

2-(2-Hydroxy-3-methoxyphenyl)-6H-perimidin-6-one

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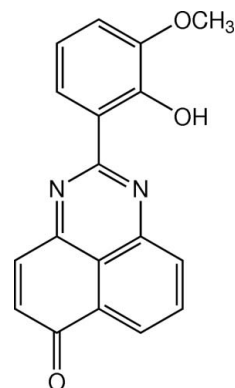
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.066; wR factor = 0.210; data-to-parameter ratio = 25.6.

The molecule of the title perimidine derivative, $\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}_3$, is essentially planar, the dihedral angle between the benzene and perimidine rings being 3.25 (5°). The hydroxy and methoxy groups lie in the plane of the benzene ring to which they are bound [$\text{O}-\text{C}-\text{C}-\text{C} = 179.96$ (11°) and $\text{C}-\text{O}-\text{C}-\text{C} = -177.96$ (12°)]. An intramolecular $\text{O}-\text{H}\cdots\text{N}$ interaction generates an $S(6)$ ring motif. In the crystal, molecules are linked by pairs of $\text{C}-\text{H}\cdots\text{O}$ interactions into dimers, which generate $S(16)$ ring motifs. These dimers are arranged into sheets parallel to the ac plane and further stacked down the b axis by $\pi-\pi$ interactions, with centroid-centroid distances in the range 3.5066 (8)– 3.7241 (7) Å.

Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For background to perimidines and their applications, see: Claramunt *et al.* (1995); del Valle *et al.* (1997); Herbert *et al.* (1987); Llamas-Saiz *et al.* (1995); Pozharskii & Dalnikovskaya (1981); Varsha *et al.* (2010). For related structures, see: Llamas-Saiz *et al.* (1995); Varsha *et al.* (2010). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}_3$	$V = 2706.8$ (2) Å ³
$M_r = 304.30$	$Z = 8$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 25.4718$ (17) Å	$\mu = 0.10$ mm ⁻¹
$b = 7.0666$ (3) Å	$T = 100$ K
$c = 15.0815$ (6) Å	$0.67 \times 0.11 \times 0.05$ mm
$\beta = 94.373$ (3)°	

Data collection

Bruker APEX DUO CCD area-detector diffractometer	42939 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	6529 independent reflections
$T_{\min} = 0.933$, $T_{\max} = 0.994$	3471 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.072$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.066$	255 parameters
$wR(F^2) = 0.210$	All H-atom parameters refined
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.57$ e Å ⁻³
6529 reflections	$\Delta\rho_{\text{min}} = -0.29$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O2}-\text{H1O2}\cdots\text{N2}$	0.91 (2)	1.73 (2)	2.5583 (15)	151 (2)
$\text{C15}-\text{H15}\cdots\text{O2}^i$	0.970 (18)	2.437 (18)	3.3686 (17)	160.8 (12)

Symmetry code: (i) $-x + 2, y, -z + \frac{3}{2}$.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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‡ Thomson Reuters ResearcherID: A-3561-2009.

§ Thomson Reuters ResearcherID: A-5085-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5107).

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supplementary materials

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2-(2-Hydroxy-3-methoxyphenyl)-6H-perimidin-6-one

H.-K. Fun, K. Chanawanno and S. Chantrapromma

Comment

Perimidines (*peri*-naphtho-fused perimidine ring systems) have received wide interests due to their applications in photo-physics (del Valle *et al.*, 1997), usage as coloring materials for polyester fibers (Claramunt *et al.*, 1995) and fluorescent materials (Varsha *et al.*, 2010). They are also noted for their biological activity displaying antiulcer, antifungal, antimicrobial and antitumor properties (Claramunt *et al.*, 1995; Herbert *et al.*, 1987; Pozharskii & Dalnikovskaya, 1981). In an attempt to synthesize a Co(II) Schiff base complex by the reaction of *o*-vanillin, 1,8-diaminonaphthalene and CoCl₂·6H₂O, the unexpected product was the perimidine derivative, (I), reported here, Fig 1.

