Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[(*E*)-2-(2-Methoxyphenyl)vinyl]-5,5-dimethylcyclohex-2-enone

Zeenat Fatima,[a] Govindaraj Senthilkumar,[b] A. Vadivel,[b] Haridoss Manikandan[b] and Devadasan Velmurugan[a]*

[a]Center of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Department of Chemistry, Annamalai University, Annamalainagar 608 002, Tamilnadu, India
Correspondence e-mail: shirai2011@gmail.com

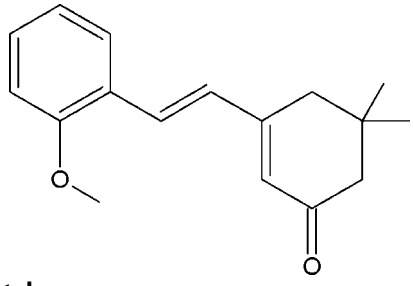
Received 23 March 2014; accepted 24 March 2014

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.085; wR factor = 0.283; data-to-parameter ratio = 20.1.

The title compound, $C_{17}H_{20}O_2$, has an *E* conformation about the bridging C=C bond. The cyclohexene ring adopts an envelope conformation with the dimethyl-substituted C atom as the flap. Its mean plane makes a dihedral angle of 7.20 (12)° with the benzene ring. In the crystal, neighbouring molecules are connected *via* C—H···O hydrogen bonds, forming chains running along the *a*-axis direction.

Related literature

For the pharmacological activity of cyclohexanone derivatives, see: Puetz *et al.* (2003); Rajveer *et al.* (2010). For related structures, see: Fatima *et al.* (2013); Hema *et al.* (2006). For ring puckering parametes, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{17}H_{20}O_2$
M_r = 256.33
Monoclinic, $P2_1/n$
a = 7.208 (4) Å
b = 13.824 (7) Å
c = 15.022 (8) Å
β = 92.13 (2)°
V = 1495.8 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.978, T_{max} = 0.986
10491 measured reflections
3517 independent reflections
2489 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.283
S = 1.06
3517 reflections
175 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14B···O1^{i}	0.97	2.62	3.554 (4)	161

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

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: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors thank the TBI X-ray facility, CAS in Crystallography and Biophysics, University of Madras, India, for the data collection and ZF thanks the UGC for a meritorious fellowship.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2717).

References

Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Fatima, Z., Senthilkumar, G., Vadivel, A., Manikandan, H. & Velmurugan, D. (2013). *Acta Cryst.* E**69**, o1121.
Hema, R., Parthasarathi, V., Ravikumar, K., Pandiarajan, K. & Murugavel, K. (2006). *Acta Cryst.* E**62**, o703–o705.
Puetz, C., Buschmann, H. & Koegel, B. (2003). US Patent Appl. No. 20030096811.
Rajveer, C., Stephenrathinaraj, B., Sudharshini, S., Kumaraswamy, D., Bhupendra, S. & Choudhury, P. K. (2010). *Res. J. Pharm. Bio. Chem. Sci.* **1**, 99–107.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2014). E**70**, o509 [doi:10.1107/S1600536814006527]

3-[(*E*)-2-(2-Methoxyphenyl)vinyl]-5,5-dimethylcyclohex-2-enone

Zeenat Fatima, Govindaraj Senthilkumar, A. Vadivel, Haridoss Manikandan and Devadasan Velmurugan

S1. Comment

Cyclohexanone is an aliphatic cyclic ketone. Cyclohexanone derivatives have potent pharmacological activity in the treatment of a broad spectrum of medical conditions (Puetz *et al.*, 2003). The cyclohexanone moiety constitutes an important structural feature in several anti-inflammatory, analgesic, local anesthetic and antihistaminic drugs (Rajveer *et al.*, 2010). As part of our studies in this area (Fatima *et al.*, 2013; Hema *et al.*, 2006), we have undertaken a single-crystal structure determination of the title compound.

