



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

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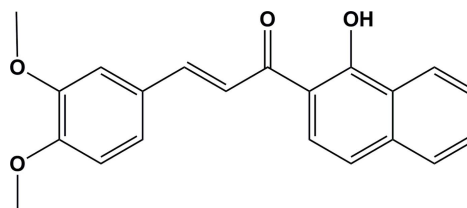
The molecular structure of the title compound, C₂₁H₁₈O₄, consists of a 3,4-dimethoxyphenyl ring and a naphthalene ring system linked *via* a prop-2-en-1-one spacer. The molecule is almost planar, with a dihedral angle between the benzene ring and the naphthalene ring system of 2.68 (12)°. There is an intramolecular O—H···O hydrogen bond involving the adjacent hydroxy and carbonyl groups. The molecule has an *E* conformation about the C=C bond and the carbonyl group is *syn* with respect to the C=C bond. In the crystal, molecules are linked by bifurcated C—H···(O,O) hydrogen bonds, enclosing an R₂¹(6) ring motif, and by a further C—H···O hydrogen bond, forming undulating sheets extending in *b*- and *c*-axis directions. There are π – π interactions between the sheets, involving inversion-related naphthalene and benzene rings [intercentroid distance = 3.7452 (17) Å], forming a three-dimensional structure.

Keywords: crystal structure; 1,3-diphenyl-2-propene-1-ones; chalcones; α,β -unsaturated carbonyl system; bifurcated C—H···O hydrogen bonds; O—H···O intramolecular hydrogen bond.

CCDC reference: 1051679

1. Related literature

For the biological activity of chalcone derivatives, see: Sashidhara *et al.* (2011); Go *et al.* (2005); Mukherjee *et al.* (2001); Liu *et al.* (2003); Sivakumar *et al.* (2007); Viana *et al.* (2003); Ducki *et al.* (1998); Rahman *et al.* (2007). For a related structure, see: Ahn *et al.* (2013). For the synthesis, see: Ezhilarasi *et al.* (2014); Sathya *et al.* (2014).



2. Experimental

2.1. Crystal data

C ₂₁ H ₁₈ O ₄	$V = 1707.5 (3) \text{ \AA}^3$
$M_r = 334.35$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.8784 (10) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 15.4108 (15) \text{ \AA}$	$T = 293 \text{ K}$
$c = 11.2288 (11) \text{ \AA}$	$0.30 \times 0.25 \times 0.20 \text{ mm}$
$\beta = 92.674 (2)^\circ$	

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer	34671 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2004)	3568 independent reflections
$T_{\min} = 0.973$, $T_{\max} = 0.982$	1992 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.051$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$	230 parameters
$wR(F^2) = 0.247$	H-atom parameters constrained
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
3568 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2A···O1	0.82	1.75	2.482 (3)	148
C7—H7···O3 ⁱ	0.93	2.57	3.368 (4)	144
C7—H7···O4 ⁱ	0.93	2.59	3.445 (4)	152
C18—H18···O2 ⁱⁱ	0.93	2.43	3.333 (4)	165

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 and SAINT (Bruker, 2004); data reduction: SAINT and XPREP (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: SHELXL2014 and PLATON (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5109).

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supporting information

Acta Cryst. (2015). E71, o371–o372 [https://doi.org/10.1107/S2056989015008087]

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

K. S. Ezhilarasi, D. Reuben Jonathan, R. Vasanthi, B. K. Revathi and G. Usha

S1. Synthesis and crystallization

The title compound was synthesized following the reported procedures (Ezhilarasi *et al.*, 2014; Sathya *et al.*, 2014).

S2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically and treated as riding atoms: C—H = 0.93–0.96 Å, O—H = 0.82 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{O}, \text{C})$ for other H atoms.

S3. Comment

Chalcones are 1,3-diphenyl-2-propene-1-ones, in which two aromatic rings are linked by a three carbon α,β -unsaturated carbonyl system. These are abundant in edible plants and are considered to be precursors of flavonoids and isoflavonoids (Rahman *et al.*, 2007). The presence of the enone functionality in the chalcone moiety confers biological activity upon it, such as antiinflammatory (Sashidhara *et al.*, 2011), antifungal (Go *et al.*, 2005) antioxidant (Mukherjee *et al.*, 2001), anti-malarial (Liu *et al.*, 2003) antituberculosis (Sivakumar *et al.*, 2007), analgesic (Viana *et al.*, 2003], and antitumor (Ducki *et al.*, 1998) activities. As part of our attempts to investigate the substituent effects of chalcones on molecular structures and hence activities, the title compound was synthesized and its crystal structure was determined.

