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Crystal structure of (*E*)-3-(2,4-dimethoxyphenyl)-1-(1-hydroxynaphthalen-2-yl)prop-2-en-1-one

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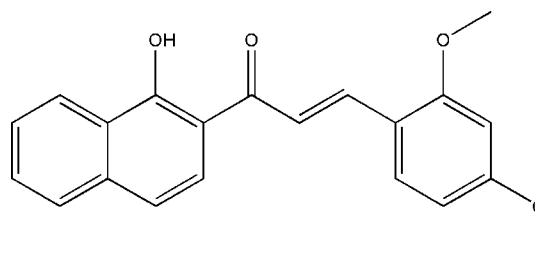
In the title compound, $C_{21}H_{18}O_4$, the $C=C$ bond of the central enone group adopts an *E* conformation. The dihedral angle formed by the benzene ring and the naphthalene ring system is $6.60(2)^\circ$. The methoxy groups on the benzene ring are essentially coplanar with the ring; the $C-C-O-C$ torsion angles being $1.6(2)$ and $-177.1(1)^\circ$. The hydroxy group attached to the naphthalene ring is involved in an intramolecular $O-H\cdots O$ hydrogen bond. The relative conformation of the two double bonds in the enone group is *s-cisoid*. In the crystal, weak $C-H\cdots O$ hydrogen bonds link the molecules into chains propagating along $[010]$.

Keywords: crystal structure; chalcone; enone; benzochalcone; naphthalene.

CCDC reference: 1019819

1. Related literature

For the synthesis and biological properties of chalcone derivatives, see: Fuchigami *et al.* (2014); Kim *et al.* (2014); Mai *et al.* (2014); Smit & D'Na (2014). For details concerning benzo-chalcone derivatives, see: Juvale *et al.* (2013); Shin *et al.* (2013). For related structures, see: Ahn *et al.* (2013); Lim & Koh (2013).



2. Experimental

2.1. Crystal data

$C_{21}H_{18}O_4$	$V = 3242.2(4) \text{ \AA}^3$
$M_r = 334.35$	$Z = 8$
Monoclinic, $C2/c$	Cu $K\alpha$ radiation
$a = 14.1148(9) \text{ \AA}$	$\mu = 0.77 \text{ mm}^{-1}$
$b = 14.7489(9) \text{ \AA}$	$T = 147 \text{ K}$
$c = 15.5929(10) \text{ \AA}$	$0.19 \times 0.12 \times 0.08 \text{ mm}$
$\beta = 92.804(4)^\circ$	

2.2. Data collection

Bruker Kappa APEX DUO CCD diffractometer	8800 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2007)	2755 independent reflections
$T_{\min} = 0.669$, $T_{\max} = 0.753$	2505 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.026$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.095$	
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
2755 reflections	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
232 parameters	

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O4-H4O\cdots O1$	0.97 (2)	1.59 (2)	2.499 (1)	155.1 (19)
$C10-H10A\cdots O1^i$	0.98	2.57	3.538 (2)	167
$C11-H11B\cdots O2^{ii}$	0.98	2.58	3.442 (2)	147

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2770).

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supporting information

Acta Cryst. (2014). E70, o1034–o1035 [doi:10.1107/S1600536814018704]

Crystal structure of (*E*)-3-(2,4-dimethoxyphenyl)-1-(1-hydroxynaphthalen-2-yl)prop-2-en-1-one

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S1. Synthesis and crystallization

To a solution of 2,4-dimethoxybenzaldehyde (830 mg, 5 mmol) in 50 ml of ethanol was added 1-hydroxy-2-acetonaphthone (930 mg, 1 mmol) and the temperature was adjusted to around 275–276 K in an ice-bath. To the cooled reaction mixture 5 ml of 50% aqueous KOH solution was added, and the reaction mixture was stirred at room temperature for 24 h. This mixture was poured into iced water (100 ml) and was acidified (pH = 3) with 6 N HCl solution to give a precipitate. Filtration and washing with water afforded the crude solid of the title compound (520 mg, 31%). Recrystallization of the solid from ethanol gave single crystals which were suitable for X-ray diffraction (M.p. 434–435 K).

