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# 1-(2-Hydroxy-4-methoxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one

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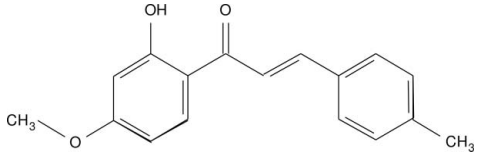
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.057; $wR$ factor = 0.184; data-to-parameter ratio = 12.8.

The molecule of the title compound, $C_{17}H_{16}O_3$, exists in the $E$ conformation with respect to the central C=C bond, is almost planar(r.m.s. deviation = 0.003 Å) and has an intramolecular O—H···O hydrogen bond, which generates an $S$(6) ring. In the crystal, molecules are linked by C—H···O interactions.

## Related literature

For the biological activity of compounds with a chalcone backbone, see: Jayashree *et al.* (2009); Epifano *et al.* (2007); Onyilagna *et al.* (1997); Satyanarayana *et al.* (2004); Deshpande *et al.* (1999); Hsieh *et al.* (2000); Khatib *et al.* (2005); Barford *et al.* (2002); Nielsen *et al.* (1995); Severi *et al.* (1998); Siva Kumar *et al.* (2007). For a related structure, see: Thippeswamy *et al.* (2010). For puckering parameters, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_{17}H_{16}O_3$
$M_r$ = 268.30
Monoclinic, $P2_1/c$
$a$ = 11.340 (2) Å
$b$ = 6.8350 (7) Å
$c$ = 20.449 (4) Å
$\beta$ = 117.710 (4)°
$V$ = 1403.2 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.26 × 0.24 × 0.22 mm

### Data collection

MacScience DIPLabo 32001 diffractometer
4137 measured reflections
2346 independent reflections
1502 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.184
$S$ = 1.05
2346 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O18—H18···O11 | 0.82 | 1.77 | 2.502 (3) | 148 |
| C13—H13···O18$^{i}$ | 0.93 | 2.56 | 3.282 (3) | 135 |

Symmetry code: (i) $x, y-1, z$.

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2240).

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# supporting information

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## 1-(2-Hydroxy-4-methoxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one

**G. B. Thippeswamy, D. Vijay Kumar, B. S. Jayashree, M. A. Sridhar and J. Shashidhara Prasad**

### S1. Comment

Chalcones (1,3-diarylpropenones) are well known intermediates for the synthesis of various heterocyclic compounds. The compounds with chalcone backbone have been reported to possess various biological activities such as anti-oxidant (Jayashree *et al.*, 2009), anti-inflammatory (Hsieh *et al.*, 2000), anti-cancer (Epifano *et al.*, 2007), anti-hyperglycemic (Satyanarayana *et al.*, 2004), anti-viral (Onyilagna *et al.*, 1997), anti-leishmanial (Nielsen *et al.*,1995), anti-tubercular (Siva Kumar *et al.*, 2007), immunomodulatory (Barford *et al.*, 2002), inhibition of various enzymes like leukotriene B (Deshpande *et al.*, 1999), tyrosinase kinase (Khatib *et al.*, 2005) and aldose reductase (Severi *et al.*, 1998) *etc*. The presence of a reactive alph, beta-unsaturated ketone function in chalcones is found to be responsible for their activity. In the present communication, we report the synthesis and crystal structure of substituted 2-hydroxy-chalcone. In the title compound, C17H16O3, the dihedral angle between the ring systems is 9.57 (13)°. The central prop-2-en-1-oneunit is planar (r.m.s. deviation = 0.003 Å) and is oriented at a dihedral angle of 2.46 (10)° with respect to the methoxyphenyl ring and at 7.46 (10)° with respect to the methylphenyl ring. The angles C2—C1—O11, C12—C1—O11 and C2—C1—C12 are 118.5 (3)°, 119.9 (2)° and 121.5 (2)° respectively which indicate that the position of C1 atom is nearly in trigonal geometry. The bond lengths and bond angles of the molecule are comparable with the values reported for 1-(2-hydroxy-5-methylphenyl)-3-(3-methylthiophen-2-yl) prop-2-en-1-one (Thippeswamy *et al.*,2010). The atoms C4, C7 in methyl-phenyl ring deviate by -0.018 (2) Å, -0.014 (3) Å, and the atoms C12, C15 in methoxyphenyl ring deviate by -0.002 (2) Å, -0.003 (3)Å respectively from Cremer and Pople plane (Cremer *et al.*,1975) which show that the two six-membered rings are in planar conformation. The packing of the molecules is characterized by intramolecular hydrogen bond of type O–H–O.

