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(*E*)-3-(Anthracen-9-yl)-1-(furan-2-yl)-prop-2-en-1-one[1]

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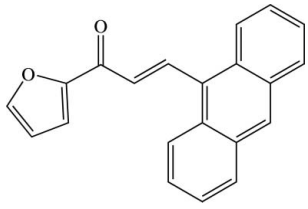
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.118; data-to-parameter ratio = 16.1.

In the molecule of the title heteroaryl chalcone derivative, $C_{21}H_{14}O_2$, the almost planar prop-2-en-1-one unit [r.m.s. deviation = 0.0087 (1) Å] forms dihedral angles of 5.81 (7) and 49.85 (6)°, respectively, with the furan ring and anthracene ring system. In the crystal structure, the molecules are linked into a two-dimensional network parallel to (100) by C—H···O hydrogen bonds and $\pi\cdots\pi$ interactions involving the furan rings [centroid–centroid distance = 3.7205 (6) Å].

Related literature

For background and applications of chalcones, see: Gaber *et al.* (2008); Niu *et al.* (2006); Xu *et al.* (2005). For related structures, see: Chantrapromma *et al.* (2009, 2010); Fun *et al.* (2009); Suwunwong *et al.* (2009). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{21}H_{14}O_2$
M_r = 298.32
Monoclinic, $P2_1/c$
a = 21.5743 (4) Å
b = 5.4571 (1) Å
c = 12.8394 (2) Å
β = 104.099 (1)°
V = 1466.09 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.55 × 0.25 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.955, T_{max} = 0.994
19468 measured reflections
4251 independent reflections
3549 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 1.03
4251 reflections
264 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.98 (2)	2.34 (2)	3.2871 (14)	165 (1)
C6—H6···O1^{i}	0.94 (2)	2.40 (2)	3.3366 (13)	173 (1)
C19—H19···O1^{ii}	0.98 (1)	2.47 (1)	3.3419 (13)	148 (1)

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

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5032).

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[1] This paper is dedicated to His Majesty King Bhumibol Adulyadej of Thailand (King Rama IX) for his sustainable development of the country.
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supporting information

Acta Cryst. (2010). E**66**, o800–o801 [doi:10.1107/S1600536810005982]

(*E*)-3-(Anthracen-9-yl)-1-(furan-2-yl)prop-2-en-1-one

Jirapa Horkaew, Thitipone Suwunwong, Suchada Chantrapromma, Chatchanok Karalai and Hoong-Kun Fun

S1. Comment

Chalcones have been studied for their wide range of applications including laser activity (Gaber *et al.*, 2008) and fluorescence properties (Niu *et al.*, 2006; Xu *et al.*, 2005). We have previously reported crystal structures of several chalcone derivatives containing the anthracene moiety which exist in *E* configuration (Suwunwong *et al.*, 2009) or *Z* configuration (Chantrapromma *et al.*, 2009, 2010; Fun *et al.*, 2009). The title compound was synthesized on account of its fluorescence properties. The crystal structure determination was undertaken to elucidate its conformation and to study the structure and fluorescence activity relationship.

The molecule of the title chalcone derivative (Fig. 1) exists in an *E* configuration with respect to the C6═C7 ethenyl bond, with a C5—C6—C7—C8 torsion angle of 178.00 (9)°. The anthracene ring system (C8–C21) is essentially planar (r.m.s. deviation = 0.0258 (1) Å). The prop-2-en-1-one unit (C5–C7/O1) is also planar (r.m.s. deviation = 0.0087 (1) Å; O1—C5—C6—C7 = 2.92 (15)°) and it forms dihedral angles of 5.81 (7) and 49.85 (6)°, respectively, with the furan ring and anthracene ring system. The interplanar angle between the furan ring and anthracene ring system is 48.53 (5)°. The bond distances show normal values (Allen *et al.*, 1987) and are comparable with those in closely related structures (Chantrapromma, Horkaew *et al.*, 2009; Chantrapromma, Suwunwong *et al.*, 2010; Fun *et al.*, 2009; Suwunwong *et al.*, 2009).