S2. Refinement details

The OH H atom was located in a difference Fourier map and freely refined. The C-bound H atoms were placed in calculated positions and refined as riding atoms: C–H = 0.95 - 0.98 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and = $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

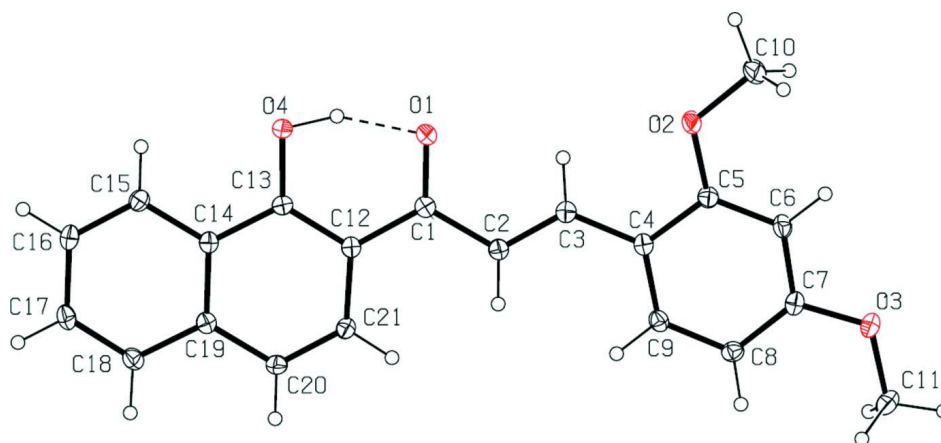
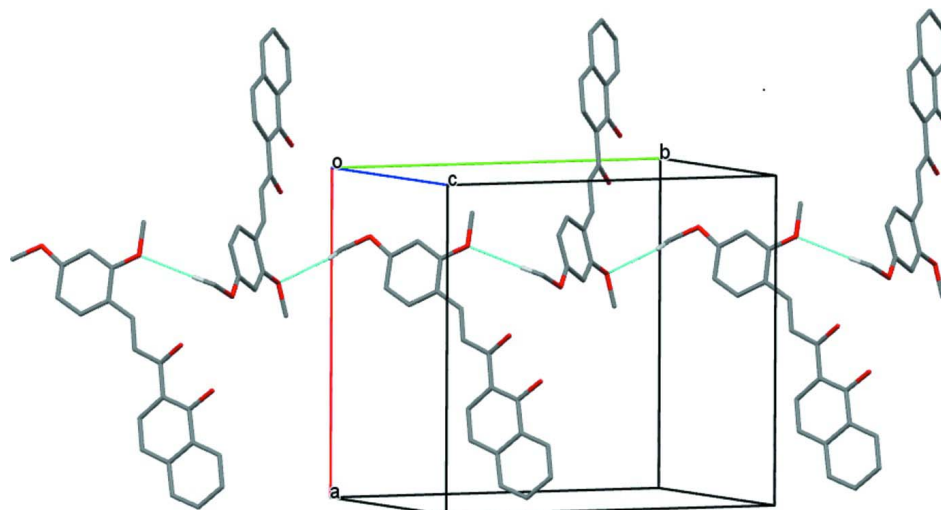


Figure 1

The molecular structure of the title molecule, with atom labelling. The displacement ellipsoids are drawn at the 50% probability level

**Figure 2**

A partial view along the *c* axis of the crystal packing of the title compound. The C—H···O hydrogen bonds are shown as dashed lines (see Table 1 for details; H atoms not involved in hydrogen bonding have been omitted for clarity).

