Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Naphthalen-1-yl){2-[(5,6,7,8-tetrahydronaphthalen-2-yl)carbonyl]phenyl}methanone

J. Kanchanadevi,[a] G. Anbalagan,[b] R. Sivasakthikumaran,[c] A. K. Mohanakrishnan,[c] B. Gunasekaran[d] and V. Manivannan[e]*

[a]Department of Physics, Velammal Institute of Technology, Panchetty, Chennai 601 204, India, [b]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, [c]Department of Organic Chemistry, University of Madras, Maraimalai Campus, Chennai 600 025, India, [d]Department of Physics & Nano Technology, SRM University, SRM Nagar, Kattankulathur, Kancheepuram Dist, Chennai 603 203 Tamil Nadu, India, and [e]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamil Nadu, India
Correspondence e-mail: phdguna@gmail.com, crystallography2010@gmail.com

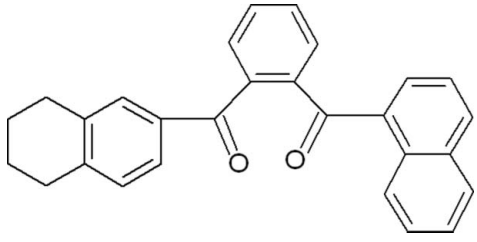
Received 14 June 2013; accepted 30 June 2013

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.100; data-to-parameter ratio = 18.4.

The title compound $C_{28}H_{22}O_2$, basically consists of three ring systems, *viz*. a central benzene ring, with a lateral napthalene group to which it subtends a dihedral angle of 66.56 (4)° and a tetrahydropyran ring exhibiting a half-chair conformation. The molecular structure is stabilized by a weak intramolecular C—H···O interaction, while the crystal packing features weak C—H···π contacts.

Related literature

For the biological activity of diketones, see: Bennett *et al.* (1999); Sugawara *et al.* (2001). For related structures, see: Jagadeesan *et al.* (2011, 2013)



Experimental

Crystal data

$C_{28}H_{22}O_2$
M_r = 390.46
Orthorhombic, $P2_12_12_1$
a = 10.5625 (5) Å
b = 13.6374 (8) Å
c = 14.4927 (8) Å
V = 2087.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.985, T_{max} = 0.989
13047 measured reflections
4998 independent reflections
3511 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.100
S = 1.03
4998 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

*Cg*3 is the centroid of the C12–C17 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1	0.93	2.29	2.856 (2)	118
C4—H4···*Cg*3^{i}	0.93	2.54	3.419 (1)	159
C25—H25*A*···*Cg*3^{ii}	0.97	2.94	3.849 (5)	157

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2509).

References

Bennett, I., Broom, N. J. P., Cassels, R., Elder, J. S., Masson, N. D. & O'Hanlon, P. J. (1999). *Bioorg. Med. Chem. Lett.* **9**, 1847–1852.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Jagadeesan, G., Sethusankar, K., Sivasakthikumaran, R. & Mohanakrishnan, A. K. (2011). *Acta Cryst.* E**67**, o3036.
Jagadeesan, G., Sethusankar, K., Sivasakthikumaran, R. & Mohanakrishnan, A. K. (2013). *Acta Cryst.* E**69**, o26.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Sugawara, Y., Kawai, H., Matsumoto, T., Okano, K. & Takizawa, S. (2001). US Patent No. 6184245 B1.

supporting information

Acta Cryst. (2013). E**69**, o1201 [doi:10.1107/S1600536813018035]

(Naphthalen-1-yl){2-[(5,6,7,8-tetrahydronaphthalen-2-yl)carbonyl]phenyl}-methanone

J. Kanchanadevi, G. Anbalagan, R. Sivasakthikumaran, A. K. Mohanakrishnan, B. Gunasekaran and V. Manivannan

S1. Comment

In recent days diketones and their derivatives are very important on account of their wide range of applications in biology and medicine. They are known to exhibit antioxidant, antitumour and antibacterial activities (Bennett *et al.*, 1999). Also they are useful as hematopoietic agents in medicine, in particular, in the treatment of cancer, chemotherapy, radiotherapy and drug therapy (Sugawara *et al.*, 2001).