The molecular structure of the title compound is shown in Fig. 1. The bond distances and angles are similar to those reported for a similar structure (Ahn *et al.*, 2013). The molecule is almost planar with a dihedral angle between the benzene and naphthalene rings of $2.65 (1)^\circ$. The torsion angles of $\text{C}20\text{—O}3\text{—C}16\text{—C}17 = 171.3 (3)^\circ$ and $\text{C}21\text{—O}4\text{—C}17\text{—C}16 = -174.0 (3)^\circ$, indicates the *trans* orientation of the two methoxy groups.

In the crystal, molecules are linked by bifurcated C—H \cdots (O,O) hydrogen bonds, enclosing an $R_2^1(6)$ ring motif, and a further C—H \cdots O hydrogen bond forming undulating sheets extending in the *b* and *c* directions. (Fig. 2 and Table 1). There are $\pi\text{—}\pi$ interactions between the sheets, involving inversion related naphthalene and benzene rings, resulting in a three-dimensional structure [$\text{Cg}2\cdots\text{Cg}3^i = 3.7452 (17) \text{ \AA}$; Cg2 and Cg3 are the centroids of rings and C14—C19; symmetry code: (i) $-x, -y+1, -z+1$].

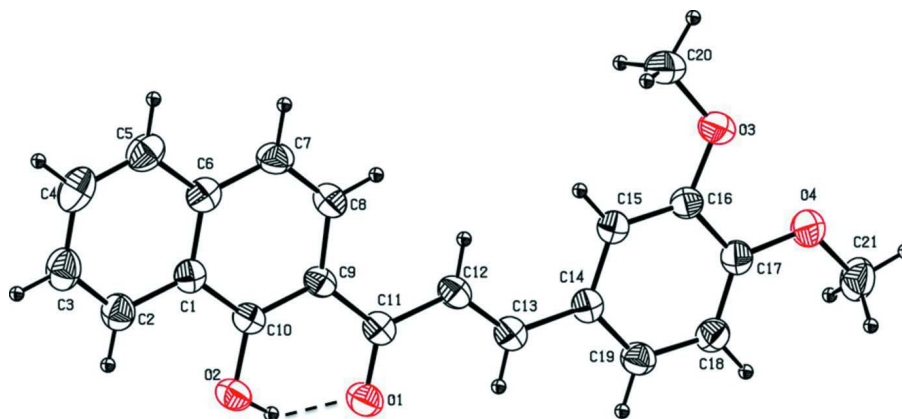


Figure 1

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

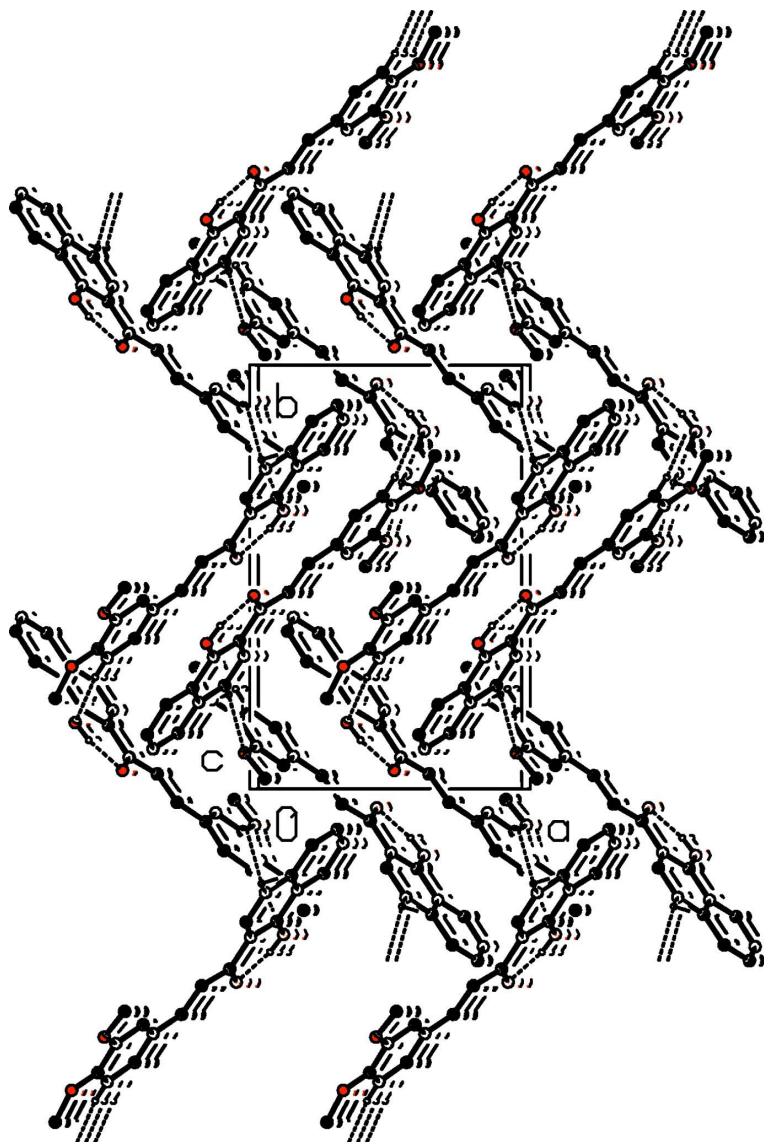


Figure 2

A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1 for details).

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

Crystal data

$C_{21}H_{18}O_4$

$M_r = 334.35$

Monoclinic, $P2_1/n$

$a = 9.8784$ (10) Å

$b = 15.4108$ (15) Å

$c = 11.2288$ (11) Å

$\beta = 92.674$ (2)°

$V = 1707.5$ (3) Å³

$Z = 4$

$F(000) = 704$

$D_x = 1.301$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3582 reflections

$\theta = 2.3$ – 26.6 °

$\mu = 0.09$ mm⁻¹

