Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl (9-oxo-9,10-dihydroacridin-10-yl)-acetate

Karol Krzymiński, Artur Sikorski and Jerzy Błażejowski*

University of Gdańsk, Faculty of Chemistry, J. Sobieskiego 18, 80-952 Gdańsk, Poland
Correspondence e-mail: bla@chem.univ.gda.pl

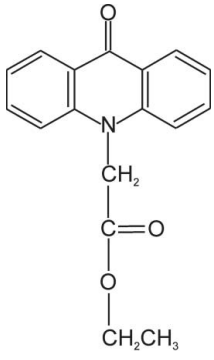
Received 12 August 2007; accepted 31 August 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.095; data-to-parameter ratio = 12.7.

In the crystal structure of the title compound, $C_{17}H_{15}NO_3$, molecules related by a center of symmetry are arranged in pairs that are stabilized *via* π–π interactions between the acridinone units. Adjacent pairs, with the acridinone rings arranged in a herringbone pattern, are linked through a network of π–π and C—H···O interactions.

Related literature

For general background, see: Agiamarnioti *et al.* (2006); Bożyk *et al.* (2003); Faller *et al.* (1997); Reymond *et al.* (1996). For related structures, see: Dobrzynska & Turowska-Tyrk (1997); Dzyabchenko *et al.* (1980); Zavodnik *et al.* (1979, 1981).



Experimental

Crystal data

$C_{17}H_{15}NO_3$
M_r = 281.30
Monoclinic, $P2_1/n$
a = 11.3232 (3) Å
b = 10.3380 (2) Å
c = 11.8925 (3) Å
β = 96.069 (2)°
V = 1384.33 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 (2) K
0.26 × 0.26 × 0.12 mm

Data collection

Oxford Diffraction GEMINI R ULTRA diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.978, T_{max} = 0.991
8822 measured reflections
2426 independent reflections
1776 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
S = 0.98
2426 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected torsion angles (°).

C1—C11—C12—C4	−3.34 (19)	C11—C9—C13—C14	3.50 (18)
N10—C16—C17—O18	170.44 (10)	C12—N10—C14—C13	−4.00 (18)
N10—C16—C17—O21	−10.40 (19)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O21^{i}	0.95	2.53	3.4155 (17)	154
C5—H5···O15^{ii}	0.95	2.37	3.2781 (15)	161
C16—H16*A*···O15^{ii}	0.99	2.34	3.3061 (16)	164

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

Table 3
π–π interactions (Å, °).

*Cg*1 is the centroid of ring C9/C11/C12/N10/C14/C13, *Cg*2 is the centroid of ring C1–C4/C12/C11 and *Cg*3 is the centroid of ring C5–C8/C13/C14. *Cg*···*Cg* is the distance between ring centroids. The dihedral angle is that between the planes of rings *CgI* and *CgJ*. The interplanar distance is the perpendicular distance of *CgI* from ring *J*. The offset is computed as the third side of the right-angled triangle involving the *Cg*···*Cg* distance.

CgI	*CgJ*	*Cg*···*Cg*	Dihedral angle	Interplanar distance	Offset
1	2^{iii}	3.780 (1)	3.1 (2)	3.492 (3)	1.361 (3)
2	1^{iii}	3.780 (1)	3.1 (2)	3.417 (3)	1.422 (3)
3	3^{iv}	3.660 (1)	0.0 (2)	3.530 (3)	1.853 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

This study was financed from the State Funds for Scientific Research (grant BW/8000-5-0047-7). The authors thank Oxford Diffraction Ltd, Abingdon, Oxfordshire, England, and Dr N. Brooks of this company for the data collection and for providing access to crystallographic experimental facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2311).

  doi:10.1107/S1600536807042663

References

Agiamarnioti, K., Triantis, T., Papadopoulos, K. & Scorilas, A. (2006). *J. Photochem. Photobiol. A Chem.* **181**, 126–131.

Bouzyk, A., Jóźwiak, L., Kolendo, A. Yu. & Błażejowski, J. (2003). *Spectrochim. Acta Part A*, **59**, 543–558.