In the molecule of the title perimidine derivative (I), C₁₈H₁₂N₂O₃, the perimidine ring system (N1–N2/C7–C17) is planar with an *r.m.s* deviation 0.0126 (11) Å. The whole molecule is essentially planar with the dihedral angle between the perimidine and phenyl rings being 3.25 (5)°. Both the hydroxy and methoxy groups are co-planar with the attached benzene ring with torsion angles O2–C2–C3–C4 = 179.96 (11)° and C18–O3–C3–C2 = -177.96 (12)°. An intramolecular O—H…N interaction generates an S(6) ring motif (Bernstein *et al.*, 1995) and helps to stabilize the planarity of the molecule (Fig. 1). Bond distances are normal (Allen *et al.*, 1987) and are comparable to those found in related structures (Llamas-Saiz *et al.*, 1995; Varsha *et al.*, 2010).

In the crystal structure (Fig. 2), the molecules are linked by two C—H…O interactions (Table 1) into dimers which generate S(16) ring motifs. These dimers are arranged into sheets parallel to the *ac* plane and further stacked down the *b* axis by π - π interactions with centroid to centroid distances $Cg_1 \cdots Cg_2^{ii} = 3.7241$ (7) Å; $Cg_2 \cdots Cg_3^{ii} = 3.5066$ (8) Å; $Cg_2 \cdots Cg_4^{ii} = 3.7055$ (8) Å and $Cg_2 \cdots Cg_4^{iii} = 3.5988$ (8) Å (symmetry codes (ii) = 2 - *x*, 1 - *y*, 1 - *z* and (iii) = 2 - *x*, 2 - *y*, 2 - *z*). *Cg*1, *Cg*2, *Cg*3, and *Cg*4 are the centroids of the N1–N2/C7–C8/C6–C17, C1–C6, C8–C12/C17, and C12–C17 rings, respectively.

Experimental

The title compound was synthesized by adding a solution of 1,8-diaminonaphthalene (0.50 g, 3.16 mmol) in ethanol (20 ml) dropwise to a solution of *o*-vanillin (0.96 g, 6.32 mmol) in ethanol (10 ml). The reaction mixture was stirred for 0.5 h at room temperature and a pale-orange precipitate was obtained. After filtration, the pale-orange solid was washed with diethyl ether. A solution of the pale-orange solid (0.20 g, 0.47 mmol) in ethanol (20 ml) was slowly added to a solution of CoCl₂·6H₂O (0.11 g, 0.47 mmol) in 10 ml of ethanol followed by triethylamine (0.06 ml, 0.47 mmol). The mixture was refluxed for 3 h. The title compound was obtained as a purple solid and washed with diethyl ether. The purple needle-shaped single crystals of the unexpected perimidine derivative of the title compound suitable for *x*-ray structure determination were recrystallized from ethanol by slow evaporation of the solvent at room temperature over several days, Mp. 507–508 K.

Refinement

All H atoms (except H13) were located in difference maps and refined isotropically. H13 was refined with U_{iso} constrained to be $1.2U_{\text{eq}}$ (C13). The highest residual electron density peak is located at 0.68 \AA from C16 and the deepest hole is located at 0.48 \AA from C16.

Figures

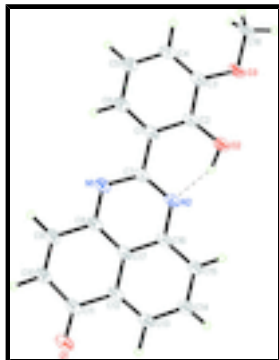


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. An intramolecular hydrogen bond is drawn as a dashed line.