The geometric parameters of the title molecule (Fig. 1) agree well with those of reported similar structures (Jagadeesan *et al.*, 2011, 2013). The central phenyl ring (C1—C6) makes a dihedral angle of 66.56 (4) ° with the napthelene ring (C8—C17) system, while the tetrahydropyran ring exhibits a half-chair conformation.

The molecular structure is stabilized by a weak intramolecular a C—H···O interaction and the crystal packing is controlled by weak C—H···π contacts (Table 1).

S2. Experimental

To a stirred solution of benzo[*c*]furan (1.0 g, 2.67 mmol) in dry THF (20 ml), lead tetraacetate (LTA) (1.18 g, 2.66 mmol) was added and then stirred at 50 ° C for half an hour. The reaction mixture was then poured into water (200 ml) and extracted with ethyl acetate (2 *x* 20 ml), washed with brine solution and dried (Na2SO4). Removal of solvent in vacuum followed by crystallization from methanol furnished the compound as a colourless solid with a Yield of 94%.

S3. Refinement

H atoms were positioned geometrically and refined using the riding model with $(C—H)_{aromatic}$ = 0.93 Å and $(C—H)_{CH2}$ 0.97 Å. In all cases $U_{iso}(H)$ = 1.2Ueq(C.

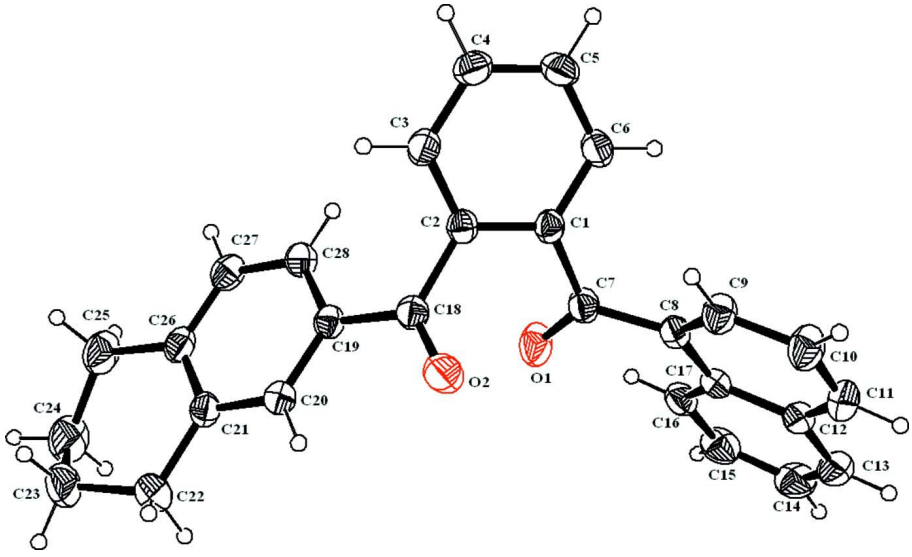


Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

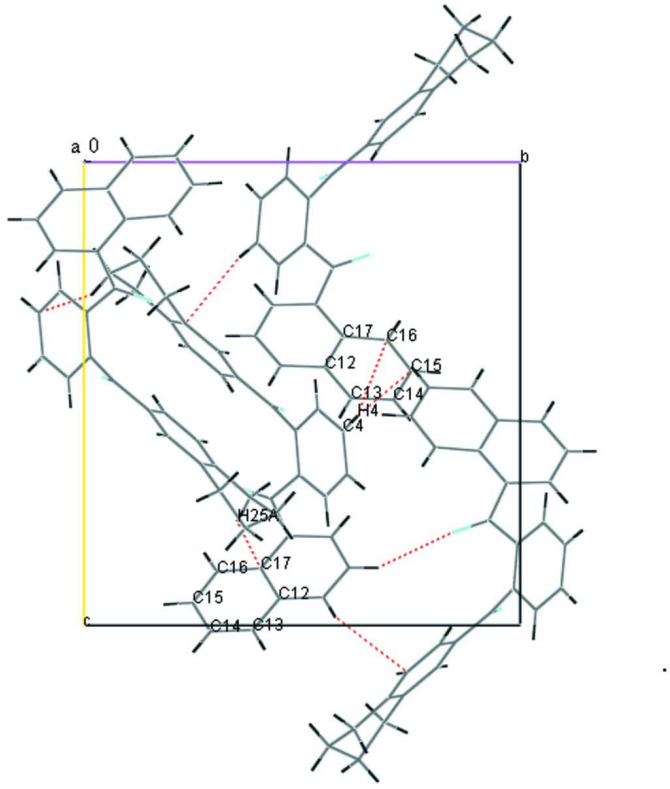


Figure 2

Packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

(Naphthalen-1-yl){2-[(5,6,7,8-tetrahydronaphthalen-2-yl)carbonyl]phenyl}methanone

Crystal data