### S2. Experimental

The title compound was prepared by dissolving 2-hydroxy-4- methoxyacetophenone 0.05 m mol in 15 ml of ethanol taken in a conical flask. To this 5 ml of 20° aqueous sodium hydroxide was added and kept for stirring at room temperature. To this mixture, 4-methylbenzaldehyde 0.05 m mol was added and continued stirring till the completion of reaction. The progress of the reaction was monitored by TLC using n-hexane and ethyl acetate as solvent system. After completion of the reaction, the mixture was poured into ice cold water, mixed properly and acidified with dilute hydrochloric acid. The title compound separates as precipitate which was collected by filtration and crystallized from methanol. The compound was chafacterized by spectroscope technique. The IR spectrum was recorded in KBr on FTIR-8400 (Shimadzu). The 1H NMR spectrum was recorded in CdCl3 solution at 400 MHz on AMX 400 MHz High Resolution Multinuclear FT-NMR Spectrometer (Bruker) with tetramethylsilane (TMS) as internal standard.

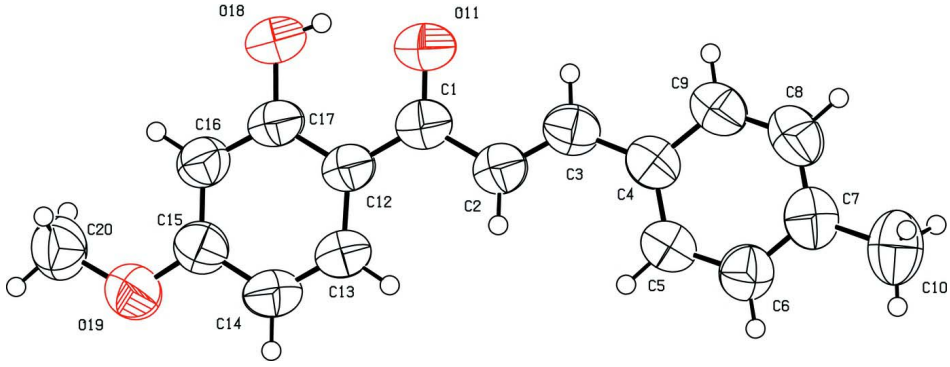


**Figure 1**

Crystal structure of the title compound with 50% probability displacement ellipsoids.