In the crystal structure, the molecules are linked into a two-dimensional network parallel to the (100) by C—H···O hydrogen bonds (Fig. 2 and Table 1) and $\pi\cdots\pi$ interactions between the furan rings at (x, y, z) and (-x, 1-y, -z) [centroid···centroid distance = 3.7205 (6) Å].

S2. Experimental

The title compound was synthesized by the condensation of anthracene-9-carbaldehyde (0.41 g, 2 mmol) with 2-furyl-methylketone (0.22 g, 2 mmol) in ethanol (30 ml) in the presence of 30 % aqueous NaOH (5 ml) at room temperature. The reaction mixture was stirred at 278 K for 3 h and then a yellow solid appeared was collected by filtration, washed with acetone and dried in air. Yellow plate-shaped single crystals of the title compound suitable for *X*-ray structure determination were recrystalized from acetone-ethanol (1:1 v/v) by slow evaporation of the solvent at room temperature after several days (m.p. 423-424 K).

S3. Refinement

All H atoms were located in a difference map and refined isotropically [C–H = 0.941 (15)–1.009 (14) Å].

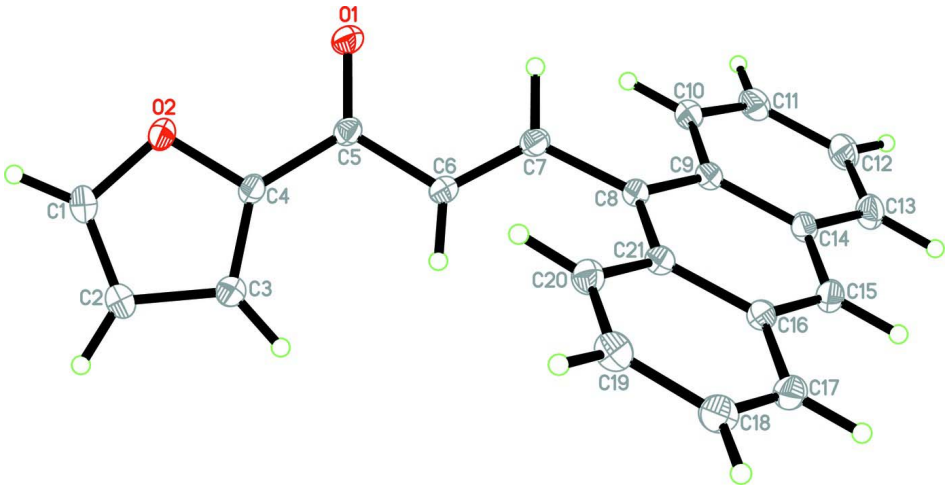

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

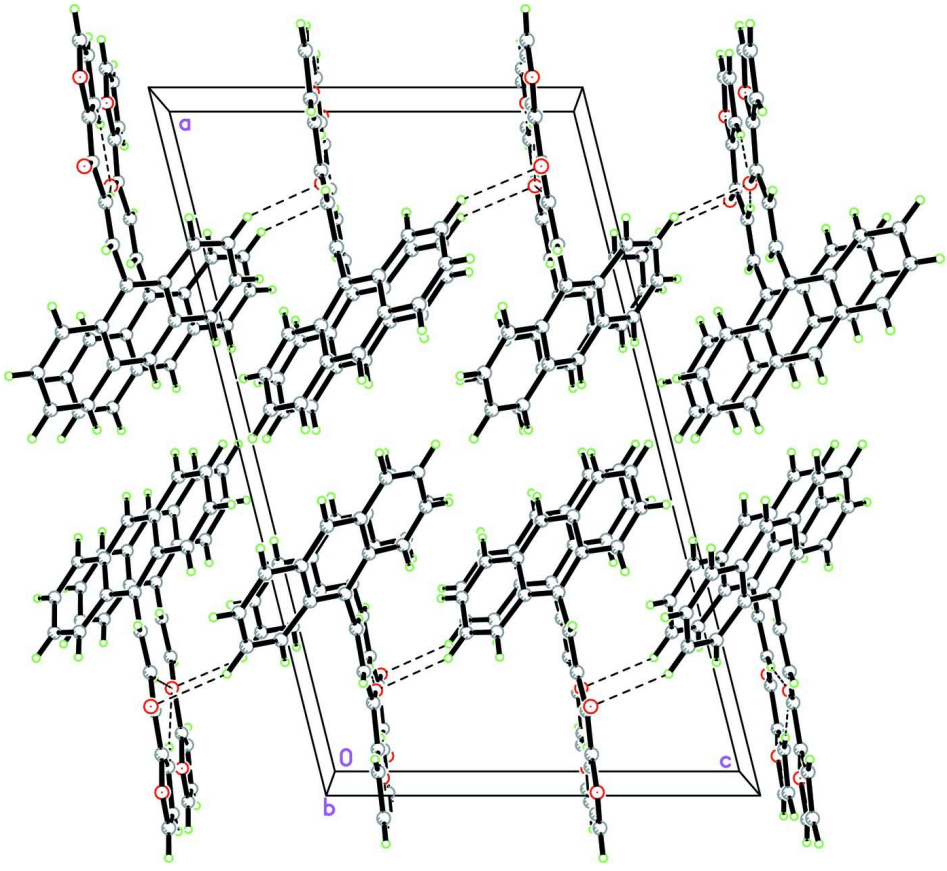

Figure 2

The crystal packing of the title compound viewed along the *b* axis. C—H···O hydrogen bonds are shown as dashed lines.

(*E*)-3-(anthracen-9-yl)-1-(furan-2-yl)prop-2-en-1-one

Crystal data

$C_{21}H_{14}O_2$
$M_r = 298.32$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 21.5743$ (4) Å
$b = 5.4571$ (1) Å
$c = 12.8394$ (2) Å
$\beta = 104.099$ (1)°
$V = 1466.09$ (4) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.352$ Mg m^{-3}
Melting point = 423–424 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4251 reflections
$\theta = 2.9$–$30.0°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Plate, yellow
0.55 × 0.25 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.955$, $T_{max} = 0.994$
19468 measured reflections
4251 independent reflections
3549 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.9°$
$h = -26 \rightarrow 30$
$k = -7 \rightarrow 7$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.118$
$S = 1.03$
4251 reflections
264 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.4737P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-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 120.0 (1) K.

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 $F^2 > \sigma(F^2)$ 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	0.13071 (4)	0.32065 (14)	0.15881 (6)	0.02003 (17)
O2	0.00592 (3)	0.46137 (14)	0.12589 (6)	0.01846 (17)

