Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2-Hydroxyethyl)-6-[(2-hydroxyethyl)amino]-5-nitro-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione

Wen Qin,[a,b] Ye Zhang,[b] Heng-Shan Wang[a]* and Yong Zhang[c]

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China, [b]Department of Chemistry and Engineering Technology, Guilin Normal College, Guilin 541004, People's Republic of China, and [c]College of Chemistry and Chemical Engineering, Suzhou University, Suzhou 215006, People's Republic of China
Correspondence e-mail: wang_hengshan@yahoo.com.cn

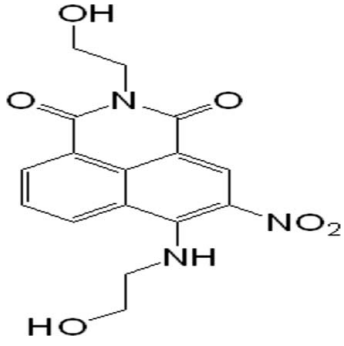
Received 13 August 2007; accepted 2 September 2007

Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.086; data-to-parameter ratio = 5.8.

The title compound, $C_{16}H_{15}N_3O_6$, exhibits weak intermolecular C—H···O and O—H···O hydrogen bonds, which stabilize the structure. π–π stacking interactions are also found, the centroid-to-centroid distance within the stacks being 3.4401 Å. The title compound represents a new derivative of 1, 8-naphthalimides.

Related literature

For related literature, see: Konstantinova *et al.* (2000); Mitchell *et al.* (1998); Xu *et al.* (2004); Tao & Qian (1999).



Experimental

Crystal data

$C_{16}H_{15}N_3O_6$
M_r = 345.31
Triclinic, $P\overline{1}$
a = 4.7125 (12) Å
b = 8.032 (2) Å
c = 9.997 (3) Å
α = 80.490 (15)°
β = 81.977 (15)°
γ = 77.324 (14)°
V = 361.98 (17) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 193 (2) K
0.30 × 0.18 × 0.15 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.964, T_{max} = 0.982
3566 measured reflections
1318 independent reflections
1107 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.086
S = 1.05
1318 reflections
229 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4^{i}	0.84	2.12	2.931 (3)	161
O3—H3···O5^{i}	0.84	2.45	3.161 (3)	143
O3—H3···N2^{i}	0.84	2.64	3.472 (4)	171
O6—H6···O2^{ii}	0.84	1.97	2.790 (3)	165
N3—H3*A*···O5	0.88	1.88	2.595 (4)	138
N3—H3*A*···O6	0.88	2.26	2.693 (4)	110
C11—H11···O4^{iii}	0.95	2.57	3.435 (4)	152
C13—H13*A*···O6^{iv}	0.99	2.49	3.376 (5)	149

Symmetry codes: (i) $x-1, y, z-1$; (ii) $x+1, y, z+1$; (iii) $x-1, y-1, z$; (iv) $x-1, y+1, z-1$.

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors thank the National Natural Science Foundation of China (Nos. 20362002 and 20442005), the 100 Young and Middle-aged Disciplinary Leaders in Guangxi Higher Education Institutions, and the Science Foundation of Guangxi Province (No. 0575046), as well as the Foundation of Guangxi Universities of the People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2026).

References

Jacobson, R. (1998). Private Communication to the Rigaku Corporation, Tokyo, Japan.
Konstantinova, A., Spirieva, A. & Petkova, T. (2000). *Dyes Pigments*, **45**, 125–129.
Mitchell, K. A., Brown, R. G., Yuan, D., Chang, S. H., Utecht, R. E. & Lewis, D. E. (1998). *J. Photochem. Photobiol. A Chem.* **115**, 157–161.
Rigaku (1999). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2000). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tao, Z. F. & Qian, S. H. (1999). *Dyes Pigments*, **43**, 139–145.
Xu, Y. F., Huang, X. Y., Qian, X. H. & Yao, W. (2004). *Bioorg. Med. Chem.* **12**, 2335–2341.

supplementary materials

Acta Cryst. (2007). E**63**, o3995 [**doi:10.1107/S160053680704295X**]

2-(2-Hydroxyethyl)-6-[(2-hydroxyethyl)amino]-5-nitro-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione

W. Qin, Y. Zhang, H.-S. Wang and Y. Zhang

Comment

The structure of 1,8-naphthalic anhydride is used as a source of fine chemicals. The use of its N-substituted derivatives as important dyes (Konstantinova *et al.*, 2000), fluorescent tapes (Mitchell *et al.*, 1998) and photochemical DNA cleaving reagents (Xu *et al.*, 2004), prompted us to the synthesis of the title copound which is being reported in this article..