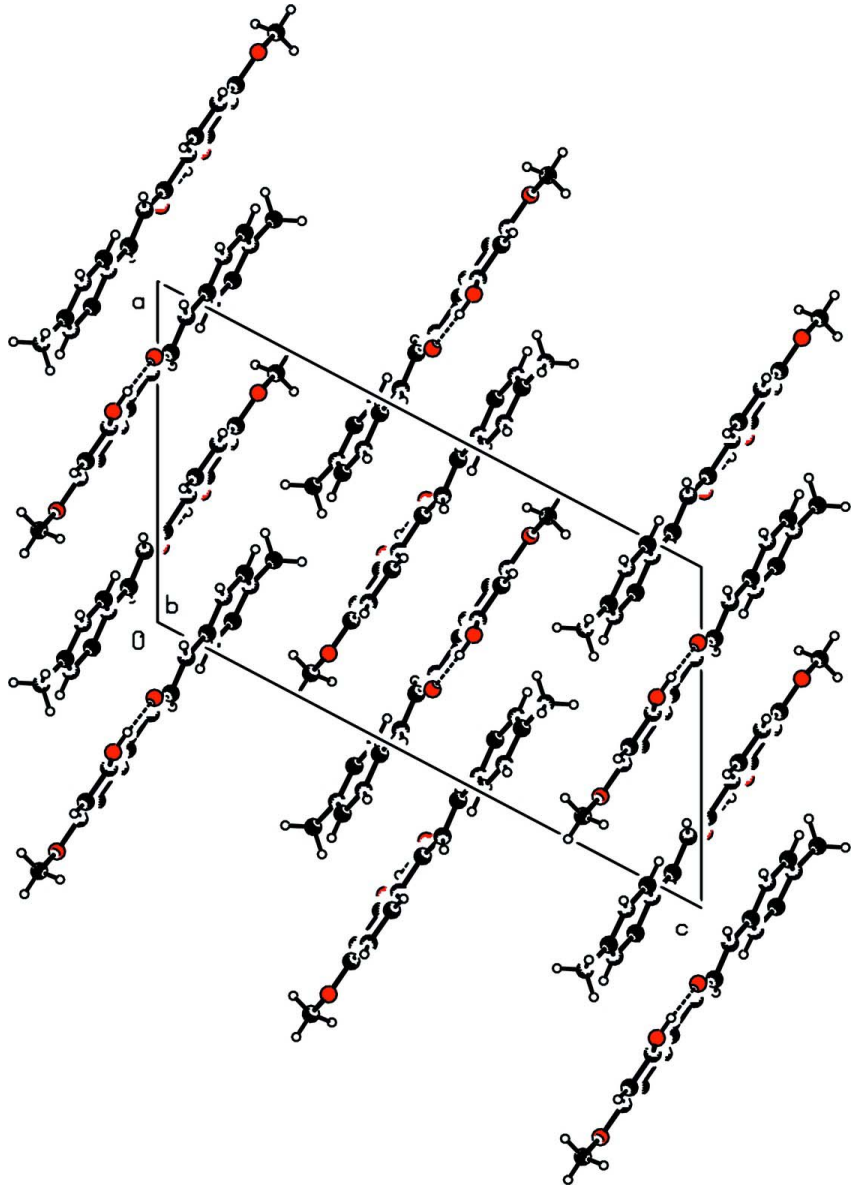


**Figure 2**

The packing of the title compound, viewed down the *b* axis.

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*Crystal data*

$C_{17}H_{16}O_3$
$M_r = 268.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.340\ (2)$ Å
$b = 6.8350\ (7)$ Å
$c = 20.449\ (4)$ Å
$\beta = 117.710\ (4)°$
$V = 1403.2\ (4)$ Å$^3$
$Z = 4$
$F(000) = 568$
$D_x = 1.270$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4137 reflections
$\theta = 2.2–25.0°$
$\mu = 0.09$ mm$^{-1}$
$T = 293$ K
Block, yellow
0.26 × 0.24 × 0.22 mm

*Data collection*

MacScience DIPLabo 32001 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ scans
4137 measured reflections
2346 independent reflections
1502 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -13 \rightarrow 13$
$k = -7 \rightarrow 7$
$l = -24 \rightarrow 24$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.184$
$S = 1.05$
2346 reflections
184 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
$w = 1/[\sigma^2(F_o^2) + (0.1052P)^2 + 0.0529P]$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.032 (8)

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O11 | 0.22698 (19) | 0.0248 (2) | 0.50576 (11) | 0.1003 (8) |
| O18 | 0.4503 (2) | 0.1776 (2) | 0.58182 (12) | 0.1010 (8) |
| O19 | 0.82822 (19) | −0.2381 (3) | 0.68536 (10) | 0.0952 (8) |
| C1 | 0.2778 (3) | −0.1418 (3) | 0.51232 (13) | 0.0769 (9) |
| C2 | 0.1894 (3) | −0.3084 (4) | 0.47598 (14) | 0.0781 (9) |
| C3 | 0.0588 (3) | −0.2910 (4) | 0.44711 (13) | 0.0788 (9) |
| C4 | −0.0439 (2) | −0.4376 (4) | 0.40885 (12) | 0.0745 (9) |
| C5 | −0.0165 (3) | −0.6329 (4) | 0.40093 (13) | 0.0771 (9) |
| C6 | −0.1187 (3) | −0.7615 (4) | 0.36199 (14) | 0.0829 (10) |
| C7 | −0.2504 (3) | −0.7042 (4) | 0.33000 (13) | 0.0853 (10) |
| C8 | −0.2767 (3) | −0.5123 (5) | 0.34017 (15) | 0.0941 (11) |
| C9 | −0.1758 (3) | −0.3830 (4) | 0.37904 (14) | 0.0876 (10) |
| C10 | −0.3608 (3) | −0.8452 (5) | 0.28614 (16) | 0.1111 (14) |
| C12 | 0.4201 (2) | −0.1668 (3) | 0.55578 (12) | 0.0695 (8) |
| C13 | 0.4837 (3) | −0.3491 (3) | 0.56897 (14) | 0.0777 (9) |
| C14 | 0.6169 (3) | −0.3701 (3) | 0.61167 (14) | 0.0833 (10) |