Dobrzynska, D. & Turowska-Tyrk, I. (1997). *Acta Cryst.* C**53**, 238–239.

Dzyabchenko, A. V., Zavodnik, V. E. & Bel'skii, V. K. (1980). *Kristallografiya*, **25**, 72–79.

Faller, T., Hutton, K., Okafo, G., Gribble, A., Camilleri, P. & Games, D. E. (1997). *Chem. Commun.* pp. 1529–1530.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.31.7. Oxford Diffraction Poland, Wrocław, Poland.

Reymond, J. L., Koch, T., Schroer, J. & Tierney, E. (1996). *Proc. Natl Acad. Sci. USA*, **93**, 4251–4256.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Zavodnik, V. E., Chetkina, L. A. & Val'kova, G. A. (1979). *Kristallografiya*, **24**, 592–596.

Zavodnik, V. E., Chetkina, L. A. & Val'kova, G. A. (1981). *Kristallografiya*, **26**, 392–396.

supplementary materials

Acta Cryst. (2007). E**63**, o3972-o3973 [**doi:10.1107/S1600536807042663**]

Ethyl (9-oxo-9,10-dihydroacridin-10-yl)acetate

K. Krzyminski, A. Sikorski and J. Blazejowski

Comment

9-Acridinones strongly fluoresce in visible region (Bożyk *et al.*, 2003) which brings about that they can serve as emitting fragments of fluorogenic indicators or labels. 9-Acridinone derivatives attached through a spacer to macromolcules have been applied among others in fluorometric assay of peptides (Faller *et al.*, 1997) and avidin or streptavidin (Agiamarnioti *et al.*, 2006). A highly sensitive assay for antibody catalysis has also been demonstrated by using a number of 9-acridinone labelled compounds (Reymond *et al.*, 1996). Our investigations have been focused on search for 9-acridinone indicators exhibiting moderate polarity and ability to be transported through cell membranes and accumulated selectivity in various tissues. Ethyl 9-(2-oxoacridin-10(9*H*)-yl)acetate, (I), is the ethyl ester of (9-oxoacridin-10(9*H*)-yl) acetic acid whose crystal structure was determined in the past (Dobrzynska & Turowska-Tyrk, 1997).

The parameters characterizing the geometry (Figure 1) of the title compound (Table 1) are typical for 9-acridinones (Dobrzynska & Turowska-Tyrk, 1997; Dzyabchenko *et al.*, 1980; Zavodnik *et al.*, 1979; Zavodnik *et al.*, 1981).

In the monoclinic crystal structure of (I), molecules related by a centre of symmetry are arranged in pairs stabilized *via* π-π interactions between acridinone units (Table 3, Figure 2). With average deviation from planarity of 0.030 Å, acridinone ring systems (given by C1—C9, N10, C11—C14 atoms) are parallel in pairs, whereas those in adjacent pairs are inclined to each other either at 0.0 (1)° (parallely oriented pairs) or 85.8 (1)° (perpendicularly oriented pairs). Parallely oriented pairs are linked by π-π interactions (Table 3, Figure 2), while perpendicularly oriented pairs - through the network of C—H···O interactions involving acridinone and carbonyl O atoms (Table 2, Figure 2). The view along the *c* axis demonstrates the arrangement of the acridinone ring in a herringbone pattern.

Experimental

The title compound was synthesized by treating 9(10*H*)-acridinone with five molar excess of ethyl iodoacetate, both dissolved in dry dimethylsulfoxide, in the presence of anhydrous potassium carbonate (323 K, 8 h). The reaction mixture was poured into diluted hydrochloric acid, and the crude product was isolated by filtration and purified by gravitational column chromatography (SiO_2, chloroform/ethanol, 10:1 *v*/*v*). Yellow crystals of (I) suitable for X-ray investigations were grown from acetone [m.p. = 455–457 K; elemental analysis (% calculated/found): C 72.58/72.36, H 5.37/5.26, N 4.98/4.96].