The molecular structure of the title compound is shown in Fig. 1. Its overall geometry is comparable to that found for 2-(3',3'-dimethylallyl)-1*H*-benz[de]iso-quindine-1,3(2*H*)-dione (Tao & Qian), apart from the hydroxyethyl, the hydroxyethyl-amino and nitro groups substituting in 1,8-naphthalimide moiety.2-(2-Hydroxyethyl)-6-[(2-hydroxyethyl)amino]-5-nitro-1*H*-benzo[de]isoquinoline-1,3(2*H*)-dione All the atoms in 1,8-naphthalimide moiety are almost coplanar.

In the crystal packing (Fig. 2), there are weak intermolecular C—H···O and O—H···O hydrogen bonds, which stabilize the structure. The π-π stacking interactions are also found while the intermolecular distance within the stacks is 3.440 Å. These contacts also partially take part in the stabilization of the structure.

Experimental

The mixture of 3-nitro-1,8-naphthalic anhydride (0.32 g, 1 mmol) and hydroxyethyl amine (0.122 g, 2.0 mmol) was refluxed in ethanol (30 ml) for about 6 h, and cooled to afford the yellow powder of the title compound. Upon recrystallization from *N*,*N*-dimethylformamide, light-brown crystls were obtained (Yield 50%, m.p. 514–516 K)

Refinement

H atoms bound to C atoms were positioned geometrically and included in the refinement in the riding-model approximation [*d*(C—H) = 0.95, 0.98, 0.99 and 1.00 Å for aromatic, methyl, CH_2 and C_H groups, respectively, and with U_{iso}(H) = 1.5U_{eq} for (mehtyl C) and 1.2U_{eq} (C) for all others.

Figures

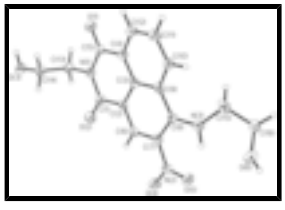


Fig. 1. The structure of the title copmpound showing 50% probability displacement ellipsoids and the atom labelling scheme. H atoms are represented by small spheres of arbitrary radius.

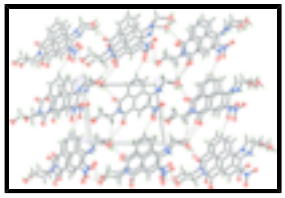


Fig. 2. Packing diagram showing a plane of molecules with H bonds indicated by dashed lines.

2-(2-Hydroxyethyl)-6-[(2-hydroxyethyl)amino]-5-nitro- 1*H*-benzo[de]isoquinoline-1,3(2*H*)-dione

Crystal data

$C_{16}H_{15}N_3O_6$	$Z = 1$
$M_r = 345.31$	$F_{000} = 180$
Triclinic, *P*1	$D_x = 1.584$ Mg m^{-3}
Hall symbol: P 1	Mo *K*α radiation λ = 0.71070 Å
$a = 4.7125$ (12) Å	Cell parameters from 1321 reflections
$b = 8.032$ (2) Å	θ = 3.1–25.3º
$c = 9.997$ (3) Å	μ = 0.12 mm^{-1}
α = 80.490 (15)º	$T = 193$ (2) K
β = 81.977 (15)º	Block, light-brown
γ = 77.324 (14)º	0.30 × 0.18 × 0.15 mm
$V = 361.98$ (17) Å^3	

Data collection

Rigaku Mercury diffractometer	1107 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.034$
Monochromator: graphite	$\theta_{max} = 25.4$º
$T = 193(2)$ K	$\theta_{min} = 3.1$º
ω scans	$h = -5 \rightarrow 5$
Absorption correction: multi-scan (Jacobson, 1998)	$k = -9 \rightarrow 8$
$T_{min} = 0.964$, $T_{max} = 0.982$	$l = -12 \rightarrow 12$
3566 measured reflections	Standard reflections: ?
1318 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.086$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
1318 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}

229 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Extinction correction: none