In the title compound, Fig. 1, the cyclohexene ring (C9—C14) adopts an envelope conformation with atom C13 as the flap: puckering parameters (Cremer & Pople, 1975) are Q = 0.464 (3) Å, θ = 52.3 (4) °, and φ = 232.2 (4) °. Its mean plane makes a dihedral angle of 7.20 (12)° with the benzene ring (C1—C6).

In the crystal, hydrogen bonded chains running along the *a*-axis direction are generated by connecting neighbouring molecules via C—H···O hydrogen bonds (Table 1 and Fig. 2).

S2. Experimental

A mixture of isophorone (0.01 mol), 2-methoxybezaldehyde (0.01 mol) and sodium hydroxide solution (10 ml, 10%) in ethanol (25 ml) was stirred at room temperature until the starting material disappeared. The resulting mixture was poured into crushed ice and the precipitate was filtered off, dried and recrystallized from ethanol giving p. colourless block-like crystals [Yield = 93%; M.p. = 373-375 K].

S3. Refinement

The H atoms were placed in calculated positions and refined as riding atoms: C—H = 0.93 - 0.97 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and = 1.2U_{eq}(C) for other H atoms.

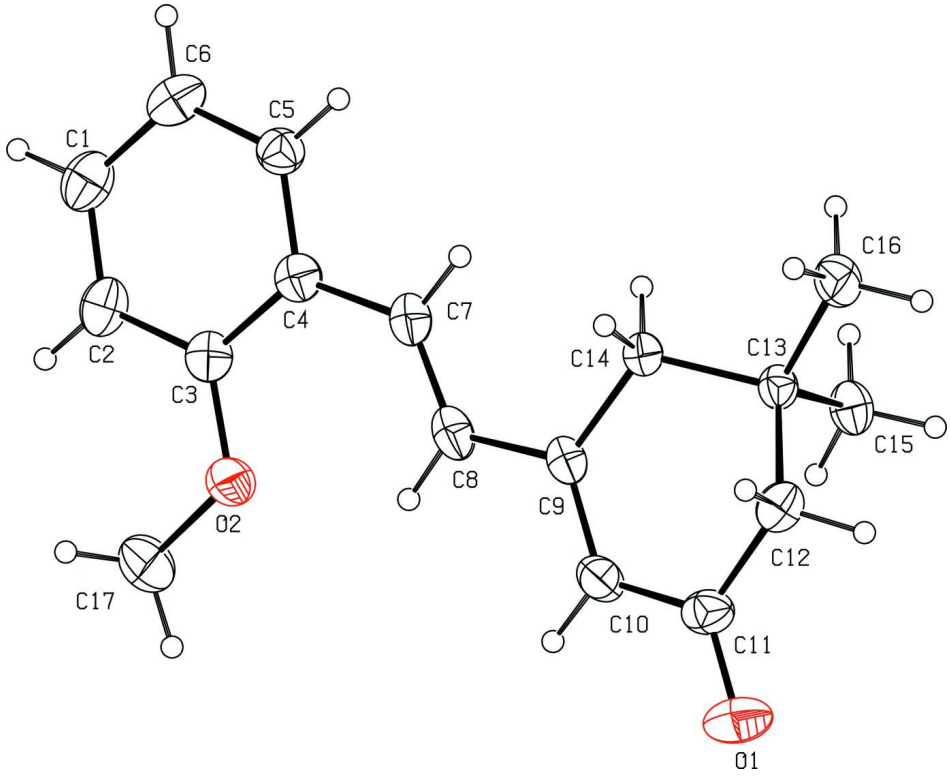


Figure 1

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

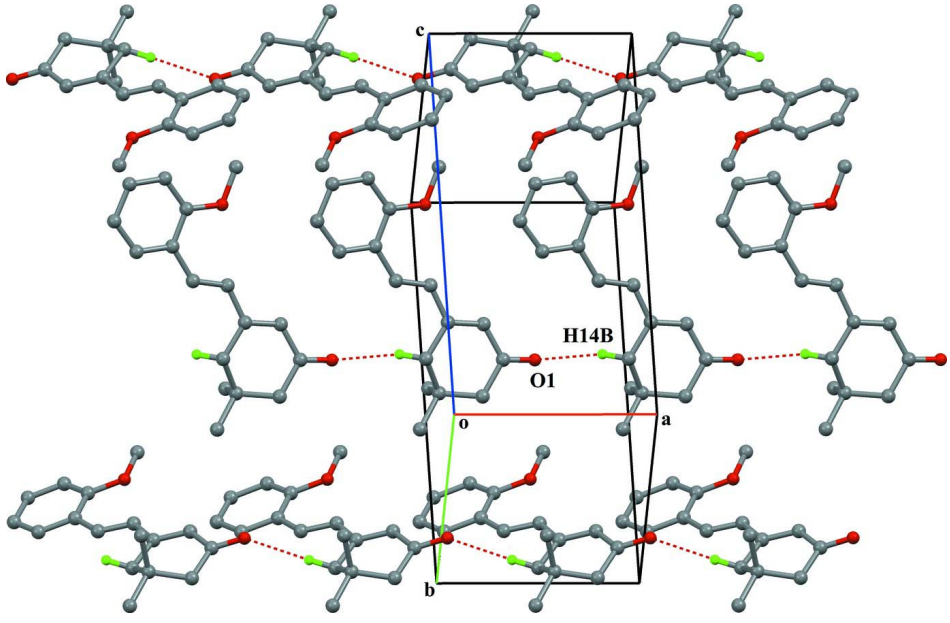


Figure 2

