A—C10—H10C	109.5
C3—C2—H2	119.9	H10B—C10—H10C	109.5
C1—C2—H2	119.9	C16—C11—C12	118.78 (19)
C2—C3—C4	121.3 (2)	C16—C11—C8	120.87 (19)
C2—C3—H3	119.3	C12—C11—C8	120.32 (18)
C4—C3—H3	119.3	C13—C12—C11	120.4 (2)
C3—C4—C5	119.5 (2)	C13—C12—H12	119.8
C3—C4—H4	120.3	C11—C12—H12	119.8
C5—C4—H4	120.3	C14—C13—C12	120.0 (2)
C4—C5—C6	120.7 (2)	C14—C13—H13	120.0
C4—C5—H5	119.7	C12—C13—H13	120.0
C6—C5—H5	119.7	C15—C14—C13	120.2 (2)
C5—C6—C1	119.60 (19)	C15—C14—H14	119.9
C5—C6—C7	121.7 (2)	C13—C14—H14	119.9
C1—C6—C7	118.66 (19)	C14—C15—C16	120.2 (2)
O2—C7—C8	124.90 (19)	C14—C15—H15	119.9
O2—C7—C6	114.51 (18)	C16—C15—H15	119.9
C8—C7—C6	120.6 (2)	C15—C16—C11	120.3 (2)
C7—C8—C9	119.96 (18)	C15—C16—H16	119.8
C7—C8—C11	123.1 (2)	C11—C16—H16	119.8
C9—C8—C11	116.93 (18)		
C9—N1—C1—C6	-6.3 (3)	C6—C7—C8—C11	175.7 (2)
C10—N1—C1—C6	177.3 (2)	C1—N1—C9—O1	-173.6 (2)
C9—N1—C1—C2	173.3 (2)	C10—N1—C9—O1	2.9 (3)
C10—N1—C1—C2	-3.0 (3)	C1—N1—C9—C8	6.6 (3)
N1—C1—C2—C3	-180.0 (2)	C10—N1—C9—C8	-177.0 (2)
C6—C1—C2—C3	-0.3 (4)	C7—C8—C9—O1	178.3 (2)
C1—C2—C3—C4	-1.1 (5)	C11—C8—C9—O1	-0.4 (3)
C2—C3—C4—C5	0.7 (5)	C7—C8—C9—N1	-1.8 (3)
C3—C4—C5—C6	1.0 (5)	C11—C8—C9—N1	179.48 (19)

C4—C5—C6—C1	-2.3 (4)	C7—C8—C11—C16	118.9 (3)
C4—C5—C6—C7	178.0 (3)	C9—C8—C11—C16	-62.4 (3)
N1—C1—C6—C5	-178.4 (2)	C7—C8—C11—C12	-63.2 (3)
C2—C1—C6—C5	1.9 (3)	C9—C8—C11—C12	115.5 (2)
N1—C1—C6—C7	1.4 (3)	C16—C11—C12—C13	1.7 (4)
C2—C1—C6—C7	-178.3 (2)	C8—C11—C12—C13	-176.3 (2)
C5—C6—C7—O2	1.2 (3)	C11—C12—C13—C14	-1.4 (4)
C1—C6—C7—O2	-178.5 (2)	C12—C13—C14—C15	-0.2 (5)
C5—C6—C7—C8	-177.1 (2)	C13—C14—C15—C16	1.6 (5)
C1—C6—C7—C8	3.2 (3)	C14—C15—C16—C11	-1.3 (4)
O2—C7—C8—C9	179.0 (2)	C12—C11—C16—C15	-0.3 (4)
C6—C7—C8—C9	-2.9 (3)	C8—C11—C16—C15	177.6 (2)
O2—C7—C8—C11	-2.4 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2O...O1 <sup>i</sup>	0.82	1.89	2.655 (2)	156

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