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.0483 (6)	0.6442 (3)	0.4925 (3)	0.0350 (6)
O2	−0.4438 (5)	0.2532 (3)	0.4083 (2)	0.0310 (6)
O3	−0.1177 (6)	0.6283 (3)	0.0831 (3)	0.0369 (7)
H3	−0.2257	0.5893	0.0411	0.055*
O4	0.5170 (6)	0.5645 (3)	0.8901 (3)	0.0352 (7)
O5	0.5728 (5)	0.3339 (3)	1.0369 (2)	0.0302 (6)
O6	0.4894 (5)	−0.0077 (3)	1.2695 (3)	0.0327 (6)
H6	0.4856	0.0642	1.3223	0.049*
N1	−0.1985 (6)	0.4477 (3)	0.4497 (3)	0.0223 (6)
N2	0.4703 (6)	0.4170 (4)	0.9316 (3)	0.0254 (7)
N3	0.2847 (6)	0.0970 (4)	1.0246 (3)	0.0268 (7)
H3A	0.4202	0.1329	1.0579	0.032*
C1	−0.0264 (7)	0.5052 (4)	0.5296 (4)	0.0239 (8)
C2	0.0537 (7)	0.3942 (4)	0.6543 (3)	0.0204 (8)
C3	−0.0248 (7)	0.2296 (4)	0.6918 (3)	0.0199 (8)
C4	−0.1870 (8)	0.1753 (4)	0.6044 (4)	0.0224 (8)
C5	−0.2869 (7)	0.2916 (4)	0.4813 (3)	0.0225 (8)
C6	0.2177 (7)	0.4469 (4)	0.7355 (3)	0.0203 (7)
H6A	0.2746	0.5550	0.7094	0.024*
C7	0.3036 (7)	0.3451 (4)	0.8560 (3)	0.0212 (8)
C8	0.2187 (7)	0.1832 (4)	0.9034 (3)	0.0213 (8)
C9	0.0624 (7)	0.1209 (4)	0.8121 (3)	0.0209 (8)
C10	−0.0009 (8)	−0.0452 (4)	0.8333 (4)	0.0256 (8)
H10	0.0634	−0.1235	0.9104	0.031*
C11	−0.1535 (8)	−0.0975 (4)	0.7455 (4)	0.0299 (9)
H11	−0.1930	−0.2105	0.7631	0.036*
C12	−0.2508 (7)	0.0134 (4)	0.6310 (4)	0.0273 (8)
H12	−0.3600	−0.0226	0.5721	0.033*