C1	−0.04942 (5)	0.5903 (2)	0.11274 (9)	0.0201 (2)
H1	−0.0880 (7)	0.489 (3)	0.1018 (12)	0.030 (4)*
C2	−0.03863 (5)	0.8346 (2)	0.11454 (9)	0.0208 (2)
H2	−0.0701 (8)	0.964 (3)	0.1084 (13)	0.034 (4)*
C3	0.02854 (5)	0.8641 (2)	0.12983 (8)	0.0177 (2)
H3	0.0517 (7)	1.019 (3)	0.1342 (11)	0.027 (4)*
C4	0.05367 (5)	0.63332 (19)	0.13651 (8)	0.0152 (2)
C5	0.11877 (5)	0.54141 (19)	0.15040 (8)	0.0150 (2)
C6	0.16862 (5)	0.72918 (19)	0.15159 (8)	0.0163 (2)
C7	0.22914 (5)	0.66214 (19)	0.15739 (8)	0.0159 (2)
C8	0.28183 (5)	0.83333 (19)	0.15569 (8)	0.01475 (19)
C9	0.34004 (5)	0.80973 (19)	0.23544 (8)	0.0153 (2)
C10	0.34956 (5)	0.6249 (2)	0.31680 (8)	0.0183 (2)
C11	0.40571 (5)	0.6100 (2)	0.39433 (9)	0.0214 (2)
C12	0.45582 (5)	0.7804 (2)	0.39679 (9)	0.0231 (2)
C13	0.44862 (5)	0.9614 (2)	0.32146 (9)	0.0214 (2)
C14	0.39083 (5)	0.9814 (2)	0.23836 (8)	0.0166 (2)
C15	0.38256 (5)	1.1693 (2)	0.16251 (8)	0.0181 (2)
C16	0.32655 (5)	1.19033 (19)	0.08122 (8)	0.0164 (2)
C17	0.31916 (5)	1.3816 (2)	0.00291 (9)	0.0201 (2)
C18	0.26502 (6)	1.3994 (2)	−0.07801 (9)	0.0218 (2)
C19	0.21559 (5)	1.2226 (2)	−0.08673 (8)	0.0209 (2)
C20	0.22049 (5)	1.0396 (2)	−0.01267 (8)	0.0183 (2)
C21	0.27525 (5)	1.01872 (19)	0.07639 (8)	0.0154 (2)
H6	0.1563 (7)	0.895 (3)	0.1471 (11)	0.021 (3)*
H7	0.2399 (6)	0.482 (3)	0.1653 (11)	0.019 (3)*
H10	0.3158 (7)	0.507 (3)	0.3176 (11)	0.024 (4)*
H11	0.4105 (8)	0.479 (3)	0.4498 (13)	0.035 (4)*
H12	0.4960 (7)	0.766 (3)	0.4544 (13)	0.033 (4)*
H13	0.4831 (8)	1.086 (3)	0.3216 (13)	0.032 (4)*
H15	0.4171 (7)	1.291 (3)	0.1670 (11)	0.024 (4)*
H17	0.3534 (7)	1.501 (3)	0.0097 (12)	0.027 (4)*
H18	0.2611 (8)	1.533 (3)	−0.1306 (13)	0.036 (4)*
H19	0.1780 (7)	1.232 (3)	−0.1469 (11)	0.025 (4)*
H20	0.1864 (7)	0.916 (3)	−0.0210 (11)	0.025 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0184 (4)	0.0134 (4)	0.0265 (4)	−0.0007 (3)	0.0020 (3)	0.0008 (3)
O2	0.0144 (3)	0.0166 (4)	0.0236 (4)	−0.0032 (3)	0.0031 (3)	0.0005 (3)
C1	0.0134 (5)	0.0248 (5)	0.0216 (5)	−0.0011 (4)	0.0031 (4)	0.0001 (4)
C2	0.0154 (5)	0.0222 (5)	0.0244 (5)	0.0021 (4)	0.0042 (4)	0.0002 (4)
C3	0.0165 (5)	0.0165 (5)	0.0196 (5)	−0.0007 (4)	0.0034 (4)	−0.0002 (4)
C4	0.0142 (4)	0.0148 (5)	0.0161 (4)	−0.0026 (4)	0.0027 (3)	0.0000 (3)
C5	0.0147 (4)	0.0143 (5)	0.0149 (4)	−0.0017 (3)	0.0016 (3)	−0.0006 (3)
C6	0.0161 (5)	0.0125 (4)	0.0199 (4)	−0.0013 (4)	0.0038 (4)	−0.0004 (4)
C7	0.0163 (5)	0.0139 (5)	0.0170 (4)	−0.0011 (4)	0.0030 (3)	−0.0004 (3)