The crystal packing of the title compound viewed along the *b* axis. The hydrogen bonds are shown as dashed lines (see Table 1 for details; H-atoms not involved in hydrogen bonding have been excluded for clarity).

3-[(*E*)-2-(2-Methoxyphenyl)vinyl]-5,5-dimethylcyclohex-2-enone

Crystal data

$C_{17}H_{20}O_2$
$M_r = 256.33$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.208$ (4) Å
$b = 13.824$ (7) Å
$c = 15.022$ (8) Å
$\beta = 92.13$ (2)°
$V = 1495.8$ (14) Å^3
$Z = 4$
$F(000) = 552$
$D_x = 1.138$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3517 reflections
$\theta = 2.0$–$28.6°$
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.978$, $T_{max} = 0.986$
10491 measured reflections
3517 independent reflections
2489 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 28.6°$, $\theta_{min} = 2.0°$
$h = -9 \rightarrow 9$
$k = -18 \rightarrow 17$
$l = -19 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.085$
$wR(F^2) = 0.283$
$S = 1.06$
3517 reflections
175 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
$w = 1/[\sigma^2(F_o^2) + (0.1498P)^2 + 0.8245P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.4696 (5)	0.6141 (2)	0.2237 (2)	0.0617 (8)
H1	1.5376	0.6552	0.1884	0.074*
C2	1.2899 (4)	0.5897 (2)	0.1978 (2)	0.0533 (7)
H2	1.2377	0.6147	0.1451	0.064*