Refinement

Methyl H atoms were placed in calculated positions with C—H = 0.98 Å and torsion angle was refined to fit the electron density, U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 (aromatic) and 0.99 Å (methylene), and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C).

Figures

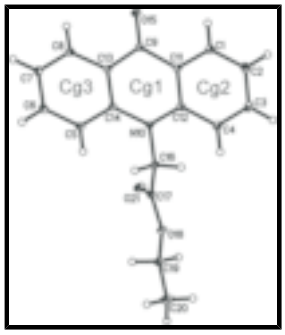


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 25% probability level and H atoms are shown as small spheres of arbitrary radius.

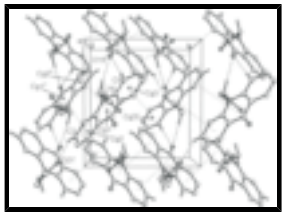


Fig. 2. The arrangement of the molecules of (I) in the crystal structure viewed approximately along the *c* axis. The C—H···O interactions are represented by dashed lines and π-π interactions by dotted lines. H atoms not involved in C—H···O interactions have been omitted. [Symmetry codes: (i) 3/2 − *x*, *y* − 1/2, 1/2 − *z*; (ii) *x* − 1/2, 1/2 − *y*, *z* − 1/2; (iii) 1 − *x*, −*y*, 1 − *z*; (iv) 1 − *x*, 1 − *y*, 1 − *z*].

Ethyl (9-oxo-9,10-dihydroacridin-10-yl)acetate

Crystal data

$C_{17}H_{15}NO_3$	F_{000} = 592
M_r = 281.30	D_x = 1.350 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2420 reflections
a = 11.3232 (3) Å	θ = 3.3–25.0º
b = 10.3380 (2) Å	μ = 0.09 mm^{-1}
c = 11.8925 (3) Å	*T* = 100 (2) K
β = 96.069 (2)º	Block, yellow
V = 1384.33 (6) Å^3	0.26 × 0.26 × 0.12 mm
Z = 4	

Data collection

Oxford Diffraction GEMINI R ULTRA diffractometer	2426 independent reflections
Radiation source: fine-focus sealed tube	1776 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 100(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 3.3º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	*h* = −12→13
T_{min} = 0.978, T_{max} = 0.991	*k* = −12→12
8822 measured reflections	*l* = −14→11

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.066P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.095$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.98$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
2426 reflections	$\Delta\rho_{min} = -0.20$ e Å^{-3}
191 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
Primary atom site location: structure-invariant direct methods	Extinction coefficient: none
Secondary atom site location: difference Fourier map	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.74768 (11)	0.07698 (13)	0.59379 (11)	0.0255 (3)
H1	0.7852	0.0956	0.6673	0.031*
C2	0.79552 (12)	−0.01492 (14)	0.53008 (12)	0.0301 (4)
H2	0.8643	−0.0614	0.5594	0.036*
C3	0.74185 (12)	−0.03963 (14)	0.42115 (12)	0.0318 (4)
H3	0.7762	−0.1013	0.3751	0.038*
C4	0.64007 (12)	0.02402 (13)	0.37971 (12)	0.0272 (3)
H4	0.6049	0.0057	0.3053	0.033*
C5	0.33185 (11)	0.34410 (12)	0.42677 (11)	0.0235 (3)
H5	0.2908	0.3207	0.3559	0.028*
C6	0.29030 (11)	0.44419 (13)	0.48748 (11)	0.0263 (3)
H6	0.2210	0.4894	0.4576	0.032*
C7	0.34785 (12)	0.48082 (13)	0.59227 (12)	0.0267 (3)
H7	0.3188	0.5508	0.6332	0.032*
C8	0.44674 (11)	0.41402 (12)	0.63490 (11)	0.0238 (3)
H8	0.4859	0.4377	0.7066	0.029*
C9	0.59786 (11)	0.24433 (12)	0.62432 (11)	0.0220 (3)
N10	0.48050 (9)	0.17667 (10)	0.40685 (8)	0.0211 (3)
C11	0.64392 (11)	0.14521 (12)	0.55352 (11)	0.0209 (3)
C12	0.58718 (11)	0.11590 (12)	0.44574 (11)	0.0213 (3)
C13	0.49175 (11)	0.31132 (12)	0.57522 (10)	0.0202 (3)
C14	0.43467 (10)	0.27592 (12)	0.46854 (10)	0.0194 (3)