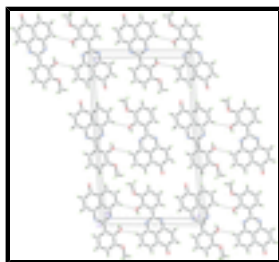


Fig. 2. The crystal packing of the title compound viewed down the b axis. Hydrogen bonds were drawn as dashed lines.

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Crystal data

$\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}_3$

$M_r = 304.30$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 25.4718 (17) \text{ \AA}$

$b = 7.0666 (3) \text{ \AA}$

$c = 15.0815 (6) \text{ \AA}$

$\beta = 94.373 (3)^\circ$

$V = 2706.8 (2) \text{ \AA}^3$

$Z = 8$

$F(000) = 1264$

$D_x = 1.493 \text{ Mg m}^{-3}$

Melting point = $507\text{--}508 \text{ K}$

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

Cell parameters from 6529 reflections

$\theta = 1.6\text{--}36.3^\circ$

$\mu = 0.10 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Needle, purple

$0.67 \times 0.11 \times 0.05 \text{ mm}$

Data collection

Bruker APEX DUO CCD area-detector
diffractometer

6529 independent reflections

Radiation source: sealed tube graphite	3471 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.072$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$\theta_{\text{max}} = 36.3^\circ$, $\theta_{\text{min}} = 1.6^\circ$
$T_{\text{min}} = 0.933$, $T_{\text{max}} = 0.994$	$h = -42 \rightarrow 34$
42939 measured reflections	$k = -11 \rightarrow 11$
	$l = -24 \rightarrow 25$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.066$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.210$	All H-atom parameters refined
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.110P)^2]$
6529 reflections	where $P = (F_o^2 + 2F_c^2)/3$
255 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.57 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	1.20986 (4)	0.86652 (17)	0.36853 (7)	0.0390 (3)
O2	0.93604 (4)	0.76137 (15)	0.66009 (7)	0.0305 (2)
H1O2	0.9692 (9)	0.784 (3)	0.6441 (15)	0.068 (7)*
O3	0.83728 (4)	0.69274 (15)	0.67439 (7)	0.0307 (2)
N1	1.00314 (4)	0.71962 (15)	0.40931 (7)	0.0230 (2)
N2	1.01534 (4)	0.77988 (14)	0.56606 (7)	0.0217 (2)
C1	0.92971 (5)	0.68964 (16)	0.50224 (9)	0.0213 (2)
C2	0.90819 (5)	0.70778 (17)	0.58472 (9)	0.0229 (3)
C3	0.85404 (5)	0.66982 (18)	0.59105 (9)	0.0245 (3)