| | | | | |
|---|---|---|---|---|
| C15 | 0.6964 (3) | −0.2045 (4) | 0.64370 (14) | 0.0771 (9) |
| C16 | 0.6383 (3) | −0.0211 (3) | 0.63231 (14) | 0.0775 (10) |
| C17 | 0.5025 (3) | −0.0035 (3) | 0.58930 (13) | 0.0735 (9) |
| C20 | 0.9130 (3) | −0.0751 (4) | 0.71775 (17) | 0.1034 (12) |
| H2 | 0.22610 | −0.42800 | 0.47330 | 0.0940* |
| H3 | 0.02810 | −0.16830 | 0.45180 | 0.0950* |
| H5 | 0.07130 | −0.67620 | 0.42210 | 0.0920* |
| H6 | −0.09840 | −0.89080 | 0.35710 | 0.0990* |
| H8 | −0.36460 | −0.47010 | 0.32020 | 0.1130* |
| H9 | −0.19680 | −0.25530 | 0.38550 | 0.1050* |
| H10A | −0.42770 | −0.83800 | 0.30230 | 0.1670* |
| H10B | −0.32560 | −0.97570 | 0.29340 | 0.1670* |
| H10C | −0.39960 | −0.81220 | 0.23470 | 0.1670* |
| H13 | 0.43250 | −0.45980 | 0.54770 | 0.0930* |
| H14 | 0.65550 | −0.49360 | 0.61970 | 0.1000* |
| H16 | 0.69040 | 0.08900 | 0.65340 | 0.0930* |
| H18 | 0.36950 | 0.17260 | 0.55550 | 0.1510* |
| H20A | 0.90600 | 0.01340 | 0.67960 | 0.1550* |
| H20B | 1.00340 | −0.11930 | 0.74500 | 0.1550* |
| H20C | 0.88710 | −0.00910 | 0.75050 | 0.1550* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O11 | 0.0982 (14) | 0.0672 (11) | 0.1254 (16) | 0.0151 (9) | 0.0435 (12) | 0.0038 (10) |
| O18 | 0.1048 (15) | 0.0578 (10) | 0.1353 (16) | 0.0064 (9) | 0.0516 (12) | 0.0001 (9) |
| O19 | 0.0834 (14) | 0.0929 (13) | 0.1058 (14) | 0.0051 (10) | 0.0411 (11) | −0.0085 (10) |
| C1 | 0.0879 (18) | 0.0692 (14) | 0.0771 (15) | 0.0051 (12) | 0.0414 (14) | 0.0029 (11) |
| C2 | 0.0831 (18) | 0.0705 (14) | 0.0819 (16) | 0.0012 (12) | 0.0393 (13) | −0.0014 (11) |
| C3 | 0.0831 (19) | 0.0788 (15) | 0.0731 (15) | 0.0096 (13) | 0.0352 (14) | 0.0036 (12) |
| C4 | 0.0741 (17) | 0.0851 (16) | 0.0634 (14) | 0.0081 (12) | 0.0313 (12) | 0.0052 (11) |
| C5 | 0.0742 (16) | 0.0832 (16) | 0.0737 (15) | 0.0129 (12) | 0.0343 (13) | 0.0039 (12) |
| C6 | 0.0848 (19) | 0.0857 (16) | 0.0788 (16) | −0.0035 (14) | 0.0385 (14) | −0.0054 (13) |
| C7 | 0.0818 (19) | 0.1053 (19) | 0.0654 (15) | −0.0058 (15) | 0.0314 (13) | 0.0042 (13) |
| C8 | 0.0705 (17) | 0.114 (2) | 0.0881 (18) | 0.0105 (15) | 0.0288 (14) | 0.0126 (16) |
| C9 | 0.0760 (18) | 0.0920 (17) | 0.0909 (18) | 0.0163 (14) | 0.0355 (15) | 0.0095 (14) |
| C10 | 0.096 (2) | 0.141 (3) | 0.0857 (19) | −0.0278 (19) | 0.0334 (16) | −0.0083 (18) |
| C12 | 0.0817 (17) | 0.0599 (12) | 0.0743 (14) | 0.0020 (11) | 0.0426 (13) | 0.0004 (10) |
| C13 | 0.0884 (18) | 0.0621 (13) | 0.0843 (16) | 0.0032 (11) | 0.0415 (14) | −0.0045 (11) |
| C14 | 0.096 (2) | 0.0649 (14) | 0.0892 (17) | 0.0089 (12) | 0.0433 (15) | −0.0031 (12) |