O15	0.64646 (8)	0.27032 (9)	0.72029 (7)	0.0296 (3)
C16	0.42514 (12)	0.14381 (13)	0.29409 (10)	0.0226 (3)
H16A	0.3399	0.1672	0.2881	0.027*
H16B	0.4308	0.0493	0.2824	0.027*
C17	0.48365 (11)	0.21345 (12)	0.20307 (11)	0.0224 (3)
O18	0.44395 (8)	0.16691 (8)	0.10116 (7)	0.0251 (3)
C19	0.49230 (12)	0.22930 (14)	0.00575 (11)	0.0269 (3)
H19B	0.5781	0.2099	0.0073	0.032*
H19A	0.4824	0.3243	0.0100	0.032*
C20	0.42657 (16)	0.17831 (15)	−0.10081 (12)	0.0428 (4)
H20C	0.4328	0.0838	−0.1020	0.064*
H20B	0.4610	0.2145	−0.1662	0.064*
H20A	0.3428	0.2033	−0.1040	0.064*
O21	0.55459 (8)	0.29938 (9)	0.21883 (8)	0.0341 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0215 (7)	0.0294 (8)	0.0253 (7)	−0.0023 (6)	0.0007 (6)	0.0009 (6)
C2	0.0221 (8)	0.0314 (8)	0.0365 (9)	0.0054 (6)	0.0022 (7)	0.0000 (7)
C3	0.0308 (8)	0.0309 (8)	0.0348 (9)	0.0037 (6)	0.0087 (7)	−0.0051 (7)
C4	0.0287 (8)	0.0291 (8)	0.0238 (8)	−0.0002 (6)	0.0029 (6)	−0.0043 (6)
C5	0.0232 (7)	0.0267 (7)	0.0194 (7)	−0.0019 (6)	−0.0028 (6)	0.0018 (6)
C6	0.0210 (7)	0.0275 (8)	0.0295 (8)	0.0018 (6)	−0.0015 (6)	0.0029 (6)
C7	0.0260 (8)	0.0248 (7)	0.0291 (8)	0.0027 (6)	0.0018 (6)	−0.0043 (6)
C8	0.0244 (7)	0.0267 (7)	0.0200 (7)	−0.0025 (6)	0.0007 (6)	−0.0026 (6)
C9	0.0207 (7)	0.0264 (7)	0.0186 (7)	−0.0029 (6)	0.0007 (6)	0.0013 (6)
N10	0.0207 (6)	0.0259 (6)	0.0160 (6)	0.0000 (5)	−0.0006 (5)	−0.0019 (5)
C11	0.0183 (7)	0.0225 (7)	0.0219 (7)	−0.0022 (5)	0.0021 (6)	0.0015 (6)
C12	0.0206 (7)	0.0219 (7)	0.0216 (7)	−0.0021 (5)	0.0034 (6)	0.0018 (6)
C13	0.0182 (7)	0.0226 (7)	0.0199 (7)	−0.0031 (5)	0.0018 (5)	0.0005 (6)
C14	0.0195 (7)	0.0204 (7)	0.0183 (7)	−0.0041 (6)	0.0020 (6)	0.0003 (5)
O15	0.0279 (5)	0.0393 (6)	0.0198 (5)	0.0057 (4)	−0.0055 (4)	−0.0047 (4)
C16	0.0236 (7)	0.0259 (7)	0.0179 (7)	−0.0035 (6)	0.0005 (6)	−0.0040 (6)
C17	0.0207 (7)	0.0242 (7)	0.0216 (7)	−0.0008 (6)	−0.0005 (6)	−0.0033 (6)
O18	0.0305 (5)	0.0283 (5)	0.0166 (5)	−0.0085 (4)	0.0027 (4)	−0.0011 (4)
C19	0.0308 (8)	0.0290 (7)	0.0221 (8)	−0.0046 (6)	0.0082 (6)	0.0010 (6)
C20	0.0590 (11)	0.0476 (9)	0.0222 (8)	−0.0208 (8)	0.0055 (8)	0.0000 (7)
O21	0.0375 (6)	0.0378 (6)	0.0270 (6)	−0.0165 (5)	0.0032 (5)	−0.0067 (5)