$T = 293$ K

Block, redish

$0.30 \times 0.25 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and φ scan

Absorption correction: multi-scan
(*SADABS*; Bruker, 2004)

$T_{\min} = 0.973$, $T_{\max} = 0.982$

34671 measured reflections

3568 independent reflections

1992 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\text{max}} = 26.6^\circ$, $\theta_{\text{min}} = 2.3^\circ$

$h = -12 \rightarrow 12$

$k = -19 \rightarrow 19$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.068$

$wR(F^2) = 0.247$

$S = 1.08$

3568 reflections

230 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.125P)^2 + 0.6413P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL2014* (Sheldrick,
2015), $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.212 (16)

Special details

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.

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	-0.0402 (2)	0.54423 (14)	0.26187 (18)	0.0626 (6)
O2	0.1324 (2)	0.65677 (13)	0.22420 (16)	0.0568 (6)
H2A	0.0852	0.6136	0.2119	0.085*
O3	-0.5102 (2)	0.41489 (16)	0.74635 (18)	0.0691 (7)
O4	-0.6337 (2)	0.28908 (15)	0.63862 (19)	0.0664 (7)
C1	0.1882 (3)	0.76195 (17)	0.3705 (2)	0.0468 (7)
C2	0.2833 (3)	0.8011 (2)	0.2974 (3)	0.0589 (8)
H2	0.2972	0.7784	0.2222	0.071*
C3	0.3548 (3)	0.8720 (2)	0.3366 (3)	0.0702 (10)
H3	0.4157	0.8983	0.2872	0.084*
C4	0.3372 (4)	0.9050 (2)	0.4501 (4)	0.0757 (10)
H4	0.3872	0.9530	0.4762	0.091*
C5	0.2474 (3)	0.8680 (2)	0.5235 (3)	0.0667 (9)
H5	0.2372	0.8907	0.5993	0.080*
C6	0.1701 (3)	0.79568 (19)	0.4855 (3)	0.0533 (8)
C7	0.0772 (3)	0.7555 (2)	0.5598 (3)	0.0599 (8)
H7	0.0658	0.7770	0.6361	0.072*
C8	0.0047 (3)	0.68597 (19)	0.5208 (3)	0.0552 (8)