supplementary materials

C4	0.82297 (5)	0.61425 (18)	0.51641 (10)	0.0269 (3)
H4	0.7846 (8)	0.588 (3)	0.5190 (13)	0.053 (5)*
C5	0.84470 (5)	0.59241 (19)	0.43503 (9)	0.0271 (3)
H5	0.8242 (6)	0.542 (2)	0.3839 (11)	0.032 (4)*
C6	0.89730 (5)	0.62922 (18)	0.42762 (9)	0.0242 (3)
H6	0.9121 (6)	0.608 (3)	0.3716 (12)	0.039 (5)*
C7	0.98576 (5)	0.73220 (16)	0.49261 (9)	0.0208 (2)
C8	1.05351 (5)	0.75829 (17)	0.40160 (9)	0.0222 (2)
C9	1.07449 (5)	0.7429 (2)	0.31468 (9)	0.0271 (3)
H9	1.0495 (6)	0.696 (2)	0.2625 (11)	0.027 (4)*
C10	1.12551 (5)	0.7780 (2)	0.30472 (9)	0.0281 (3)
H10	1.1420 (6)	0.761 (2)	0.2446 (11)	0.031 (4)*
C11	1.16293 (5)	0.83502 (19)	0.37912 (9)	0.0269 (3)
C12	1.14203 (5)	0.84961 (17)	0.46741 (9)	0.0233 (3)
C13	1.17405 (5)	0.89476 (19)	0.54295 (9)	0.0268 (3)
H13	1.2155 (6)	0.916 (2)	0.5341 (11)	0.032*
C14	1.15283 (5)	0.90293 (19)	0.62651 (10)	0.0284 (3)
H14	1.1753 (6)	0.931 (2)	0.6784 (10)	0.029 (4)*
C15	1.10056 (5)	0.86583 (18)	0.63559 (9)	0.0257 (3)
H15	1.0859 (6)	0.865 (2)	0.6931 (12)	0.036 (4)*
C16	1.06736 (5)	0.81935 (16)	0.55893 (9)	0.0218 (2)
C17	1.08818 (5)	0.81121 (16)	0.47560 (8)	0.0206 (2)
C18	0.78320 (6)	0.6497 (2)	0.68447 (12)	0.0338 (3)
H18A	0.7621 (7)	0.737 (3)	0.6464 (12)	0.039 (5)*
H18B	0.7746 (6)	0.521 (3)	0.6683 (10)	0.032 (4)*
H18C	0.7805 (7)	0.666 (2)	0.7467 (12)	0.035 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0255 (5)	0.0525 (7)	0.0408 (6)	-0.0050 (5)	0.0157 (4)	0.0022 (5)
O2	0.0225 (5)	0.0393 (6)	0.0313 (5)	-0.0060 (4)	0.0121 (4)	-0.0095 (4)
O3	0.0201 (4)	0.0387 (6)	0.0353 (5)	-0.0036 (4)	0.0158 (4)	-0.0050 (4)
N1	0.0213 (5)	0.0227 (5)	0.0261 (6)	0.0006 (4)	0.0090 (4)	0.0043 (4)
N2	0.0189 (5)	0.0195 (5)	0.0278 (6)	-0.0018 (4)	0.0099 (4)	-0.0012 (4)
C1	0.0201 (5)	0.0168 (5)	0.0282 (6)	0.0001 (4)	0.0088 (5)	0.0031 (4)
C2	0.0204 (6)	0.0202 (5)	0.0290 (7)	-0.0007 (4)	0.0089 (5)	-0.0003 (4)
C3	0.0222 (6)	0.0220 (5)	0.0309 (7)	0.0002 (4)	0.0112 (5)	0.0011 (5)
C4	0.0186 (6)	0.0244 (6)	0.0383 (8)	-0.0017 (5)	0.0073 (5)	0.0059 (5)
C5	0.0235 (6)	0.0268 (6)	0.0313 (7)	-0.0019 (5)	0.0036 (5)	0.0066 (5)
C6	0.0245 (6)	0.0234 (6)	0.0254 (6)	-0.0002 (4)	0.0066 (5)	0.0054 (5)
C7	0.0213 (5)	0.0171 (5)	0.0253 (6)	0.0013 (4)	0.0092 (5)	0.0019 (4)
C8	0.0212 (5)	0.0196 (5)	0.0266 (6)	0.0013 (4)	0.0079 (5)	0.0041 (4)
C9	0.0265 (6)	0.0316 (6)	0.0244 (6)	0.0006 (5)	0.0096 (5)	0.0042 (5)
C10	0.0273 (6)	0.0330 (7)	0.0254 (7)	0.0006 (5)	0.0118 (5)	0.0051 (5)
C11	0.0249 (6)	0.0271 (6)	0.0304 (7)	0.0000 (5)	0.0127 (5)	0.0043 (5)
C12	0.0204 (5)	0.0213 (5)	0.0297 (6)	-0.0008 (4)	0.0109 (5)	0.0026 (5)
C13	0.0219 (6)	0.0261 (6)	0.0336 (7)	-0.0046 (5)	0.0090 (5)	0.0000 (5)