Geometric parameters (Å, °)

C1—C2	1.363 (2)	C9—C11	1.4574 (18)
C1—C11	1.4100 (17)	C9—O15	1.2428 (14)
C1—H1	0.9500	N10—C12	1.3962 (16)
C2—C3	1.3951 (19)	N10—C14	1.3932 (16)
C2—H2	0.9500	N10—C16	1.4591 (15)
C3—C4	1.3725 (19)	C11—C12	1.4048 (17)
C3—H3	0.9500	C13—C14	1.4099 (16)

C4—C12	1.4061 (19)	C16—C17	1.5102 (19)
C4—H4	0.9500	C16—H16A	0.9900
C5—C6	1.3731 (19)	C16—H16B	0.9900
C5—C14	1.4060 (17)	C17—O18	1.3369 (15)
C5—H5	0.9500	C17—O21	1.1990 (15)
C6—C7	1.3962 (18)	O18—C19	1.4610 (16)
C6—H6	0.9500	C19—C20	1.4961 (18)
C7—C8	1.3666 (18)	C19—H19B	0.9900
C7—H7	0.9500	C19—H19A	0.9900
C8—C13	1.4026 (18)	C20—H20C	0.9800
C8—H8	0.9500	C20—H20B	0.9800
C9—C13	1.4546 (17)	C20—H20A	0.9800
C2—C1—C11	121.73 (12)	C1—C11—C9	119.45 (11)
C2—C1—H1	119.1	N10—C12—C11	120.09 (12)
C11—C1—H1	119.1	N10—C12—C4	121.58 (11)
C1—C2—C3	118.96 (12)	C11—C12—C4	118.33 (11)
C1—C2—H2	120.5	C8—C13—C14	119.69 (11)
C3—C2—H2	120.5	C8—C13—C9	119.09 (11)
C4—C3—C2	120.83 (14)	C14—C13—C9	121.22 (12)
C4—C3—H3	119.6	N10—C14—C5	121.58 (11)
C2—C3—H3	119.6	N10—C14—C13	120.28 (11)
C3—C4—C12	120.96 (12)	C5—C14—C13	118.14 (12)
C3—C4—H4	119.5	N10—C16—H16A	109.3
C12—C4—H4	119.5	C17—C16—H16A	109.3
C6—C5—C14	120.59 (12)	N10—C16—H16B	109.3
C6—C5—H5	119.7	C17—C16—H16B	109.3
C14—C5—H5	119.7	H16B—C16—H16B	107.9
C5—C6—C7	121.35 (12)	C16—C17—O18	110.32 (10)
C5—C6—H6	119.3	C16—C17—O21	125.35 (12)
C7—C6—H6	119.3	C17—O18—C19	115.31 (9)
C8—C7—C6	118.74 (13)	O18—C17—O21	124.32 (12)
C8—C7—H7	120.6	O18—C19—C20	107.97 (11)
C6—C7—H7	120.6	O18—C19—H19B	110.1
C7—C8—C13	121.47 (11)	C20—C19—H19B	110.1
C7—C8—H8	119.3	O18—C19—H19A	110.1
C13—C8—H8	119.3	C20—C19—H19A	110.1
O15—C9—C13	122.17 (12)	H19B—C19—H19A	108.4
O15—C9—C11	122.13 (11)	C19—C20—H20C	109.5
N10—C16—C17	111.68 (10)	C19—C20—H20B	109.5
C11—C9—C13	115.70 (11)	H20C—C20—H20B	109.5
C12—N10—C14	120.95 (10)	C19—C20—H20A	109.5
C14—N10—C16	120.51 (10)	H20C—C20—H20A	109.5
C12—C11—C1	119.10 (12)	H20B—C20—H20A	109.5
C12—C11—C9	121.45 (11)		
C11—C1—C2—C3	1.6 (2)	C9—C11—C12—C4	176.68 (12)
C1—C2—C3—C4	−2.3 (2)	C3—C4—C12—N10	−176.76 (12)
C2—C3—C4—C12	0.1 (2)	C3—C4—C12—C11	2.7 (2)
C14—C5—C6—C7	−0.4 (2)	C7—C8—C13—C14	0.3 (2)