$C_{28}H_{22}O_2$
$M_r = 390.46$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.5625$ (5) Å
$b = 13.6374$ (8) Å
$c = 14.4927$ (8) Å
$V = 2087.6$ (2) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.242$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5023 reflections
$\theta = 2.4$–$27.9°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, colourless
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.985$, $T_{max} = 0.989$
13047 measured reflections
4998 independent reflections
3511 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.4°$
$h = -13 \rightarrow 8$
$k = -17 \rightarrow 11$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.100$
$S = 1.03$
4998 reflections
272 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
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.1006P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0063 (11)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.33655 (16)	0.99371 (12)	0.82430 (11)	0.0415 (4)
C2	0.32842 (16)	0.98524 (12)	0.92015 (11)	0.0412 (4)
C3	0.23477 (17)	1.03566 (13)	0.96667 (13)	0.0490 (4)
H3	0.2288	1.0302	1.0305	0.059*
C4	0.15021 (18)	1.09395 (15)	0.91969 (15)	0.0579 (5)
H4	0.0873	1.1273	0.9519	0.070*
C5	0.15820 (18)	1.10309 (15)	0.82597 (15)	0.0569 (5)
H5	0.1011	1.1428	0.7944	0.068*
C6	0.25110 (17)	1.05336 (13)	0.77827 (13)	0.0517 (5)
H6	0.2565	1.0599	0.7145	0.062*
C7	0.42627 (17)	0.92891 (14)	0.77308 (12)	0.0476 (4)
C8	0.49710 (16)	0.96879 (13)	0.69309 (12)	0.0439 (4)

