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

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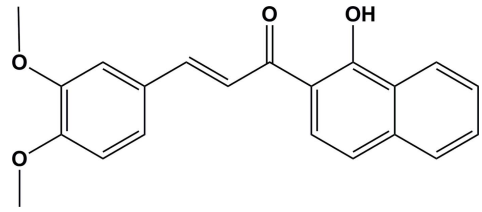
The molecular structure of the title compound, $C_{21}H_{18}O_4$, consists of a 3,4-dimethoxyphenyl ring and a naphthalene ring system linked *via* a prop-2-en-1-one spacer. The molecule is almost planar, with a dihedral angle between the benzene ring and the naphthalene ring system of 2.68 (12)°. There 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 $R_2^1(6)$ ring motif, and by a further C—H···O hydrogen bond, forming undulating sheets extending in *b*- and *c*-axis directions. There are $\pi$–$\pi$ 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; $\alpha,\beta$-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

$C_{21}H_{18}O_4$
$M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.30 × 0.25 × 0.20 mm

### 2.2. Data collection

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

### 2.3. Refinement

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| 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

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# 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 $U_{iso}$(H)= 1.5$U_{eq}$(C) for methyl H atoms and 1.2Ueq(O,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 $\alpha,\beta$-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)°. The torsion angles of C20—O3—C16—C17 = 171.3 (3)° and C21—O4—C17—C16 = -174.0 (3)°, indicates the *trans* orientation of the two methoxy groups.

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

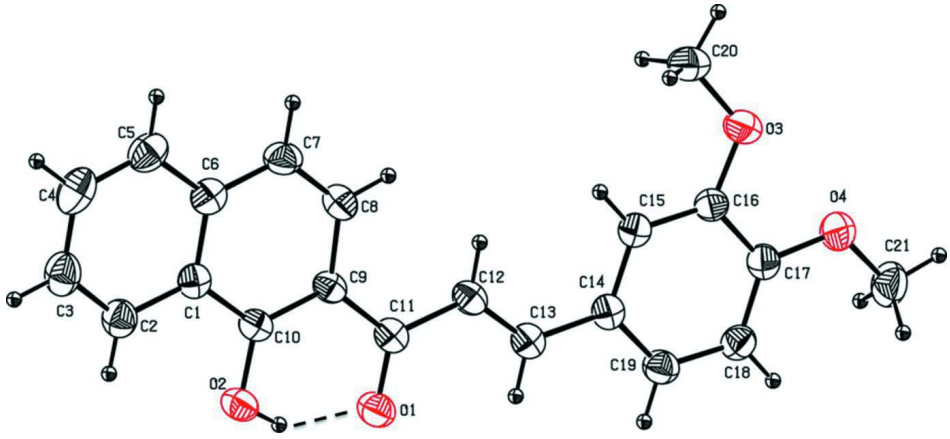


**Figure 1**

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

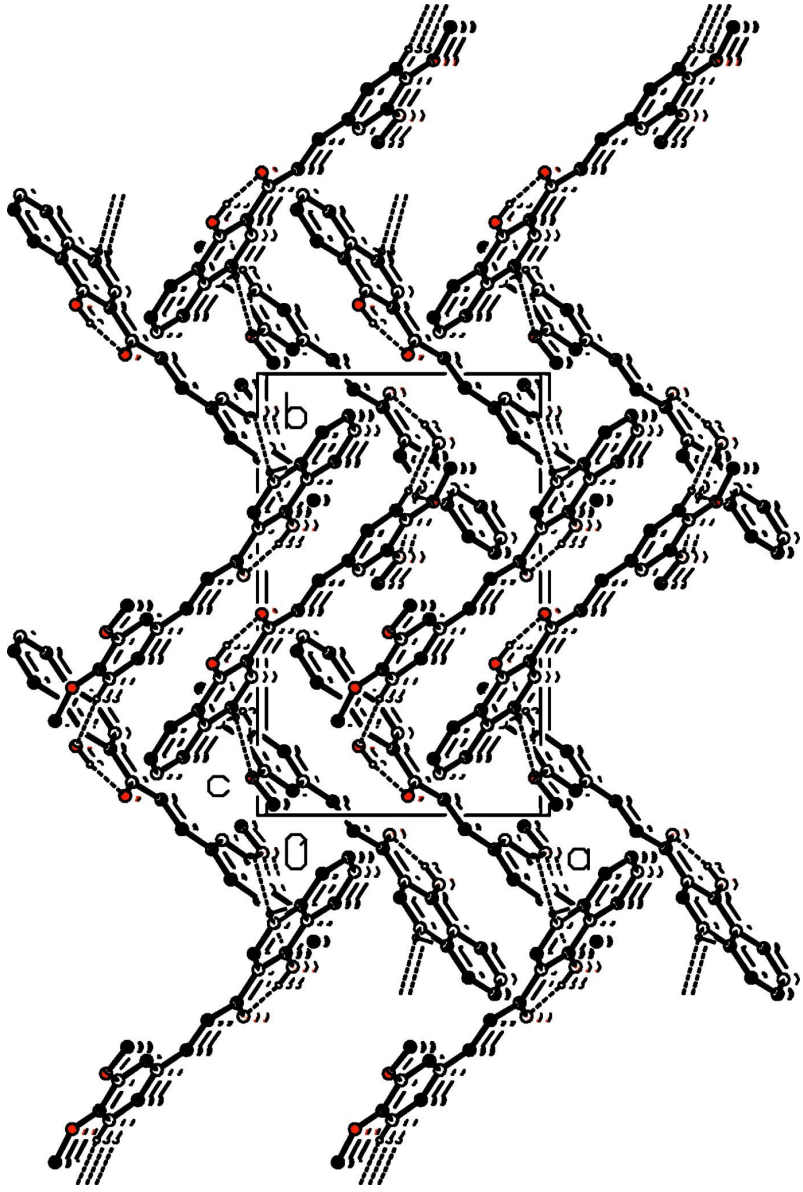


**Figure 2**

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*

$C_{21}H_{18}O_4$
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Monoclinic, $P2_1/n$
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$c = 11.2288$ (11) Å
$\beta = 92.674$ (2)°
$V = 1707.5$ (3) Å$^3$
$Z = 4$
$F(000) = 704$
$D_x = 1.301$ 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 × 0.25 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ 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 $I > 2\sigma(I)$
$R_{int}$ = 0.051
$\theta_{max}$ = 26.6°, $\theta_{min}$ = 2.3°
$h$ = −12→12
$k$ = −19→19
$l$ = −14→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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |

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| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*A*···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.