C14	0.0248 (6)	0.0295 (6)	0.0319 (7)	-0.0057 (5)	0.0077 (5)	-0.0041 (5)
C15	0.0245 (6)	0.0263 (6)	0.0273 (7)	-0.0051 (5)	0.0100 (5)	-0.0033 (5)
C16	0.0211 (5)	0.0175 (5)	0.0281 (6)	-0.0020 (4)	0.0104 (4)	-0.0016 (4)
C17	0.0210 (5)	0.0168 (5)	0.0253 (6)	0.0000 (4)	0.0094 (4)	0.0024 (4)
C18	0.0192 (6)	0.0437 (9)	0.0405 (9)	-0.0047 (6)	0.0145 (6)	-0.0017 (7)

Geometric parameters (Å, °)

O1—C11	1.2384 (16)	C8—C17	1.4196 (18)
O2—C2	1.3474 (16)	C8—C9	1.4568 (19)
O2—H1O2	0.91 (2)	C9—C10	1.3427 (19)
O3—C3	1.3676 (16)	C9—H9	1.028 (16)
O3—C18	1.4301 (16)	C10—C11	1.472 (2)
N1—C8	1.3256 (16)	C10—H10	1.035 (17)
N1—C7	1.3663 (17)	C11—C12	1.4747 (18)
N2—C7	1.3345 (17)	C12—C13	1.3868 (19)
N2—C16	1.3664 (16)	C12—C17	1.4127 (17)
C1—C2	1.4030 (18)	C13—C14	1.4098 (19)
C1—C6	1.4102 (19)	C13—H13	1.085 (16)
C1—C7	1.4769 (17)	C14—C15	1.3739 (18)
C2—C3	1.4155 (17)	C14—H14	0.955 (15)
C3—C4	1.3827 (19)	C15—C16	1.4179 (18)
C4—C5	1.393 (2)	C15—H15	0.970 (17)
C4—H4	1.000 (19)	C16—C17	1.4019 (18)
C5—C6	1.3777 (18)	C18—H18A	0.976 (18)
C5—H5	0.966 (16)	C18—H18B	0.963 (17)
C6—H6	0.963 (18)	C18—H18C	0.954 (18)
C2—O2—H1O2	105.4 (14)	C9—C10—C11	122.77 (12)
C3—O3—C18	116.32 (11)	C9—C10—H10	122.6 (9)
C8—N1—C7	116.80 (11)	C11—C10—H10	114.6 (9)
C7—N2—C16	118.40 (11)	O1—C11—C10	121.75 (12)
C2—C1—C6	119.38 (11)	O1—C11—C12	121.49 (13)
C2—C1—C7	120.97 (11)	C10—C11—C12	116.75 (11)
C6—C1—C7	119.65 (11)	C13—C12—C17	119.11 (12)
O2—C2—C1	123.88 (11)	C13—C12—C11	121.84 (12)
O2—C2—C3	116.70 (11)	C17—C12—C11	119.03 (12)
C1—C2—C3	119.41 (12)	C12—C13—C14	120.14 (12)
O3—C3—C4	125.62 (12)	C12—C13—H13	116.6 (8)
O3—C3—C2	114.43 (12)	C14—C13—H13	123.2 (8)
C4—C3—C2	119.95 (12)	C15—C14—C13	121.45 (13)
C3—C4—C5	120.50 (12)	C15—C14—H14	118.9 (9)
C3—C4—H4	121.5 (11)	C13—C14—H14	119.6 (9)
C5—C4—H4	118.0 (11)	C14—C15—C16	119.02 (12)
C6—C5—C4	120.32 (13)	C14—C15—H15	122.2 (10)
C6—C5—H5	118.3 (9)	C16—C15—H15	118.7 (10)
C4—C5—H5	121.2 (9)	N2—C16—C17	119.84 (11)
C5—C6—C1	120.42 (12)	N2—C16—C15	120.32 (11)
C5—C6—H6	119.3 (10)	C17—C16—C15	119.84 (11)
C1—C6—H6	120.2 (10)	C16—C17—C12	120.44 (12)