C8	0.0136 (4)	0.0137 (4)	0.0175 (4)	−0.0003 (3)	0.0047 (3)	−0.0019 (3)
C9	0.0140 (4)	0.0155 (5)	0.0173 (4)	0.0008 (4)	0.0051 (3)	−0.0012 (4)
C10	0.0162 (5)	0.0180 (5)	0.0212 (5)	0.0012 (4)	0.0054 (4)	0.0007 (4)
C11	0.0190 (5)	0.0232 (5)	0.0219 (5)	0.0047 (4)	0.0049 (4)	0.0032 (4)
C12	0.0156 (5)	0.0286 (6)	0.0232 (5)	0.0024 (4)	0.0011 (4)	0.0001 (4)
C13	0.0139 (5)	0.0248 (6)	0.0245 (5)	−0.0009 (4)	0.0027 (4)	−0.0015 (4)
C14	0.0135 (4)	0.0177 (5)	0.0192 (4)	−0.0002 (4)	0.0050 (4)	−0.0026 (4)
C15	0.0157 (5)	0.0184 (5)	0.0213 (5)	−0.0025 (4)	0.0067 (4)	−0.0012 (4)
C16	0.0167 (5)	0.0153 (5)	0.0190 (4)	−0.0003 (4)	0.0075 (4)	−0.0014 (4)
C17	0.0217 (5)	0.0176 (5)	0.0234 (5)	−0.0010 (4)	0.0105 (4)	0.0013 (4)
C18	0.0259 (6)	0.0213 (5)	0.0207 (5)	0.0027 (4)	0.0106 (4)	0.0039 (4)
C19	0.0204 (5)	0.0243 (6)	0.0175 (5)	0.0024 (4)	0.0038 (4)	0.0011 (4)
C20	0.0170 (5)	0.0193 (5)	0.0184 (4)	−0.0003 (4)	0.0037 (4)	−0.0003 (4)
C21	0.0150 (4)	0.0149 (5)	0.0168 (4)	0.0006 (4)	0.0049 (3)	−0.0011 (4)

Geometric parameters (Å, º)

O1—C5	1.2312 (13)	C10—H10	0.973 (15)
O2—C1	1.3606 (13)	C11—C12	1.4209 (17)
O2—C4	1.3754 (12)	C11—H11	0.997 (17)
C1—C2	1.3526 (16)	C12—C13	1.3642 (17)
C1—H1	0.981 (16)	C12—H12	0.996 (16)
C2—C3	1.4235 (15)	C13—C14	1.4342 (14)
C2—H2	0.968 (17)	C13—H13	1.007 (16)
C3—C4	1.3654 (14)	C14—C15	1.3950 (15)
C3—H3	0.974 (15)	C15—C16	1.3959 (14)
C4—C5	1.4609 (14)	C15—H15	0.988 (15)
C5—C6	1.4827 (14)	C16—C17	1.4310 (15)
C6—C7	1.3406 (14)	C16—C21	1.4396 (14)
C6—H6	0.941 (15)	C17—C18	1.3645 (16)
C7—C8	1.4757 (14)	C17—H17	0.972 (15)
C7—H7	1.009 (14)	C18—C19	1.4225 (17)
C8—C21	1.4176 (14)	C18—H18	0.984 (17)
C8—C9	1.4196 (14)	C19—C20	1.3653 (15)
C9—C10	1.4303 (14)	C19—H19	0.975 (14)
C9—C14	1.4353 (14)	C20—C21	1.4346 (14)
C10—C11	1.3701 (15)	C20—H20	0.984 (15)
C1—O2—C4	105.84 (8)	C10—C11—H11	118.7 (9)
C2—C1—O2	111.43 (10)	C12—C11—H11	120.6 (9)
C2—C1—H1	134.0 (9)	C13—C12—C11	120.23 (10)
O2—C1—H1	114.6 (9)	C13—C12—H12	120.8 (9)
C1—C2—C3	106.20 (10)	C11—C12—H12	119.0 (9)
C1—C2—H2	127.0 (10)	C12—C13—C14	120.72 (10)
C3—C2—H2	126.8 (10)	C12—C13—H13	122.1 (9)
C4—C3—C2	106.24 (9)	C14—C13—H13	117.2 (9)
C4—C3—H3	127.2 (9)	C15—C14—C13	121.04 (10)
C2—C3—H3	126.6 (9)	C15—C14—C9	119.63 (9)