H8	-0.0557	0.6606	0.5715	0.066*
C9	0.0170 (3)	0.65037 (17)	0.4059 (2)	0.0439 (7)
C10	0.1113 (3)	0.68788 (17)	0.3329 (2)	0.0445 (7)
C11	-0.0608 (3)	0.57509 (17)	0.3629 (2)	0.0479 (7)
C12	-0.1620 (3)	0.53573 (18)	0.4362 (3)	0.0505 (7)
H12	-0.1748	0.5582	0.5118	0.061*
C13	-0.2369 (3)	0.46840 (19)	0.3981 (3)	0.0514 (7)
H13	-0.2211	0.4483	0.3219	0.062*
C14	-0.3399 (3)	0.42287 (18)	0.4610 (2)	0.0484 (7)
C15	-0.3725 (3)	0.44398 (18)	0.5770 (2)	0.0482 (7)
H15	-0.3268	0.4891	0.6165	0.058*
C16	-0.4709 (3)	0.39945 (19)	0.6339 (2)	0.0494 (7)
C17	-0.5390 (3)	0.33076 (19)	0.5753 (3)	0.0502 (7)
C18	-0.5085 (3)	0.30938 (19)	0.4609 (3)	0.0549 (8)
H18	-0.5543	0.2644	0.4213	0.066*
C19	-0.4089 (3)	0.35528 (19)	0.4049 (3)	0.0565 (8)
H19	-0.3881	0.3402	0.3277	0.068*
C20	-0.4327 (4)	0.4750 (3)	0.8165 (3)	0.0800 (11)
H20A	-0.4646	0.4758	0.8960	0.120*
H20B	-0.4418	0.5318	0.7820	0.120*
H20C	-0.3391	0.4580	0.8191	0.120*
C21	-0.6958 (4)	0.2140 (2)	0.5876 (3)	0.0770 (10)
H21A	-0.7562	0.1892	0.6429	0.116*
H21B	-0.6273	0.1723	0.5700	0.116*
H21C	-0.7459	0.2295	0.5155	0.116*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0739 (15)	0.0598 (13)	0.0553 (13)	-0.0084 (11)	0.0161 (10)	-0.0062 (10)
O2	0.0683 (14)	0.0591 (13)	0.0440 (11)	-0.0023 (10)	0.0119 (10)	0.0030 (9)
O3	0.0801 (15)	0.0796 (16)	0.0486 (13)	-0.0189 (12)	0.0110 (11)	-0.0048 (10)
O4	0.0678 (14)	0.0696 (15)	0.0620 (13)	-0.0185 (11)	0.0060 (11)	0.0058 (11)
C1	0.0443 (15)	0.0449 (15)	0.0511 (16)	0.0067 (12)	-0.0003 (12)	0.0070 (12)
C2	0.0584 (19)	0.0583 (18)	0.0597 (18)	-0.0032 (15)	0.0013 (15)	0.0102 (14)
C3	0.064 (2)	0.065 (2)	0.081 (2)	-0.0109 (17)	0.0006 (18)	0.0163 (18)
C4	0.067 (2)	0.058 (2)	0.101 (3)	-0.0055 (17)	-0.016 (2)	-0.0005 (19)
C5	0.065 (2)	0.058 (2)	0.076 (2)	0.0049 (16)	-0.0085 (17)	-0.0108 (16)
C6	0.0528 (17)	0.0486 (16)	0.0580 (17)	0.0084 (13)	-0.0023 (14)	-0.0008 (13)
C7	0.0643 (19)	0.065 (2)	0.0507 (17)	0.0067 (16)	0.0061 (14)	-0.0116 (15)
C8	0.0566 (18)	0.0566 (18)	0.0536 (17)	0.0026 (14)	0.0134 (14)	0.0002 (14)
C9	0.0465 (15)	0.0433 (15)	0.0424 (14)	0.0090 (11)	0.0068 (12)	0.0019 (11)
C10	0.0476 (16)	0.0442 (15)	0.0417 (15)	0.0094 (12)	0.0031 (12)	0.0041 (11)
C11	0.0500 (16)	0.0440 (15)	0.0499 (16)	0.0081 (12)	0.0056 (12)	0.0051 (12)
C12	0.0536 (17)	0.0500 (16)	0.0485 (16)	0.0039 (13)	0.0094 (13)	0.0060 (12)
C13	0.0510 (17)	0.0515 (17)	0.0519 (16)	0.0057 (13)	0.0053 (13)	0.0049 (13)
C14	0.0455 (15)	0.0469 (16)	0.0529 (17)	0.0042 (12)	0.0027 (12)	0.0064 (12)
C15	0.0475 (16)	0.0463 (15)	0.0506 (16)	0.0017 (12)	0.0001 (12)	0.0034 (12)