C9	0.52520 (18)	1.06701 (14)	0.69107 (14)	0.0543 (5)
H9	0.4900	1.1078	0.7357	0.065*
C10	0.6045 (2)	1.10767 (16)	0.62462 (15)	0.0643 (5)
H10	0.6202	1.1748	0.6243	0.077*
C11	0.6585 (2)	1.04903 (16)	0.56068 (14)	0.0618 (5)
H11	0.7140	1.0761	0.5179	0.074*
C12	0.63253 (16)	0.94787 (15)	0.55742 (12)	0.0498 (5)
C13	0.68928 (19)	0.88731 (19)	0.49028 (14)	0.0655 (6)
H13	0.7459	0.9141	0.4481	0.079*
C14	0.6619 (2)	0.79030 (19)	0.48681 (16)	0.0733 (7)
H14	0.7003	0.7509	0.4425	0.088*
C15	0.5770 (2)	0.74932 (16)	0.54904 (15)	0.0669 (6)
H15	0.5578	0.6829	0.5451	0.080*
C16	0.52150 (17)	0.80499 (13)	0.61565 (13)	0.0522 (5)
H16	0.4647	0.7762	0.6565	0.063*
C17	0.54892 (14)	0.90562 (13)	0.62354 (12)	0.0424 (4)
C18	0.42905 (17)	0.93173 (14)	0.97279 (12)	0.0446 (4)
C19	0.39317 (16)	0.85114 (13)	1.03589 (11)	0.0413 (4)
C20	0.48595 (17)	0.80906 (14)	1.09093 (12)	0.0476 (4)
H20	0.5684	0.8328	1.0874	0.057*
C21	0.45937 (17)	0.73290 (14)	1.15083 (12)	0.0504 (5)
C22	0.5631 (2)	0.6889 (2)	1.20877 (15)	0.0760 (7)
H22A	0.6168	0.7412	1.2317	0.091*
H22B	0.6147	0.6468	1.1701	0.091*
C23	0.5145 (3)	0.62984 (19)	1.28973 (16)	0.0862 (8)
H23A	0.5833	0.5917	1.3158	0.103*
H23B	0.4835	0.6740	1.3371	0.103*
C24	0.4094 (3)	0.5620 (2)	1.26035 (19)	0.0970 (9)
H24A	0.4404	0.5177	1.2131	0.116*
H24B	0.3823	0.5229	1.3127	0.116*
C25	0.2995 (2)	0.61887 (17)	1.22370 (17)	0.0791 (7)
H25A	0.2545	0.6482	1.2751	0.095*
H25B	0.2418	0.5739	1.1933	0.095*
C26	0.33552 (19)	0.69868 (14)	1.15654 (12)	0.0512 (5)
C27	0.24312 (18)	0.74029 (14)	1.10116 (13)	0.0519 (5)
H27	0.1605	0.7170	1.1047	0.062*
C28	0.27079 (17)	0.81506 (13)	1.04115 (12)	0.0468 (4)
H28	0.2075	0.8415	1.0041	0.056*
O1	0.44000 (15)	0.84526 (11)	0.79968 (10)	0.0732 (4)
O2	0.53817 (12)	0.95838 (12)	0.96392 (11)	0.0726 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0438 (10)	0.0393 (10)	0.0415 (9)	−0.0032 (8)	0.0041 (7)	0.0052 (8)
C2	0.0430 (9)	0.0389 (10)	0.0416 (9)	−0.0055 (8)	0.0013 (7)	0.0034 (7)
C3	0.0545 (11)	0.0479 (11)	0.0446 (10)	0.0008 (9)	0.0094 (8)	0.0021 (8)
C4	0.0523 (11)	0.0541 (12)	0.0674 (13)	0.0082 (10)	0.0130 (9)	0.0033 (10)