| C15 | 0.0809 (18) | 0.0813 (15) | 0.0758 (15) | 0.0040 (13) | 0.0420 (14) | −0.0022 (12) |
| C16 | 0.0836 (19) | 0.0677 (14) | 0.0885 (17) | −0.0030 (12) | 0.0461 (15) | −0.0061 (12) |
| C17 | 0.0923 (19) | 0.0577 (13) | 0.0832 (15) | 0.0049 (11) | 0.0514 (14) | 0.0018 (11) |
| C20 | 0.087 (2) | 0.112 (2) | 0.107 (2) | −0.0097 (17) | 0.0417 (17) | −0.0209 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O11—C1 | 1.255 (3) | C14—C15 | 1.405 (4) |
| O18—C17 | 1.350 (3) | C15—C16 | 1.385 (4) |
| O19—C15 | 1.352 (4) | C16—C17 | 1.378 (5) |
| O19—C20 | 1.419 (4) | C2—H2 | 0.9300 |
| O18—H18 | 0.8200 | C3—H3 | 0.9300 |
| C1—C2 | 1.470 (4) | C5—H5 | 0.9300 |
| C1—C12 | 1.445 (4) | C6—H6 | 0.9300 |
| C2—C3 | 1.320 (5) | C8—H8 | 0.9300 |
| C3—C4 | 1.458 (4) | C9—H9 | 0.9300 |
| C4—C9 | 1.379 (4) | C10—H10A | 0.9600 |
| C4—C5 | 1.397 (4) | C10—H10B | 0.9600 |
| C5—C6 | 1.375 (4) | C10—H10C | 0.9600 |
| C6—C7 | 1.380 (5) | C13—H13 | 0.9300 |
| C7—C8 | 1.382 (4) | C14—H14 | 0.9300 |
| C7—C10 | 1.502 (4) | C16—H16 | 0.9300 |
| C8—C9 | 1.370 (5) | C20—H20A | 0.9600 |
| C12—C17 | 1.412 (3) | C20—H20B | 0.9600 |
| C12—C13 | 1.402 (3) | C20—H20C | 0.9600 |
| C13—C14 | 1.356 (5) | | |
| | | | |
| O11···O18 | 2.502 (3) | H2···C5 | 2.8200 |
| O18···O11 | 2.502 (3) | H2···C13 | 2.7100 |
| O18···C13$^{i}$ | 3.282 (3) | H2···H5 | 2.3100 |
| O11···H3 | 2.3900 | H2···H13 | 2.1300 |
| O11···H9$^{ii}$ | 2.8700 | H3···O11 | 2.3900 |
| O11···H5$^{i}$ | 2.7200 | H3···H9 | 2.3400 |
| O11···H18 | 1.7700 | H5···O11$^{v}$ | 2.7200 |
| O18···H13$^{i}$ | 2.5600 | H5···C2 | 2.8200 |
| C1···C7$^{iii}$ | 3.540 (4) | H5···H2 | 2.3100 |
| C3···C5$^{iii}$ | 3.398 (4) | H6···H10B | 2.3600 |
| C3···C4$^{iii}$ | 3.551 (4) | H8···H10A | 2.5900 |
| C4···C4$^{iii}$ | 3.488 (3) | H8···C10$^{viii}$ | 2.9800 |
| C4···C3$^{iii}$ | 3.551 (4) | H9···H3 | 2.3400 |
| C5···C3$^{iii}$ | 3.398 (4) | H9···O11$^{ii}$ | 2.8700 |
| C6···C20$^{iv}$ | 3.590 (5) | H10A···H8 | 2.5900 |
| C7···C1$^{iii}$ | 3.540 (4) | H10A···C12$^{iii}$ | 2.8600 |
| C10···C12$^{iii}$ | 3.596 (4) | H10A···C17$^{iii}$ | 2.9200 |
| C12···C10$^{iii}$ | 3.596 (4) | H10B···H6 | 2.3600 |
| C13···O18$^{v}$ | 3.282 (3) | H13···O18$^{v}$ | 2.5600 |
| C20···C6$^{iv}$ | 3.590 (5) | H13···C2 | 2.6600 |
| C1···H18 | 2.3700 | H13···H2 | 2.1300 |
| C2···H13 | 2.6600 | H16···C20 | 2.5000 |
| C2···H5 | 2.8200 | H16···H20A | 2.3100 |
| C4···H20C$^{vi}$ | 2.9800 | H16···H20C | 2.2900 |
| C5···H2 | 2.8200 | H18···O11 | 1.7700 |
| C5···H20C$^{vi}$ | 2.9100 | H18···C1 | 2.3700 |