C5—C6—C7—C8	−0.7 (2)	C7—C8—C13—C9	179.52 (12)
C6—C7—C8—C13	0.7 (2)	O15—C9—C13—C8	4.02 (19)
C2—C1—C11—C12	1.2 (2)	C11—C9—C13—C8	−175.67 (11)
C2—C1—C11—C9	−178.80 (12)	O15—C9—C13—C14	−176.81 (12)
O15—C9—C11—C12	179.25 (12)	C12—N10—C14—C5	175.47 (12)
C13—C9—C11—C12	−1.06 (18)	C16—N10—C14—C5	2.45 (18)
O15—C9—C11—C1	−0.74 (19)	C16—N10—C14—C13	−177.02 (11)
C13—C9—C11—C1	178.95 (11)	C6—C5—C14—N10	−178.01 (12)
C14—N10—C12—C11	6.44 (18)	C6—C5—C14—C13	1.47 (19)
C16—N10—C12—C11	179.62 (11)	C8—C13—C14—N10	178.06 (11)
C14—N10—C12—C4	−174.07 (11)	C9—C13—C14—N10	−1.10 (18)
C16—N10—C12—C4	−0.88 (18)	C8—C13—C14—C5	−1.43 (18)
C1—C11—C12—C4	−3.34 (19)	C9—C13—C14—C5	179.41 (11)
N10—C16—C17—O18	170.44 (10)	C14—N10—C16—C17	93.93 (13)
N10—C16—C17—O21	−10.40 (19)	C12—N10—C16—C17	−79.29 (14)
C11—C9—C13—C14	3.50 (18)	O21—C17—O18—C19	−0.61 (18)
C12—N10—C14—C13	−4.00 (18)	C16—C17—O18—C19	178.56 (10)
C1—C11—C12—N10	176.17 (11)	C17—O18—C19—C20	−172.36 (12)
C9—C11—C12—N10	−3.82 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O21^{i}	0.95	2.53	3.4155 (17)	154
C5—H5···O15^{ii}	0.95	2.37	3.2781 (15)	161
C16—H16A···O15^{ii}	0.99	2.34	3.3061 (16)	164

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

π–π interactions (Å,°)

CgI	CgJ	*Cg*···*Cg*	Dihedral angle	Interplanar distance	Offset
1	2^{iii}	3.780 (1)	3.1	3.492	1.361 (3)
2	1^{iii}	3.780 (1)	3.1	3.417	1.422 (3)
3	3^{iv}	3.660 (1)	0.0	3.530	1.853 (3)

Symmetry codes: (iii) 1 − *x*, −*y*, 1 − *z*; (iv) 1 − *x*, 1 − *y*, 1 − *z*.
Notes: *Cg*1 is the centroid of ring C9/C11/C12/N10/C14/C13, *Cg*2 is the centroid of ring C1–C4/C12/C11 and *Cg*3 is the centroid of ring C5–C8/C13/C14. *Cg*···*Cg* is the distance between ring centroids. The dihedral angle is that between the planes of rings CgI and CgJ. The interplanar distance is the perpendicular distance of CgI from ring J. The offset is computed as the third side of the right-angled triangle involving the *Cg*···*Cg* distance.