C5	0.0513 (12)	0.0507 (12)	0.0688 (13)	0.0109 (9)	−0.0017 (9)	0.0126 (10)
C6	0.0575 (11)	0.0524 (12)	0.0453 (10)	0.0011 (9)	−0.0028 (9)	0.0104 (9)
C7	0.0552 (11)	0.0437 (11)	0.0438 (10)	0.0001 (9)	0.0037 (8)	0.0060 (8)
C8	0.0478 (10)	0.0430 (10)	0.0409 (9)	0.0035 (8)	0.0012 (7)	0.0055 (8)
C9	0.0651 (12)	0.0444 (11)	0.0535 (11)	−0.0031 (9)	0.0090 (9)	0.0008 (9)
C10	0.0758 (13)	0.0477 (12)	0.0693 (13)	−0.0124 (10)	0.0153 (12)	0.0074 (11)
C11	0.0614 (12)	0.0649 (14)	0.0590 (13)	−0.0073 (11)	0.0136 (10)	0.0149 (10)
C12	0.0450 (10)	0.0607 (13)	0.0436 (10)	0.0060 (9)	0.0009 (7)	0.0061 (9)
C13	0.0587 (12)	0.0831 (18)	0.0547 (12)	0.0140 (11)	0.0094 (10)	0.0021 (11)
C14	0.0760 (15)	0.0790 (18)	0.0649 (14)	0.0293 (13)	0.0060 (11)	−0.0137 (13)
C15	0.0809 (15)	0.0487 (13)	0.0710 (15)	0.0172 (11)	−0.0036 (12)	−0.0058 (11)
C16	0.0599 (11)	0.0448 (11)	0.0519 (11)	0.0078 (9)	−0.0016 (9)	0.0069 (9)
C17	0.0410 (9)	0.0454 (10)	0.0406 (9)	0.0045 (7)	−0.0052 (7)	0.0055 (8)
C18	0.0431 (10)	0.0488 (11)	0.0420 (9)	−0.0021 (8)	0.0002 (7)	0.0033 (8)
C19	0.0457 (9)	0.0416 (10)	0.0367 (8)	−0.0001 (8)	0.0023 (7)	−0.0019 (8)
C20	0.0447 (10)	0.0544 (11)	0.0435 (9)	0.0010 (9)	0.0018 (7)	0.0038 (8)
C21	0.0591 (12)	0.0530 (11)	0.0391 (10)	0.0101 (9)	0.0075 (8)	0.0043 (8)
C22	0.0740 (14)	0.0879 (18)	0.0661 (14)	0.0233 (13)	0.0023 (11)	0.0249 (13)
C23	0.110 (2)	0.0872 (19)	0.0611 (14)	0.0355 (17)	0.0091 (14)	0.0274 (13)
C24	0.121 (2)	0.0741 (18)	0.096 (2)	0.0233 (17)	0.0315 (17)	0.0412 (16)
C25	0.0948 (17)	0.0636 (15)	0.0790 (16)	0.0071 (12)	0.0311 (13)	0.0268 (13)
C26	0.0633 (13)	0.0432 (11)	0.0470 (10)	0.0069 (9)	0.0173 (8)	0.0028 (8)
C27	0.0516 (10)	0.0483 (11)	0.0560 (11)	−0.0068 (9)	0.0096 (9)	−0.0019 (9)
C28	0.0500 (10)	0.0472 (11)	0.0432 (10)	−0.0014 (8)	0.0000 (8)	−0.0009 (8)
O1	0.1049 (12)	0.0478 (8)	0.0669 (9)	0.0165 (8)	0.0289 (8)	0.0166 (7)
O2	0.0455 (8)	0.0879 (11)	0.0844 (10)	−0.0111 (7)	−0.0058 (7)	0.0355 (9)

Geometric parameters (Å, º)

C1—C6	1.386 (2)	C15—C16	1.361 (3)
C1—C2	1.397 (2)	C15—H15	0.9300
C1—C7	1.493 (2)	C16—C17	1.407 (2)
C2—C3	1.380 (2)	C16—H16	0.9300
C2—C18	1.498 (2)	C18—O2	1.215 (2)
C3—C4	1.376 (3)	C18—C19	1.479 (2)
C3—H3	0.9300	C19—C28	1.385 (2)
C4—C5	1.367 (3)	C19—C20	1.388 (2)
C4—H4	0.9300	C20—C21	1.382 (2)
C5—C6	1.379 (3)	C20—H20	0.9300
C5—H5	0.9300	C21—C26	1.391 (3)
C6—H6	0.9300	C21—C22	1.505 (3)
C7—O1	1.213 (2)	C22—C23	1.513 (3)
C7—C8	1.483 (2)	C22—H22A	0.9700
C8—C9	1.372 (2)	C22—H22B	0.9700
C8—C17	1.435 (2)	C23—C24	1.507 (4)
C9—C10	1.392 (3)	C23—H23A	0.9700
C9—H9	0.9300	C23—H23B	0.9700
C10—C11	1.350 (3)	C24—C25	1.494 (3)