(*E*)-3-(2,4-Dimethoxyphenyl)-1-(1-hydroxynaphthalen-2-yl)prop-2-en-1-one

Crystal data

C₂₁H₁₈O₄

M_r = 334.35

Monoclinic, *C2/c*

Hall symbol: -C 2yc

a = 14.1148 (9) Å

b = 14.7489 (9) Å

c = 15.5929 (10) Å

β = 92.804 (4)°

V = 3242.2 (4) Å³

Z = 8

F(000) = 1408

D_x = 1.370 Mg m⁻³

Cu *K*α radiation, λ = 1.54178 Å

Cell parameters from 4341 reflections

θ = 4.3–66.4°

μ = 0.77 mm⁻¹

T = 147 K

Needle, orange

0.19 × 0.12 × 0.08 mm

Data collection

Bruker Kappa APEX DUO CCD
diffractometer

Radiation source: Bruker ImuS

Multi-layer optics monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)

T_{min} = 0.669, *T_{max}* = 0.753

8800 measured reflections

2755 independent reflections

2505 reflections with *I* > 2σ(*I*)

R_{int} = 0.026

θ_{max} = 66.5°, θ_{min} = 4.3°

h = -16→16

k = -17→17

l = -13→18

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.036

wR (*F*²) = 0.095

S = 1.05

2755 reflections

232 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

H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 1.958P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.46036 (6)	0.17828 (6)	1.03233 (6)	0.0275 (2)
O2	0.19523 (6)	0.11183 (7)	0.85783 (7)	0.0345 (3)
O3	0.17234 (6)	-0.10692 (6)	0.63594 (6)	0.0266 (2)
O4	0.59612 (6)	0.24290 (6)	1.12130 (6)	0.0251 (2)
C1	0.51556 (9)	0.13224 (8)	0.98872 (8)	0.0210 (3)
C2	0.47622 (9)	0.07880 (8)	0.91593 (8)	0.0223 (3)
H2A	0.5173	0.0432	0.8832	0.027*
C3	0.38286 (9)	0.07983 (8)	0.89525 (8)	0.0213 (3)
H3A	0.3454	0.1177	0.9294	0.026*
C4	0.33198 (8)	0.03012 (8)	0.82693 (8)	0.0201 (3)
C5	0.23466 (9)	0.04712 (8)	0.80855 (8)	0.0226 (3)
C6	0.18419 (9)	0.00040 (9)	0.74439 (8)	0.0240 (3)
H6A	0.1190	0.0134	0.7324	0.029*
C7	0.22926 (9)	-0.06572 (9)	0.69744 (8)	0.0215 (3)
C8	0.32474 (9)	-0.08523 (9)	0.71418 (8)	0.0233 (3)
H8A	0.3557	-0.1302	0.6822	0.028*
C9	0.37358 (9)	-0.03735 (9)	0.77878 (8)	0.0222 (3)
H9A	0.4386	-0.0512	0.7908	0.027*
C10	0.09670 (11)	0.13031 (13)	0.84355 (13)	0.0516 (5)
H10A	0.0772	0.1763	0.8845	0.077*
H10B	0.0603	0.0746	0.8514	0.077*
H10C	0.0847	0.1528	0.7849	0.077*
C11	0.21279 (10)	-0.17857 (10)	0.58794 (9)	0.0339 (3)
H11A	0.1648	-0.2029	0.5466	0.051*
H11B	0.2349	-0.2269	0.6272	0.051*
H11C	0.2665	-0.1551	0.5571	0.051*
C12	0.61749 (8)	0.13277 (8)	1.01100 (8)	0.0193 (3)
C13	0.65294 (8)	0.18928 (8)	1.07709 (7)	0.0190 (3)
C14	0.75210 (8)	0.19224 (8)	1.10073 (7)	0.0193 (3)
C15	0.78867 (9)	0.25063 (8)	1.16617 (8)	0.0220 (3)
H15A	0.7470	0.2893	1.1952	0.026*
C16	0.88385 (9)	0.25175 (9)	1.18786 (8)	0.0251 (3)