C13	−0.2808 (8)	0.5604 (5)	0.3226 (4)	0.0271 (8)
H13A	−0.2958	0.6823	0.3338	0.033*
H13B	−0.4741	0.5465	0.3034	0.033*
C14	−0.0527 (8)	0.5139 (5)	0.2042 (4)	0.0324 (9)
H14A	0.1427	0.5197	0.2266	0.039*
H14B	−0.0475	0.3944	0.1894	0.039*
C15	0.1779 (8)	−0.0454 (4)	1.1135 (4)	0.0268 (8)
H15A	0.2988	−0.1572	1.0924	0.032*
H15B	−0.0274	−0.0427	1.1002	0.032*
C16	0.1987 (8)	−0.0229 (5)	1.2586 (4)	0.0298 (8)
H16A	0.0589	0.0819	1.2829	0.036*
H16B	0.1493	−0.1234	1.3220	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0485 (16)	0.0283 (14)	0.0310 (16)	−0.0174 (12)	−0.0105 (12)	0.0057 (11)
O2	0.0355 (14)	0.0332 (14)	0.0283 (15)	−0.0107 (11)	−0.0100 (12)	−0.0053 (11)
O3	0.0543 (19)	0.0443 (17)	0.0191 (15)	−0.0272 (14)	−0.0125 (13)	0.0061 (12)
O4	0.0468 (17)	0.0327 (15)	0.0326 (15)	−0.0215 (13)	−0.0102 (12)	−0.0004 (11)
O5	0.0357 (15)	0.0341 (14)	0.0240 (15)	−0.0108 (11)	−0.0122 (12)	−0.0001 (11)
O6	0.0351 (15)	0.0335 (14)	0.0320 (17)	−0.0054 (12)	−0.0121 (12)	−0.0065 (11)
N1	0.0257 (15)	0.0229 (15)	0.0178 (16)	−0.0048 (12)	−0.0050 (12)	0.0007 (11)
N2	0.0271 (17)	0.0287 (17)	0.0234 (18)	−0.0114 (14)	−0.0015 (14)	−0.0051 (13)
N3	0.0280 (17)	0.0281 (15)	0.0258 (18)	−0.0092 (13)	−0.0064 (13)	0.0000 (13)
C1	0.0228 (19)	0.027 (2)	0.022 (2)	−0.0060 (16)	−0.0024 (15)	−0.0040 (15)
C2	0.0190 (18)	0.0206 (18)	0.021 (2)	−0.0047 (14)	0.0021 (15)	−0.0034 (14)
C3	0.0185 (18)	0.0219 (18)	0.019 (2)	−0.0046 (15)	0.0004 (15)	−0.0040 (14)
C4	0.0233 (18)	0.0199 (18)	0.024 (2)	−0.0046 (14)	0.0022 (15)	−0.0056 (14)
C5	0.0243 (19)	0.026 (2)	0.018 (2)	−0.0075 (16)	−0.0031 (16)	−0.0030 (15)
C6	0.0188 (17)	0.0230 (18)	0.019 (2)	−0.0073 (14)	0.0005 (14)	−0.0011 (13)
C7	0.0196 (18)	0.0215 (19)	0.024 (2)	−0.0065 (15)	0.0005 (15)	−0.0065 (15)
C8	0.0196 (18)	0.0272 (19)	0.017 (2)	−0.0056 (15)	−0.0015 (15)	−0.0027 (15)
C9	0.0186 (17)	0.0212 (18)	0.022 (2)	−0.0041 (14)	0.0028 (15)	−0.0036 (14)
C10	0.031 (2)	0.0255 (19)	0.020 (2)	−0.0068 (16)	−0.0031 (15)	0.0001 (14)
C11	0.037 (2)	0.0217 (17)	0.034 (2)	−0.0101 (16)	−0.0050 (17)	−0.0049 (15)
C12	0.028 (2)	0.032 (2)	0.026 (2)	−0.0112 (16)	−0.0066 (16)	−0.0046 (16)
C13	0.0290 (19)	0.0309 (19)	0.021 (2)	−0.0071 (16)	−0.0092 (15)	0.0046 (14)
C14	0.030 (2)	0.048 (2)	0.020 (2)	−0.0107 (18)	−0.0049 (16)	−0.0004 (16)
C15	0.029 (2)	0.0255 (18)	0.026 (2)	−0.0083 (16)	−0.0032 (16)	0.0009 (15)
C16	0.034 (2)	0.0304 (18)	0.026 (2)	−0.0132 (16)	−0.0049 (16)	0.0033 (15)

Geometric parameters (Å, °)

O1—C1	1.227 (4)	C4—C5	1.482 (5)
O2—C5	1.225 (4)	C6—C7	1.396 (5)
O3—C14	1.420 (4)	C6—H6A	0.9500
O3—H3	0.8400	C7—C8	1.431 (4)
O4—N2	1.245 (4)	C8—C9	1.458 (5)