C10—H10	0.9300	C24—H24A	0.9700
C11—C12	1.407 (3)	C24—H24B	0.9700
C11—H11	0.9300	C25—C26	1.509 (3)
C12—C13	1.410 (3)	C25—H25A	0.9700
C12—C17	1.425 (2)	C25—H25B	0.9700
C13—C14	1.355 (3)	C26—C27	1.385 (3)
C13—H13	0.9300	C27—C28	1.372 (2)
C14—C15	1.389 (3)	C27—H27	0.9300
C14—H14	0.9300	C28—H28	0.9300

C6—C1—C2	119.15 (17)	C16—C17—C12	117.86 (17)
C6—C1—C7	121.42 (16)	C16—C17—C8	124.35 (16)
C2—C1—C7	118.98 (16)	C12—C17—C8	117.79 (16)
C3—C2—C1	119.25 (16)	O2—C18—C19	122.04 (16)
C3—C2—C18	120.16 (15)	O2—C18—C2	118.26 (16)
C1—C2—C18	120.21 (16)	C19—C18—C2	119.67 (15)
C4—C3—C2	120.75 (17)	C28—C19—C20	118.71 (16)
C4—C3—H3	119.6	C28—C19—C18	122.48 (15)
C2—C3—H3	119.6	C20—C19—C18	118.80 (15)
C5—C4—C3	120.29 (18)	C21—C20—C19	121.89 (16)
C5—C4—H4	119.9	C21—C20—H20	119.1
C3—C4—H4	119.9	C19—C20—H20	119.1
C4—C5—C6	119.83 (18)	C20—C21—C26	118.70 (16)
C4—C5—H5	120.1	C20—C21—C22	120.15 (18)
C6—C5—H5	120.1	C26—C21—C22	121.15 (17)
C5—C6—C1	120.72 (17)	C21—C22—C23	113.45 (19)
C5—C6—H6	119.6	C21—C22—H22A	108.9
C1—C6—H6	119.6	C23—C22—H22A	108.9
O1—C7—C8	122.21 (16)	C21—C22—H22B	108.9
O1—C7—C1	118.32 (15)	C23—C22—H22B	108.9
C8—C7—C1	119.45 (16)	H22A—C22—H22B	107.7
C9—C8—C17	119.25 (16)	C24—C23—C22	111.0 (2)
C9—C8—C7	118.93 (16)	C24—C23—H23A	109.4
C17—C8—C7	121.44 (16)	C22—C23—H23A	109.4
C8—C9—C10	122.27 (19)	C24—C23—H23B	109.4
C8—C9—H9	118.9	C22—C23—H23B	109.4
C10—C9—H9	118.9	H23A—C23—H23B	108.0
C11—C10—C9	119.54 (19)	C25—C24—C23	110.7 (2)
C11—C10—H10	120.2	C25—C24—H24A	109.5
C9—C10—H10	120.2	C23—C24—H24A	109.5
C10—C11—C12	121.43 (18)	C25—C24—H24B	109.5
C10—C11—H11	119.3	C23—C24—H24B	109.5
C12—C11—H11	119.3	H24A—C24—H24B	108.1
C11—C12—C13	120.97 (19)	C24—C25—C26	114.05 (19)
C11—C12—C17	119.64 (18)	C24—C25—H25A	108.7
C13—C12—C17	119.39 (19)	C26—C25—H25A	108.7
C14—C13—C12	120.5 (2)	C24—C25—H25B	108.7
C14—C13—H13	119.8	C26—C25—H25B	108.7

C12—C13—H13	119.8	H25A—C25—H25B	107.6
C13—C14—C15	120.4 (2)	C27—C26—C21	119.38 (17)
C13—C14—H14	119.8	C27—C26—C25	119.43 (18)
C15—C14—H14	119.8	C21—C26—C25	121.17 (18)
C16—C15—C14	120.9 (2)	C28—C27—C26	121.45 (17)
C16—C15—H15	119.5	C28—C27—H27	119.3
C14—C15—H15	119.5	C26—C27—H27	119.3
C15—C16—C17	120.87 (18)	C27—C28—C19	119.86 (17)
C15—C16—H16	119.6	C27—C28—H28	120.1
C17—C16—H16	119.6	C19—C28—H28	120.1