H16A	0.9081	0.2916	1.2315	0.030*
C17	0.94584 (9)	0.19415 (9)	1.14567 (8)	0.0259 (3)
H17A	1.0117	0.1946	1.1616	0.031*
C18	0.91205 (9)	0.13741 (9)	1.08185 (8)	0.0246 (3)
H18A	0.9549	0.0991	1.0537	0.030*
C19	0.81422 (9)	0.13491 (8)	1.05720 (8)	0.0203 (3)
C20	0.77706 (9)	0.07710 (9)	0.99071 (8)	0.0228 (3)
H20A	0.8185	0.0382	0.9617	0.027*
C21	0.68288 (9)	0.07699 (8)	0.96827 (8)	0.0216 (3)
H21A	0.6599	0.0387	0.9229	0.026*
H4O	0.5337 (15)	0.2284 (14)	1.0965 (13)	0.059 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0193 (4)	0.0320 (5)	0.0312 (5)	0.0025 (4)	-0.0004 (4)	-0.0075 (4)
O2	0.0217 (5)	0.0350 (6)	0.0455 (6)	0.0096 (4)	-0.0106 (4)	-0.0179 (5)
O3	0.0286 (5)	0.0265 (5)	0.0242 (5)	-0.0033 (4)	-0.0046 (4)	-0.0038 (4)
O4	0.0202 (5)	0.0282 (5)	0.0267 (5)	0.0035 (4)	-0.0002 (4)	-0.0078 (4)
C1	0.0217 (6)	0.0192 (6)	0.0221 (6)	-0.0003 (5)	0.0010 (5)	0.0028 (5)
C2	0.0208 (6)	0.0227 (6)	0.0234 (6)	-0.0006 (5)	0.0006 (5)	-0.0010 (5)
C3	0.0229 (6)	0.0184 (6)	0.0224 (6)	-0.0006 (5)	-0.0001 (5)	0.0019 (5)
C4	0.0206 (6)	0.0188 (6)	0.0208 (6)	-0.0020 (5)	-0.0004 (5)	0.0037 (5)
C5	0.0228 (6)	0.0193 (6)	0.0254 (6)	0.0018 (5)	-0.0015 (5)	0.0003 (5)
C6	0.0207 (6)	0.0238 (7)	0.0270 (7)	0.0004 (5)	-0.0052 (5)	0.0009 (5)
C7	0.0251 (6)	0.0212 (6)	0.0179 (6)	-0.0055 (5)	-0.0019 (5)	0.0038 (5)
C8	0.0251 (6)	0.0234 (7)	0.0217 (6)	-0.0009 (5)	0.0046 (5)	0.0000 (5)
C9	0.0187 (6)	0.0255 (7)	0.0224 (6)	-0.0019 (5)	0.0012 (5)	0.0026 (5)
C10	0.0254 (8)	0.0575 (11)	0.0703 (12)	0.0182 (7)	-0.0136 (7)	-0.0335 (9)
C11	0.0387 (8)	0.0336 (8)	0.0291 (7)	-0.0041 (6)	-0.0006 (6)	-0.0114 (6)
C12	0.0201 (6)	0.0181 (6)	0.0197 (6)	-0.0007 (5)	-0.0004 (5)	0.0023 (5)
C13	0.0218 (6)	0.0168 (6)	0.0184 (6)	0.0011 (5)	0.0020 (5)	0.0020 (5)
C14	0.0209 (6)	0.0189 (6)	0.0178 (6)	-0.0012 (5)	-0.0009 (5)	0.0037 (5)
C15	0.0249 (6)	0.0215 (6)	0.0195 (6)	-0.0004 (5)	-0.0003 (5)	0.0008 (5)
C16	0.0266 (7)	0.0264 (7)	0.0218 (6)	-0.0045 (5)	-0.0051 (5)	0.0008 (5)
C17	0.0196 (6)	0.0320 (7)	0.0254 (6)	-0.0019 (5)	-0.0043 (5)	0.0039 (5)
C18	0.0204 (6)	0.0277 (7)	0.0255 (7)	0.0022 (5)	0.0000 (5)	0.0020 (5)
C19	0.0211 (6)	0.0207 (6)	0.0191 (6)	0.0001 (5)	-0.0004 (5)	0.0045 (5)
C20	0.0223 (6)	0.0224 (6)	0.0237 (6)	0.0030 (5)	0.0019 (5)	-0.0023 (5)
C21	0.0231 (6)	0.0204 (6)	0.0211 (6)	-0.0008 (5)	-0.0012 (5)	-0.0017 (5)