supplementary materials

N2—C7—N1	125.29 (11)	C16—C17—C8	117.41 (11)
N2—C7—C1	117.29 (11)	C12—C17—C8	122.12 (11)
N1—C7—C1	117.42 (11)	O3—C18—H18A	107.1 (10)
N1—C8—C17	122.25 (12)	O3—C18—H18B	112.2 (9)
N1—C8—C9	119.17 (12)	H18A—C18—H18B	110.1 (14)
C17—C8—C9	118.57 (11)	O3—C18—H18C	102.7 (10)
C10—C9—C8	120.76 (13)	H18A—C18—H18C	115.0 (15)
C10—C9—H9	121.4 (9)	H18B—C18—H18C	109.5 (14)
C8—C9—H9	117.7 (9)		
C6—C1—C2—O2	178.87 (11)	C8—C9—C10—C11	-0.6 (2)
C7—C1—C2—O2	-0.90 (19)	C9—C10—C11—O1	179.92 (13)
C6—C1—C2—C3	-1.62 (18)	C9—C10—C11—C12	1.0 (2)
C7—C1—C2—C3	178.60 (10)	O1—C11—C12—C13	-1.6 (2)
C18—O3—C3—C4	1.88 (19)	C10—C11—C12—C13	177.40 (12)
C18—O3—C3—C2	-177.96 (12)	O1—C11—C12—C17	-179.71 (12)
O2—C2—C3—O3	-0.19 (17)	C10—C11—C12—C17	-0.76 (17)
C1—C2—C3—O3	-179.73 (10)	C17—C12—C13—C14	-0.32 (19)
O2—C2—C3—C4	179.96 (11)	C11—C12—C13—C14	-178.48 (12)
C1—C2—C3—C4	0.42 (18)	C12—C13—C14—C15	0.4 (2)
O3—C3—C4—C5	-178.86 (12)	C13—C14—C15—C16	-0.3 (2)
C2—C3—C4—C5	0.98 (19)	C7—N2—C16—C17	0.73 (17)
C3—C4—C5—C6	-1.1 (2)	C7—N2—C16—C15	-178.36 (11)
C4—C5—C6—C1	-0.1 (2)	C14—C15—C16—N2	179.33 (12)
C2—C1—C6—C5	1.47 (18)	C14—C15—C16—C17	0.24 (19)
C7—C1—C6—C5	-178.75 (11)	N2—C16—C17—C12	-179.29 (10)
C16—N2—C7—N1	-0.21 (18)	C15—C16—C17—C12	-0.20 (18)
C16—N2—C7—C1	179.80 (10)	N2—C16—C17—C8	-0.99 (17)
C8—N1—C7—N2	-0.03 (18)	C15—C16—C17—C8	178.10 (11)
C8—N1—C7—C1	179.96 (10)	C13—C12—C17—C16	0.24 (18)
C2—C1—C7—N2	2.97 (17)	C11—C12—C17—C16	178.45 (10)
C6—C1—C7—N2	-176.80 (11)	C13—C12—C17—C8	-177.98 (11)
C2—C1—C7—N1	-177.02 (10)	C11—C12—C17—C8	0.23 (18)
C6—C1—C7—N1	3.21 (16)	N1—C8—C17—C16	0.77 (17)
C7—N1—C8—C17	-0.26 (17)	C9—C8—C17—C16	-178.10 (11)
C7—N1—C8—C9	178.60 (11)	N1—C8—C17—C12	179.04 (11)
N1—C8—C9—C10	-178.90 (12)	C9—C8—C17—C12	0.17 (17)
C17—C8—C9—C10	0.01 (19)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H1O2 \cdots N2	0.91 (2)	1.73 (2)	2.5583 (15)	151 (2)
C15—H15 \cdots O2 ⁱ	0.970 (18)	2.437 (18)	3.3686 (17)	160.8 (12)

Symmetry codes: (i) $-x+2, y, -z+3/2$.