| | | | |
|---|---|---|---|
| C6···H20C$^{vi}$ | 2.9600 | H20A···C16 | 2.7300 |
| C7···H20C$^{vi}$ | 3.0900 | H20A···H16 | 2.3100 |
| C10···H8$^{vii}$ | 2.9800 | H20C···C16 | 2.7300 |
| C12···H10A$^{iii}$ | 2.8600 | H20C···H16 | 2.2900 |
| C13···H2 | 2.7100 | H20C···C4$^{ix}$ | 2.9800 |
| C16···H20A | 2.7300 | H20C···C5$^{ix}$ | 2.9100 |
| C16···H20C | 2.7300 | H20C···C6$^{ix}$ | 2.9600 |
| C17···H10A$^{iii}$ | 2.9200 | H20C···C7$^{ix}$ | 3.0900 |
| C20···H16 | 2.5000 | | |

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|---|---|---|---|
| C15—O19—C20 | 118.1 (2) | C3—C2—H2 | 119.00 |
| C17—O18—H18 | 109.00 | C2—C3—H3 | 116.00 |
| O11—C1—C2 | 118.5 (3) | C4—C3—H3 | 116.00 |
| O11—C1—C12 | 119.9 (2) | C4—C5—H5 | 120.00 |
| C2—C1—C12 | 121.5 (2) | C6—C5—H5 | 120.00 |
| C1—C2—C3 | 121.1 (3) | C5—C6—H6 | 119.00 |
| C2—C3—C4 | 128.9 (3) | C7—C6—H6 | 119.00 |
| C3—C4—C9 | 118.9 (3) | C7—C8—H8 | 119.00 |
| C5—C4—C9 | 117.5 (3) | C9—C8—H8 | 119.00 |
| C3—C4—C5 | 123.6 (3) | C4—C9—H9 | 119.00 |
| C4—C5—C6 | 120.3 (3) | C8—C9—H9 | 119.00 |
| C5—C6—C7 | 121.9 (3) | C7—C10—H10A | 110.00 |
| C6—C7—C8 | 117.4 (3) | C7—C10—H10B | 109.00 |
| C6—C7—C10 | 121.3 (3) | C7—C10—H10C | 109.00 |
| C8—C7—C10 | 121.4 (3) | H10A—C10—H10B | 109.00 |
| C7—C8—C9 | 121.3 (3) | H10A—C10—H10C | 109.00 |
| C4—C9—C8 | 121.6 (3) | H10B—C10—H10C | 109.00 |
| C1—C12—C13 | 123.4 (2) | C12—C13—H13 | 119.00 |
| C1—C12—C17 | 120.2 (2) | C14—C13—H13 | 119.00 |
| C13—C12—C17 | 116.4 (2) | C13—C14—H14 | 120.00 |
| C12—C13—C14 | 122.5 (2) | C15—C14—H14 | 120.00 |
| C13—C14—C15 | 119.8 (2) | C15—C16—H16 | 120.00 |
| O19—C15—C16 | 124.1 (3) | C17—C16—H16 | 120.00 |
| C14—C15—C16 | 119.9 (3) | O19—C20—H20A | 109.00 |
| O19—C15—C14 | 116.0 (3) | O19—C20—H20B | 109.00 |
| C15—C16—C17 | 119.3 (2) | O19—C20—H20C | 110.00 |
| O18—C17—C16 | 117.0 (2) | H20A—C20—H20B | 109.00 |
| C12—C17—C16 | 122.1 (2) | H20A—C20—H20C | 110.00 |
| O18—C17—C12 | 120.9 (3) | H20B—C20—H20C | 109.00 |
| C1—C2—H2 | 119.00 | | |