C6—C1—C2—C3	0.6 (3)	C11—C12—C17—C8	−1.8 (2)
C7—C1—C2—C3	−171.82 (16)	C13—C12—C17—C8	177.47 (17)
C6—C1—C2—C18	−172.24 (16)	C9—C8—C17—C16	−176.47 (17)
C7—C1—C2—C18	15.3 (3)	C7—C8—C17—C16	10.7 (3)
C1—C2—C3—C4	−0.2 (3)	C9—C8—C17—C12	2.8 (2)
C18—C2—C3—C4	172.73 (17)	C7—C8—C17—C12	−170.07 (16)
C2—C3—C4—C5	−0.3 (3)	C3—C2—C18—O2	−116.9 (2)
C3—C4—C5—C6	0.3 (3)	C1—C2—C18—O2	55.9 (2)
C4—C5—C6—C1	0.2 (3)	C3—C2—C18—C19	61.0 (2)
C2—C1—C6—C5	−0.7 (3)	C1—C2—C18—C19	−126.17 (18)
C7—C1—C6—C5	171.59 (18)	O2—C18—C19—C28	−174.79 (18)
C6—C1—C7—O1	−135.5 (2)	C2—C18—C19—C28	7.4 (2)
C2—C1—C7—O1	36.8 (3)	O2—C18—C19—C20	4.2 (3)
C6—C1—C7—C8	45.7 (3)	C2—C18—C19—C20	−173.60 (16)
C2—C1—C7—C8	−142.05 (17)	C28—C19—C20—C21	−0.3 (3)
O1—C7—C8—C9	−150.0 (2)	C18—C19—C20—C21	−179.40 (16)
C1—C7—C8—C9	28.8 (3)	C19—C20—C21—C26	−0.8 (3)
O1—C7—C8—C17	22.9 (3)	C19—C20—C21—C22	179.53 (18)
C1—C7—C8—C17	−158.31 (16)	C20—C21—C22—C23	162.3 (2)
C17—C8—C9—C10	−1.2 (3)	C26—C21—C22—C23	−17.3 (3)
C7—C8—C9—C10	171.80 (18)	C21—C22—C23—C24	46.4 (3)
C8—C9—C10—C11	−1.4 (3)	C22—C23—C24—C25	−61.6 (3)
C9—C10—C11—C12	2.5 (3)	C23—C24—C25—C26	46.2 (3)
C10—C11—C12—C13	179.9 (2)	C20—C21—C26—C27	1.2 (3)
C10—C11—C12—C17	−0.8 (3)	C22—C21—C26—C27	−179.15 (19)
C11—C12—C13—C14	−178.9 (2)	C20—C21—C26—C25	−177.22 (18)
C17—C12—C13—C14	1.9 (3)	C22—C21—C26—C25	2.4 (3)
C12—C13—C14—C15	0.4 (3)	C24—C25—C26—C27	164.4 (2)
C13—C14—C15—C16	−1.3 (3)	C24—C25—C26—C21	−17.2 (3)
C14—C15—C16—C17	−0.2 (3)	C21—C26—C27—C28	−0.5 (3)
C15—C16—C17—C12	2.4 (3)	C25—C26—C27—C28	177.99 (18)
C15—C16—C17—C8	−178.34 (18)	C26—C27—C28—C19	−0.7 (3)
C11—C12—C17—C16	177.50 (17)	C20—C19—C28—C27	1.1 (3)
C13—C12—C17—C16	−3.2 (2)	C18—C19—C28—C27	−179.88 (16)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C12–C17 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1	0.93	2.29	2.856 (2)	118
C4—H4···*Cg*3^{i}	0.93	2.54	3.419 (1)	159
C25—H25*A*···*Cg*3^{ii}	0.97	2.94	3.849 (5)	157

Symmetry codes: (i) −*x*+1/2, −*y*, *z*+1/2; (ii) *x*+1/2, −*y*+1/2, −*z*+1.