Fig. 1

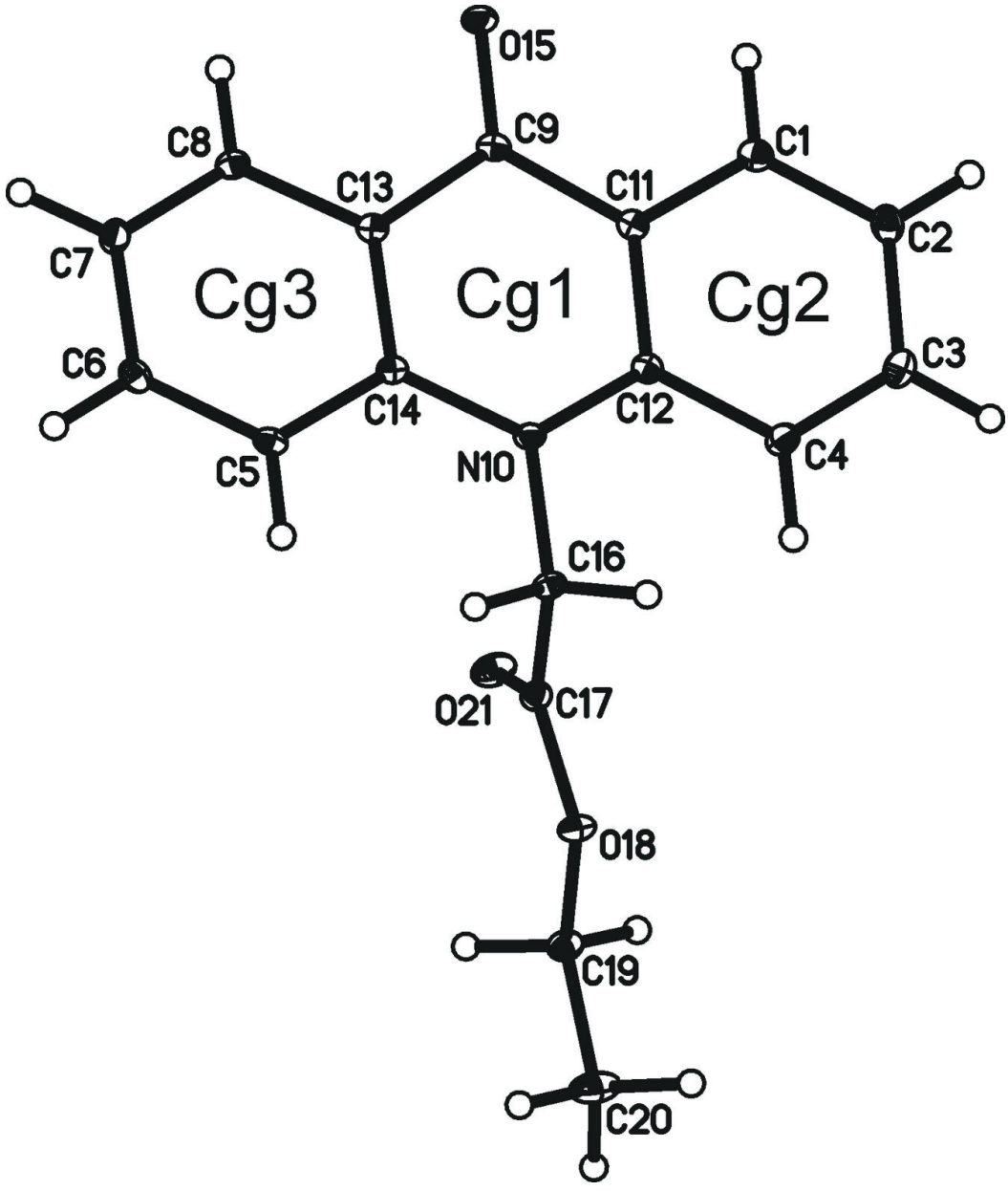

O15
C9
C8
C13
C11
C1
C7
Cg3
Cg1
Cg2
C2
C6
C14
C12
C3
C5
N10
C4
C16
O21
C17
O18
C19
C20

Fig. 2