O5—N2	1.248 (4)	C9—C10	1.406 (5)
O6—C16	1.423 (4)	C10—C11	1.376 (5)
O6—H6	0.8400	C10—H10	0.9500
N1—C5	1.381 (4)	C11—C12	1.394 (5)
N1—C1	1.405 (4)	C11—H11	0.9500
N1—C13	1.479 (5)	C12—H12	0.9500
N2—C7	1.425 (4)	C13—C14	1.520 (5)
N3—C8	1.333 (4)	C13—H13A	0.9900
N3—C15	1.464 (4)	C13—H13B	0.9900
N3—H3A	0.8800	C14—H14A	0.9900
C1—C2	1.452 (5)	C14—H14B	0.9900
C2—C6	1.367 (5)	C15—C16	1.510 (5)
C2—C3	1.428 (4)	C15—H15A	0.9900
C3—C4	1.413 (5)	C15—H15B	0.9900
C3—C9	1.419 (5)	C16—H16A	0.9900
C4—C12	1.374 (5)	C16—H16B	0.9900
C14—O3—H3	109.5	C10—C9—C8	123.9 (3)
C16—O6—H6	109.5	C3—C9—C8	119.3 (3)
C5—N1—C1	123.9 (3)	C11—C10—C9	121.9 (3)
C5—N1—C13	118.8 (3)	C11—C10—H10	119.1
C1—N1—C13	117.3 (3)	C9—C10—H10	119.1
O4—N2—O5	119.8 (3)	C10—C11—C12	120.8 (3)
O4—N2—C7	119.1 (3)	C10—C11—H11	119.6
O5—N2—C7	121.1 (3)	C12—C11—H11	119.6
C8—N3—C15	133.1 (3)	C4—C12—C11	119.3 (3)
C8—N3—H3A	113.4	C4—C12—H12	120.4
C15—N3—H3A	113.4	C11—C12—H12	120.4
O1—C1—N1	119.7 (3)	N1—C13—C14	110.0 (3)
O1—C1—C2	123.2 (3)	N1—C13—H13A	109.7
N1—C1—C2	117.1 (3)	C14—C13—H13A	109.7
C6—C2—C3	119.2 (3)	N1—C13—H13B	109.7
C6—C2—C1	118.8 (3)	C14—C13—H13B	109.7
C3—C2—C1	122.0 (3)	H13A—C13—H13B	108.2
C4—C3—C9	120.5 (3)	O3—C14—C13	110.8 (3)
C4—C3—C2	118.4 (3)	O3—C14—H14A	109.5
C9—C3—C2	121.2 (3)	C13—C14—H14A	109.5
C12—C4—C3	120.6 (3)	O3—C14—H14B	109.5
C12—C4—C5	119.0 (3)	C13—C14—H14B	109.5
C3—C4—C5	120.3 (3)	H14A—C14—H14B	108.1
O2—C5—N1	119.8 (3)	N3—C15—C16	107.1 (3)
O2—C5—C4	122.1 (3)	N3—C15—H15A	110.3
N1—C5—C4	118.1 (3)	C16—C15—H15A	110.3
C2—C6—C7	121.4 (3)	N3—C15—H15B	110.3
C2—C6—H6A	119.3	C16—C15—H15B	110.3
C7—C6—H6A	119.3	H15A—C15—H15B	108.5
C6—C7—N2	115.4 (3)	O6—C16—C15	108.5 (3)
C6—C7—C8	122.2 (3)	O6—C16—H16A	110.0
N2—C7—C8	122.3 (3)	C15—C16—H16A	110.0
N3—C8—C7	120.2 (3)	O6—C16—H16B	110.0

N3—C8—C9	123.4 (3)	C15—C16—H16B	110.0
C7—C8—C9	116.4 (3)	H16A—C16—H16B	108.4
C10—C9—C3	116.8 (3)		
C5—N1—C1—O1	178.4 (3)	O5—N2—C7—C6	−176.0 (3)
C13—N1—C1—O1	0.2 (5)	O4—N2—C7—C8	−174.3 (3)
C5—N1—C1—C2	−1.8 (4)	O5—N2—C7—C8	6.7 (4)
C13—N1—C1—C2	179.9 (3)	C15—N3—C8—C7	163.9 (3)
O1—C1—C2—C6	0.6 (5)	C15—N3—C8—C9	−16.7 (6)
N1—C1—C2—C6	−179.2 (3)	C6—C7—C8—N3	−174.4 (3)
O1—C1—C2—C3	−177.1 (3)	N2—C7—C8—N3	2.7 (5)
N1—C1—C2—C3	3.1 (4)	C6—C7—C8—C9	6.2 (4)
C6—C2—C3—C4	−178.1 (3)	N2—C7—C8—C9	−176.7 (3)
C1—C2—C3—C4	−0.4 (4)	C4—C3—C9—C10	4.7 (4)
C6—C2—C3—C9	0.5 (4)	C2—C3—C9—C10	−174.0 (3)
C1—C2—C3—C9	178.2 (3)	C4—C3—C9—C8	−177.4 (3)
C9—C3—C4—C12	−3.1 (5)	C2—C3—C9—C8	4.0 (4)
C2—C3—C4—C12	175.5 (3)	N3—C8—C9—C10	−8.7 (5)
C9—C3—C4—C5	177.8 (3)	C7—C8—C9—C10	170.7 (3)
C2—C3—C4—C5	−3.5 (4)	N3—C8—C9—C3	173.5 (3)
C1—N1—C5—O2	178.0 (3)	C7—C8—C9—C3	−7.1 (4)
C13—N1—C5—O2	−3.9 (5)	C3—C9—C10—C11	−3.2 (5)
C1—N1—C5—C4	−2.0 (5)	C8—C9—C10—C11	178.9 (3)
C13—N1—C5—C4	176.2 (3)	C9—C10—C11—C12	0.2 (5)
C12—C4—C5—O2	5.8 (5)	C3—C4—C12—C11	0.0 (5)
C3—C4—C5—O2	−175.2 (3)	C5—C4—C12—C11	179.0 (3)
C12—C4—C5—N1	−174.3 (3)	C10—C11—C12—C4	1.5 (5)
C3—C4—C5—N1	4.8 (5)	C5—N1—C13—C14	−87.6 (4)
C3—C2—C6—C7	−1.7 (4)	C1—N1—C13—C14	90.7 (4)
C1—C2—C6—C7	−179.4 (3)	N1—C13—C14—O3	−176.1 (3)
C2—C6—C7—N2	−179.1 (3)	C8—N3—C15—C16	−149.0 (4)
C2—C6—C7—C8	−1.8 (5)	N3—C15—C16—O6	−53.4 (4)
O4—N2—C7—C6	3.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4^{i}	0.84	2.12	2.931 (3)	161
O3—H3···O5^{i}	0.84	2.45	3.161 (3)	143
O3—H3···N2^{i}	0.84	2.64	3.472 (4)	171
O6—H6···O2^{ii}	0.84	1.97	2.790 (3)	165
N3—H3A···O5	0.88	1.88	2.595 (4)	138
N3—H3A···O6	0.88	2.26	2.693 (4)	110
C11—H11···O4^{iii}	0.95	2.57	3.435 (4)	152
C13—H13A···O6^{iv}	0.99	2.49	3.376 (5)	149