C3	1.1846 (4)	0.52740 (19)	0.25024 (18)	0.0472 (6)
C4	1.2616 (4)	0.49045 (18)	0.33219 (18)	0.0452 (6)
C5	1.4433 (4)	0.51557 (18)	0.35727 (18)	0.0464 (6)
H5	1.4951	0.4915	0.4104	0.056*
C6	1.5515 (4)	0.5767 (2)	0.3041 (2)	0.0617 (8)
H6	1.6732	0.5920	0.3213	0.074*
C7	1.1621 (4)	0.42686 (18)	0.39463 (18)	0.0479 (6)
H7	1.2321	0.4088	0.4452	0.057*
C8	0.9882 (4)	0.39088 (18)	0.39058 (18)	0.0500 (7)
H8	0.9143	0.4049	0.3401	0.060*
C9	0.9055 (3)	0.33023 (16)	0.46110 (16)	0.0411 (6)
C10	0.7259 (4)	0.29964 (19)	0.45218 (19)	0.0496 (7)
H10	0.6585	0.3153	0.4002	0.060*
C11	0.6334 (3)	0.24317 (19)	0.5206 (2)	0.0499 (7)
C12	0.7438 (4)	0.22367 (19)	0.60826 (18)	0.0459 (6)
H12A	0.6987	0.1644	0.6345	0.055*
H12B	0.7219	0.2760	0.6495	0.055*
C13	0.9558 (3)	0.21429 (15)	0.59556 (15)	0.0369 (5)
C14	1.0219 (3)	0.30514 (16)	0.54545 (16)	0.0396 (5)
H14A	1.0200	0.3600	0.5857	0.048*
H14B	1.1495	0.2952	0.5292	0.048*
C15	0.9938 (4)	0.12099 (17)	0.54174 (19)	0.0480 (6)
H15A	0.9532	0.0657	0.5744	0.072*
H15B	1.1244	0.1157	0.5323	0.072*
H15C	0.9272	0.1239	0.4853	0.072*
C16	1.0603 (5)	0.2081 (2)	0.68771 (18)	0.0563 (8)
H16A	1.0354	0.2652	0.7216	0.084*
H16B	1.1913	0.2031	0.6793	0.084*
H16C	1.0187	0.1521	0.7192	0.084*
C17	0.9273 (5)	0.5303 (3)	0.1418 (2)	0.0736 (10)
H17A	0.9271	0.5997	0.1389	0.110*
H17B	0.8023	0.5068	0.1344	0.110*
H17C	1.0008	0.5048	0.0952	0.110*
O1	0.4730 (3)	0.2135 (2)	0.5081 (2)	0.0762 (8)
O2	1.0044 (3)	0.49973 (15)	0.22679 (13)	0.0569 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0701 (18)	0.0601 (16)	0.0560 (17)	−0.0103 (15)	0.0175 (15)	−0.0004 (14)
C2	0.0659 (16)	0.0489 (13)	0.0464 (14)	−0.0038 (12)	0.0184 (13)	−0.0005 (11)
C3	0.0542 (14)	0.0450 (12)	0.0426 (13)	0.0002 (11)	0.0037 (12)	−0.0020 (10)
C4	0.0477 (13)	0.0433 (12)	0.0448 (13)	0.0021 (10)	0.0033 (11)	−0.0035 (10)
C5	0.0477 (13)	0.0468 (12)	0.0445 (13)	0.0005 (10)	−0.0014 (11)	−0.0020 (10)
C6	0.0517 (14)	0.0652 (17)	0.069 (2)	−0.0135 (13)	0.0093 (15)	−0.0085 (15)
C7	0.0576 (14)	0.0416 (12)	0.0446 (13)	0.0017 (11)	0.0024 (12)	0.0073 (10)
C8	0.0646 (16)	0.0446 (12)	0.0404 (13)	0.0084 (12)	−0.0033 (12)	0.0079 (10)
C9	0.0488 (12)	0.0367 (10)	0.0375 (12)	0.0056 (9)	−0.0005 (10)	0.0036 (9)

C10	0.0490 (13)	0.0494 (13)	0.0495 (14)	0.0067 (11)	−0.0090 (12)	0.0045 (11)
C11	0.0390 (12)	0.0479 (13)	0.0627 (17)	0.0036 (10)	0.0002 (12)	−0.0098 (12)
C12	0.0479 (13)	0.0456 (12)	0.0448 (13)	−0.0035 (10)	0.0127 (11)	−0.0038 (10)
C13	0.0432 (11)	0.0346 (10)	0.0327 (11)	−0.0005 (9)	0.0005 (9)	0.0022 (8)
C14	0.0409 (11)	0.0376 (11)	0.0401 (12)	−0.0020 (9)	−0.0014 (10)	0.0062 (9)
C15	0.0581 (14)	0.0363 (11)	0.0497 (14)	0.0092 (10)	0.0051 (12)	−0.0005 (10)
C16	0.0710 (18)	0.0579 (15)	0.0392 (13)	−0.0071 (13)	−0.0096 (13)	0.0101 (11)
C17	0.084 (2)	0.083 (2)	0.0520 (18)	−0.0015 (19)	−0.0171 (17)	0.0147 (16)
O1	0.0395 (10)	0.0955 (18)	0.0935 (19)	−0.0095 (11)	−0.0002 (11)	−0.0084 (14)
O2	0.0559 (11)	0.0680 (12)	0.0461 (11)	−0.0088 (9)	−0.0081 (9)	0.0163 (9)