Geometric parameters (Å, °)

O1—C1	1.2580 (15)	C10—H10B	0.9800
O2—C5	1.3612 (16)	C10—H10C	0.9800
O2—C10	1.4239 (17)	C11—H11A	0.9800
O3—C7	1.3635 (15)	C11—H11B	0.9800
O3—C11	1.4299 (17)	C11—H11C	0.9800

O4—C13	1.3408 (15)	C12—C13	1.3987 (17)
O4—H4O	0.97 (2)	C12—C21	1.4258 (17)
C1—C12	1.4634 (17)	C13—C14	1.4306 (17)
C1—C2	1.4683 (18)	C14—C15	1.4133 (17)
C2—C3	1.3414 (18)	C14—C19	1.4152 (17)
C2—H2A	0.9500	C15—C16	1.3693 (18)
C3—C4	1.4537 (17)	C15—H15A	0.9500
C3—H3A	0.9500	C16—C17	1.4059 (19)
C4—C9	1.3936 (18)	C16—H16A	0.9500
C4—C5	1.4119 (17)	C17—C18	1.3680 (19)
C5—C6	1.3832 (18)	C17—H17A	0.9500
C6—C7	1.3919 (18)	C18—C19	1.4156 (17)
C6—H6A	0.9500	C18—H18A	0.9500
C7—C8	1.3902 (18)	C19—C20	1.4227 (18)
C8—C9	1.3858 (18)	C20—C21	1.3580 (17)
C8—H8A	0.9500	C20—H20A	0.9500
C9—H9A	0.9500	C21—H21A	0.9500
C10—H10A	0.9800		
C5—O2—C10	117.97 (11)	O3—C11—H11A	109.5
C7—O3—C11	117.44 (10)	O3—C11—H11B	109.5
C13—O4—H4O	102.7 (12)	H11A—C11—H11B	109.5
O1—C1—C12	119.77 (11)	O3—C11—H11C	109.5
O1—C1—C2	119.13 (11)	H11A—C11—H11C	109.5
C12—C1—C2	121.11 (11)	H11B—C11—H11C	109.5
C3—C2—C1	120.65 (11)	C13—C12—C21	118.15 (11)
C3—C2—H2A	119.7	C13—C12—C1	119.35 (11)
C1—C2—H2A	119.7	C21—C12—C1	122.50 (11)
C2—C3—C4	127.94 (12)	O4—C13—C12	121.93 (11)
C2—C3—H3A	116.0	O4—C13—C14	116.85 (11)
C4—C3—H3A	116.0	C12—C13—C14	121.22 (11)
C9—C4—C5	116.67 (11)	C15—C14—C19	119.82 (11)
C9—C4—C3	123.29 (11)	C15—C14—C13	121.53 (11)
C5—C4—C3	120.00 (11)	C19—C14—C13	118.65 (11)
O2—C5—C6	123.18 (11)	C16—C15—C14	120.33 (12)
O2—C5—C4	115.50 (11)	C16—C15—H15A	119.8
C6—C5—C4	121.32 (12)	C14—C15—H15A	119.8
C5—C6—C7	119.80 (11)	C15—C16—C17	120.18 (12)
C5—C6—H6A	120.1	C15—C16—H16A	119.9
C7—C6—H6A	120.1	C17—C16—H16A	119.9
O3—C7—C8	124.91 (11)	C18—C17—C16	120.48 (12)
O3—C7—C6	114.42 (11)	C18—C17—H17A	119.8
C8—C7—C6	120.67 (11)	C16—C17—H17A	119.8
C9—C8—C7	118.31 (12)	C17—C18—C19	120.94 (12)
C9—C8—H8A	120.8	C17—C18—H18A	119.5
C7—C8—H8A	120.8	C19—C18—H18A	119.5
C8—C9—C4	123.21 (12)	C14—C19—C18	118.24 (11)
C8—C9—H9A	118.4	C14—C19—C20	119.51 (11)