C3—C4—O2	110.29 (9)	C13—C14—C9	119.30 (10)
C3—C4—C5	132.80 (9)	C14—C15—C16	121.51 (10)
O2—C4—C5	116.90 (9)	C14—C15—H15	119.0 (8)
O1—C5—C4	121.40 (9)	C16—C15—H15	119.5 (8)
O1—C5—C6	122.66 (9)	C15—C16—C17	120.89 (10)
C4—C5—C6	115.93 (9)	C15—C16—C21	119.67 (9)
C7—C6—C5	120.41 (10)	C17—C16—C21	119.43 (9)
C7—C6—H6	121.6 (9)	C18—C17—C16	121.01 (10)
C5—C6—H6	118.0 (9)	C18—C17—H17	120.7 (9)
C6—C7—C8	124.74 (10)	C16—C17—H17	118.3 (9)
C6—C7—H7	117.9 (8)	C17—C18—C19	119.86 (10)
C8—C7—H7	117.4 (8)	C17—C18—H18	119.4 (9)
C21—C8—C9	119.94 (9)	C19—C18—H18	120.8 (9)
C21—C8—C7	121.30 (9)	C20—C19—C18	120.81 (10)
C9—C8—C7	118.76 (9)	C20—C19—H19	120.0 (9)
C8—C9—C10	122.36 (9)	C18—C19—H19	119.2 (9)
C8—C9—C14	119.68 (9)	C19—C20—C21	121.48 (10)
C10—C9—C14	117.92 (9)	C19—C20—H20	119.7 (8)
C11—C10—C9	121.13 (10)	C21—C20—H20	118.8 (8)
C11—C10—H10	118.9 (8)	C8—C21—C20	123.23 (9)
C9—C10—H10	119.9 (8)	C8—C21—C16	119.46 (9)
C10—C11—C12	120.68 (10)	C20—C21—C16	117.25 (9)

C4—O2—C1—C2	0.05 (12)	C12—C13—C14—C15	178.54 (10)
O2—C1—C2—C3	0.07 (13)	C12—C13—C14—C9	0.46 (16)
C1—C2—C3—C4	−0.16 (12)	C8—C9—C14—C15	−0.25 (15)
C2—C3—C4—O2	0.20 (11)	C10—C9—C14—C15	−177.91 (9)
C2—C3—C4—C5	179.04 (10)	C8—C9—C14—C13	177.85 (9)
C1—O2—C4—C3	−0.16 (11)	C10—C9—C14—C13	0.20 (15)
C1—O2—C4—C5	−179.20 (8)	C13—C14—C15—C16	179.91 (10)
C3—C4—C5—O1	176.89 (11)	C9—C14—C15—C16	−2.01 (16)
O2—C4—C5—O1	−4.33 (14)	C14—C15—C16—C17	−178.97 (10)
C3—C4—C5—C6	−4.22 (16)	C14—C15—C16—C21	1.51 (15)
O2—C4—C5—C6	174.56 (8)	C15—C16—C17—C18	178.56 (10)
O1—C5—C6—C7	2.92 (15)	C21—C16—C17—C18	−1.92 (16)
C4—C5—C6—C7	−175.95 (9)	C16—C17—C18—C19	−1.51 (17)
C5—C6—C7—C8	178.00 (9)	C17—C18—C19—C20	2.45 (17)
C6—C7—C8—C21	−49.44 (15)	C18—C19—C20—C21	0.14 (17)
C6—C7—C8—C9	130.63 (11)	C9—C8—C21—C20	173.77 (9)
C21—C8—C9—C10	−179.46 (9)	C7—C8—C21—C20	−6.16 (15)
C7—C8—C9—C10	0.48 (15)	C9—C8—C21—C16	−3.49 (15)
C21—C8—C9—C14	2.99 (15)	C7—C8—C21—C16	176.57 (9)
C7—C8—C9—C14	−177.07 (9)	C19—C20—C21—C8	179.21 (10)
C8—C9—C10—C11	−178.45 (10)	C19—C20—C21—C16	−3.47 (15)
C14—C9—C10—C11	−0.86 (15)	C15—C16—C21—C8	1.27 (15)
C9—C10—C11—C12	0.87 (17)	C17—C16—C21—C8	−178.26 (9)
C10—C11—C12—C13	−0.18 (18)	C15—C16—C21—C20	−176.16 (9)
C11—C12—C13—C14	−0.48 (18)	C17—C16—C21—C20	4.31 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.98 (2)	2.34 (2)	3.2871 (14)	165 (1)
C6—H6···O1^{i}	0.94 (2)	2.40 (2)	3.3366 (13)	173 (1)
C19—H19···O1^{ii}	0.98 (1)	2.47 (1)	3.3419 (13)	148 (1)

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