C16	0.0506 (16)	0.0539 (17)	0.0435 (15)	0.0011 (13)	-0.0004 (12)	0.0036 (12)
C17	0.0481 (16)	0.0517 (16)	0.0507 (17)	0.0012 (13)	0.0007 (13)	0.0094 (13)
C18	0.0562 (18)	0.0526 (17)	0.0554 (18)	-0.0042 (14)	-0.0023 (14)	-0.0007 (13)
C19	0.0605 (18)	0.0581 (18)	0.0512 (17)	0.0002 (14)	0.0064 (14)	-0.0053 (14)
C20	0.093 (3)	0.092 (3)	0.056 (2)	-0.018 (2)	0.0084 (18)	-0.0162 (18)
C21	0.069 (2)	0.073 (2)	0.089 (3)	-0.0219 (18)	0.0025 (19)	0.0060 (19)

Geometric parameters (Å, °)

O1—C11	1.255 (3)	C9—C10	1.395 (4)
O2—C10	1.336 (3)	C9—C11	1.462 (4)
O2—H2A	0.8200	C11—C12	1.457 (4)
O3—C16	1.359 (3)	C12—C13	1.333 (4)
O3—C20	1.417 (4)	C12—H12	0.9300
O4—C17	1.361 (3)	C13—C14	1.446 (4)
O4—C21	1.418 (4)	C13—H13	0.9300
C1—C6	1.411 (4)	C14—C19	1.381 (4)
C1—C2	1.411 (4)	C14—C15	1.395 (4)
C1—C10	1.425 (4)	C15—C16	1.372 (4)
C2—C3	1.363 (5)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.402 (4)
C3—C4	1.391 (5)	C17—C18	1.374 (4)
C3—H3	0.9300	C18—C19	1.385 (4)
C4—C5	1.365 (5)	C18—H18	0.9300
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.406 (4)	C20—H20A	0.9600
C5—H5	0.9300	C20—H20B	0.9600
C6—C7	1.412 (4)	C20—H20C	0.9600
C7—C8	1.350 (4)	C21—H21A	0.9600
C7—H7	0.9300	C21—H21B	0.9600
C8—C9	1.412 (4)	C21—H21C	0.9600
C8—H8	0.9300		
C10—O2—H2A	109.5	C13—C12—C11	121.8 (3)
C16—O3—C20	117.4 (2)	C13—C12—H12	119.1
C17—O4—C21	118.0 (2)	C11—C12—H12	119.1
C6—C1—C2	119.4 (3)	C12—C13—C14	127.8 (3)
C6—C1—C10	118.6 (2)	C12—C13—H13	116.1
C2—C1—C10	122.0 (3)	C14—C13—H13	116.1
C3—C2—C1	120.2 (3)	C19—C14—C15	118.1 (3)
C3—C2—H2	119.9	C19—C14—C13	119.2 (3)
C1—C2—H2	119.9	C15—C14—C13	122.8 (3)
C2—C3—C4	120.3 (3)	C16—C15—C14	121.2 (3)
C2—C3—H3	119.9	C16—C15—H15	119.4
C4—C3—H3	119.9	C14—C15—H15	119.4
C5—C4—C3	120.9 (3)	O3—C16—C15	125.8 (3)
C5—C4—H4	119.6	O3—C16—C17	114.6 (2)
C3—C4—H4	119.6	C15—C16—C17	119.6 (3)