Fig. 1

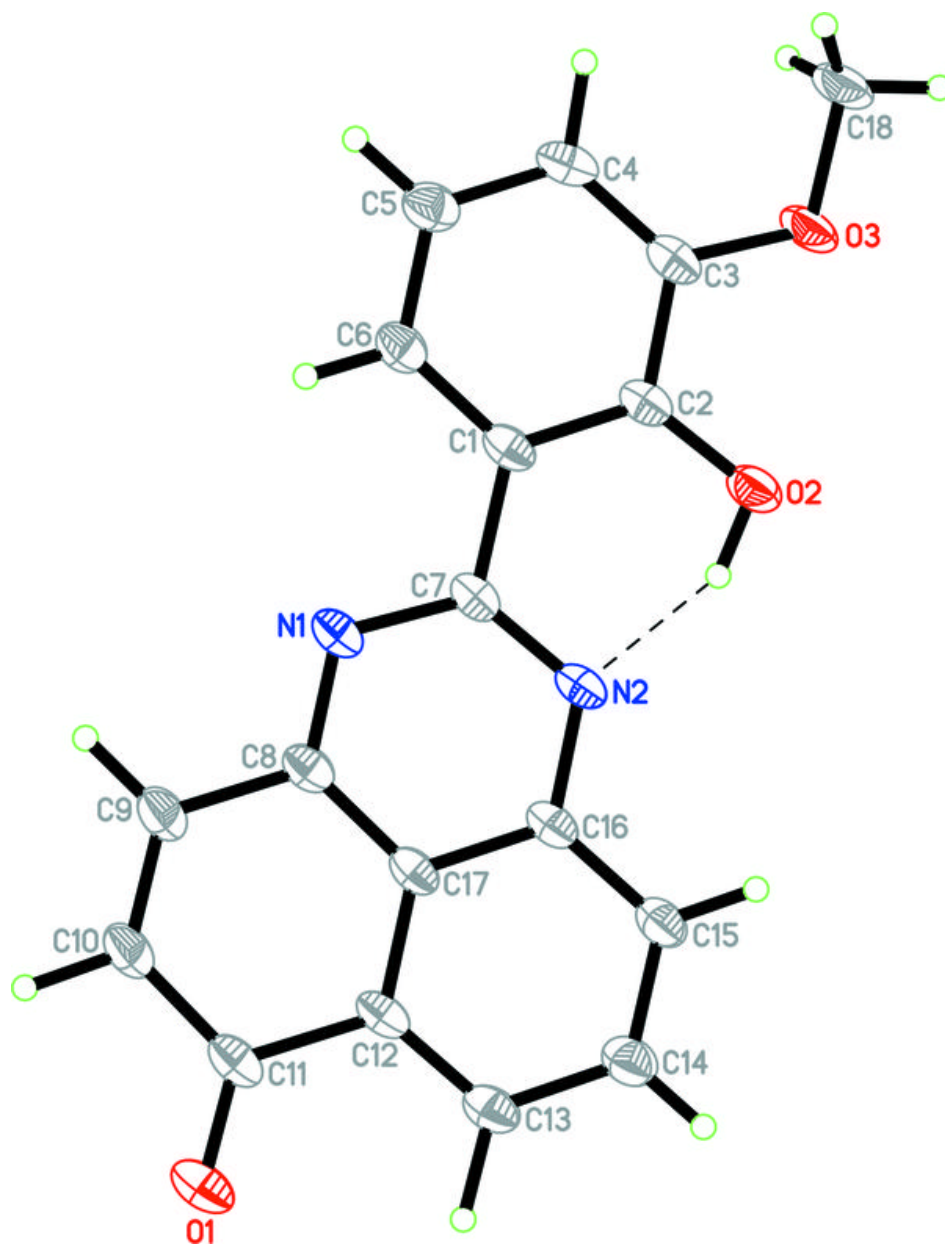


Fig. 2