C4—C9—H9A	118.4	C18—C19—C20	122.24 (11)
O2—C10—H10A	109.5	C21—C20—C19	120.66 (11)
O2—C10—H10B	109.5	C21—C20—H20A	119.7
H10A—C10—H10B	109.5	C19—C20—H20A	119.7
O2—C10—H10C	109.5	C20—C21—C12	121.79 (11)
H10A—C10—H10C	109.5	C20—C21—H21A	119.1
H10B—C10—H10C	109.5	C12—C21—H21A	119.1
O1—C1—C2—C3	0.91 (18)	C2—C1—C12—C21	-4.86 (18)
C12—C1—C2—C3	-179.00 (11)	C21—C12—C13—O4	-179.06 (10)
C1—C2—C3—C4	-178.69 (11)	C1—C12—C13—O4	0.41 (17)
C2—C3—C4—C9	9.1 (2)	C21—C12—C13—C14	0.81 (17)
C2—C3—C4—C5	-173.07 (12)	C1—C12—C13—C14	-179.73 (10)
C10—O2—C5—C6	1.6 (2)	O4—C13—C14—C15	-1.54 (17)
C10—O2—C5—C4	-178.52 (14)	C12—C13—C14—C15	178.59 (11)
C9—C4—C5—O2	178.52 (11)	O4—C13—C14—C19	178.34 (10)
C3—C4—C5—O2	0.59 (17)	C12—C13—C14—C19	-1.53 (17)
C9—C4—C5—C6	-1.56 (18)	C19—C14—C15—C16	-0.24 (18)
C3—C4—C5—C6	-179.48 (11)	C13—C14—C15—C16	179.64 (11)
O2—C5—C6—C7	-179.17 (12)	C14—C15—C16—C17	-0.57 (19)
C4—C5—C6—C7	0.91 (19)	C15—C16—C17—C18	0.90 (19)
C11—O3—C7—C8	3.18 (17)	C16—C17—C18—C19	-0.38 (19)
C11—O3—C7—C6	-177.12 (11)	C15—C14—C19—C18	0.74 (17)
C5—C6—C7—O3	-179.88 (11)	C13—C14—C19—C18	-179.15 (11)
C5—C6—C7—C8	-0.17 (19)	C15—C14—C19—C20	-179.25 (11)
O3—C7—C8—C9	179.82 (11)	C13—C14—C19—C20	0.86 (17)
C6—C7—C8—C9	0.13 (18)	C17—C18—C19—C14	-0.43 (18)
C7—C8—C9—C4	-0.87 (19)	C17—C18—C19—C20	179.56 (12)
C5—C4—C9—C8	1.56 (18)	C14—C19—C20—C21	0.52 (18)
C3—C4—C9—C8	179.41 (11)	C18—C19—C20—C21	-179.47 (12)
O1—C1—C12—C13	-4.21 (17)	C19—C20—C21—C12	-1.29 (19)
C2—C1—C12—C13	175.70 (11)	C13—C12—C21—C20	0.62 (18)
O1—C1—C12—C21	175.23 (11)	C1—C12—C21—C20	-178.83 (12)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4O \cdots O1	0.97 (2)	1.59 (2)	2.499 (1)	155.1 (19)
C10—H10A \cdots O1 ⁱ	0.98	2.57	3.538 (2)	167
C11—H11B \cdots O2 ⁱⁱ	0.98	2.58	3.442 (2)	147

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