C4—C5—C6	120.5 (3)	O4—C17—C18	124.1 (3)
C4—C5—H5	119.8	O4—C17—C16	116.0 (3)
C6—C5—H5	119.8	C18—C17—C16	119.9 (3)
C5—C6—C1	118.7 (3)	C17—C18—C19	119.6 (3)
C5—C6—C7	121.8 (3)	C17—C18—H18	120.2
C1—C6—C7	119.5 (3)	C19—C18—H18	120.2
C8—C7—C6	120.4 (3)	C14—C19—C18	121.6 (3)
C8—C7—H7	119.8	C14—C19—H19	119.2
C6—C7—H7	119.8	C18—C19—H19	119.2
C7—C8—C9	122.5 (3)	O3—C20—H20A	109.5
C7—C8—H8	118.7	O3—C20—H20B	109.5
C9—C8—H8	118.7	H20A—C20—H20B	109.5
C10—C9—C8	117.7 (3)	O3—C20—H20C	109.5
C10—C9—C11	119.3 (2)	H20A—C20—H20C	109.5
C8—C9—C11	122.9 (2)	H20B—C20—H20C	109.5
O2—C10—C9	121.7 (2)	O4—C21—H21A	109.5
O2—C10—C1	117.0 (2)	O4—C21—H21B	109.5
C9—C10—C1	121.3 (2)	H21A—C21—H21B	109.5
O1—C11—C12	119.8 (3)	O4—C21—H21C	109.5
O1—C11—C9	119.6 (2)	H21A—C21—H21C	109.5
C12—C11—C9	120.5 (2)	H21B—C21—H21C	109.5
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C6—C1—C2—C3	-1.4 (4)	C8—C9—C11—O1	-176.6 (3)
C10—C1—C2—C3	179.9 (3)	C10—C9—C11—C12	-178.7 (2)
C1—C2—C3—C4	1.6 (5)	C8—C9—C11—C12	3.4 (4)
C2—C3—C4—C5	-0.7 (5)	O1—C11—C12—C13	-1.7 (4)
C3—C4—C5—C6	-0.4 (5)	C9—C11—C12—C13	178.3 (2)
C4—C5—C6—C1	0.5 (4)	C11—C12—C13—C14	179.7 (3)
C4—C5—C6—C7	179.5 (3)	C12—C13—C14—C19	178.6 (3)
C2—C1—C6—C5	0.4 (4)	C12—C13—C14—C15	-1.7 (5)
C10—C1—C6—C5	179.1 (3)	C19—C14—C15—C16	-0.4 (4)
C2—C1—C6—C7	-178.6 (3)	C13—C14—C15—C16	179.9 (2)
C10—C1—C6—C7	0.1 (4)	C20—O3—C16—C15	-8.0 (4)
C5—C6—C7—C8	-179.8 (3)	C20—O3—C16—C17	171.3 (3)
C1—C6—C7—C8	-0.9 (5)	C14—C15—C16—O3	-180.0 (3)
C6—C7—C8—C9	-0.2 (5)	C14—C15—C16—C17	0.8 (4)
C7—C8—C9—C10	2.0 (4)	C21—O4—C17—C18	6.1 (4)
C7—C8—C9—C11	179.9 (3)	C21—O4—C17—C16	-174.0 (3)
C8—C9—C10—O2	178.1 (2)	O3—C16—C17—O4	-0.3 (4)
C11—C9—C10—O2	0.0 (4)	C15—C16—C17—O4	179.0 (2)
C8—C9—C10—C1	-2.7 (4)	O3—C16—C17—C18	179.6 (3)
C11—C9—C10—C1	179.2 (2)	C15—C16—C17—C18	-1.0 (4)
C6—C1—C10—O2	-179.0 (2)	O4—C17—C18—C19	-179.1 (3)
C2—C1—C10—O2	-0.3 (4)	C16—C17—C18—C19	0.9 (4)
C6—C1—C10—C9	1.8 (4)	C15—C14—C19—C18	0.3 (4)
C2—C1—C10—C9	-179.6 (2)	C13—C14—C19—C18	180.0 (3)
C10—C9—C11—O1	1.3 (4)	C17—C18—C19—C14	-0.6 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O2—H2A···O1	0.82	1.75	2.482 (3)	148
C7—H7···O3 ⁱ	0.93	2.57	3.368 (4)	144
C7—H7···O4 ⁱ	0.93	2.59	3.445 (4)	152
C18—H18···O2 ⁱⁱ	0.93	2.43	3.333 (4)	165

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