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| C20—O19—C15—C16 | −1.9 (4) | C5—C6—C7—C10 | 178.6 (3) |
| C20—O19—C15—C14 | 178.8 (3) | C10—C7—C8—C9 | −178.8 (3) |
| C12—C1—C2—C3 | 168.4 (3) | C6—C7—C8—C9 | 1.5 (4) |
| O11—C1—C12—C13 | 176.6 (3) | C7—C8—C9—C4 | 0.9 (4) |
| C2—C1—C12—C13 | −2.5 (4) | C17—C12—C13—C14 | 0.2 (4) |
| C2—C1—C12—C17 | 179.3 (3) | C1—C12—C13—C14 | −178.0 (3) |
| O11—C1—C12—C17 | −1.7 (4) | C13—C12—C17—O18 | −178.0 (2) |

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| O11—C1—C2—C3 | −10.7 (4) | C13—C12—C17—C16 | 0.4 (4) |
| C1—C2—C3—C4 | 179.5 (2) | C1—C12—C17—O18 | 0.4 (4) |
| C2—C3—C4—C9 | −176.0 (3) | C1—C12—C17—C16 | 178.8 (3) |
| C2—C3—C4—C5 | 4.5 (4) | C12—C13—C14—C15 | −0.9 (4) |
| C3—C4—C5—C6 | −177.9 (3) | C13—C14—C15—C16 | 0.8 (4) |
| C5—C4—C9—C8 | −2.9 (4) | C13—C14—C15—O19 | −179.9 (3) |
| C9—C4—C5—C6 | 2.6 (4) | O19—C15—C16—C17 | −179.4 (3) |
| C3—C4—C9—C8 | 177.6 (3) | C14—C15—C16—C17 | −0.2 (4) |
| C4—C5—C6—C7 | −0.4 (4) | C15—C16—C17—O18 | 178.0 (3) |
| C5—C6—C7—C8 | −1.7 (4) | C15—C16—C17—C12 | −0.5 (4) |

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*, −*y*−1, −*z*+1; (iv) −*x*+1, −*y*−1, −*z*+1; (v) *x*, *y*−1, *z*; (vi) *x*−1, −*y*−1/2, *z*−1/2; (vii) −*x*−1, *y*−1/2, −*z*+1/2; (viii) −*x*−1, *y*+1/2, −*z*+1/2; (ix) *x*+1, −*y*−1/2, *z*+1/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O18—H18···O11 | 0.82 | 1.77 | 2.502 (3) | 148 |
| C3—H3···O11 | 0.93 | 2.39 | 2.758 (3) | 103 |
| C13—H13···O18$^{v}$ | 0.93 | 2.56 | 3.282 (3) | 135 |

Symmetry code: (v) *x*, *y*−1, *z*.