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

Fig. 1

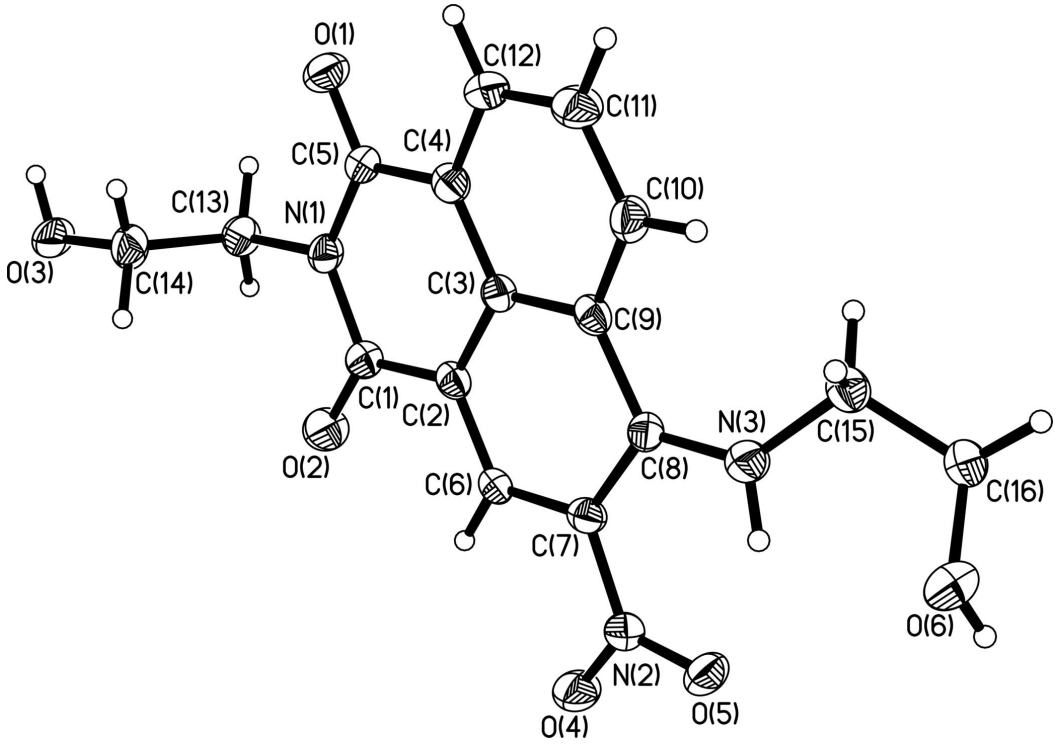

O(1)
C(12)
C(11)
C(5)
C(4)
C(10)
C(13)
N(1)
O(3)
C(14)
C(3)
C(9)
C(1)
C(2)
N(3)
C(15)
O(2)
C(8)
C(16)
C(6)
C(7)
O(6)
N(2)
O(4)
O(5)

Fig. 2