Geometric parameters (Å, º)

C1—C2	1.381 (4)	C11—O1	1.234 (3)
C1—C6	1.421 (5)	C11—C12	1.537 (4)
C1—H1	0.9300	C12—C13	1.553 (4)
C2—C3	1.408 (4)	C12—H12A	0.9700
C2—H2	0.9300	C12—H12B	0.9700
C3—O2	1.387 (3)	C13—C14	1.548 (3)
C3—C4	1.426 (4)	C13—C15	1.552 (3)
C4—C5	1.393 (4)	C13—C16	1.553 (3)
C4—C7	1.489 (4)	C14—H14A	0.9700
C5—C6	1.416 (4)	C14—H14B	0.9700
C5—H5	0.9300	C15—H15A	0.9600
C6—H6	0.9300	C15—H15B	0.9600
C7—C8	1.348 (4)	C15—H15C	0.9600
C7—H7	0.9300	C16—H16A	0.9600
C8—C9	1.493 (4)	C16—H16B	0.9600
C8—H8	0.9300	C16—H16C	0.9600
C9—C10	1.364 (4)	C17—O2	1.437 (3)
C9—C14	1.533 (3)	C17—H17A	0.9600
C10—C11	1.470 (4)	C17—H17B	0.9600
C10—H10	0.9300	C17—H17C	0.9600
C2—C1—C6	120.4 (3)	C13—C12—H12A	109.0
C2—C1—H1	119.8	C11—C12—H12B	109.0
C6—C1—H1	119.8	C13—C12—H12B	109.0
C1—C2—C3	120.7 (3)	H12A—C12—H12B	107.8
C1—C2—H2	119.7	C14—C13—C15	111.0 (2)
C3—C2—H2	119.7	C14—C13—C12	108.29 (18)
O2—C3—C2	123.0 (2)	C15—C13—C12	109.07 (19)
O2—C3—C4	116.8 (2)	C14—C13—C16	109.30 (19)
C2—C3—C4	120.1 (3)	C15—C13—C16	109.2 (2)
C5—C4—C3	118.4 (3)	C12—C13—C16	110.0 (2)
C5—C4—C7	116.5 (2)	C9—C14—C13	114.63 (19)
C3—C4—C7	125.0 (2)	C9—C14—H14A	108.6
C4—C5—C6	121.8 (3)	C13—C14—H14A	108.6
C4—C5—H5	119.1	C9—C14—H14B	108.6

C6—C5—H5	119.1	C13—C14—H14B	108.6
C5—C6—C1	118.5 (3)	H14A—C14—H14B	107.6
C5—C6—H6	120.8	C13—C15—H15A	109.5
C1—C6—H6	120.8	C13—C15—H15B	109.5
C8—C7—C4	131.2 (2)	H15A—C15—H15B	109.5
C8—C7—H7	114.4	C13—C15—H15C	109.5
C4—C7—H7	114.4	H15A—C15—H15C	109.5
C7—C8—C9	124.8 (2)	H15B—C15—H15C	109.5
C7—C8—H8	117.6	C13—C16—H16A	109.5
C9—C8—H8	117.6	C13—C16—H16B	109.5
C10—C9—C8	120.5 (2)	H16A—C16—H16B	109.5
C10—C9—C14	119.9 (2)	C13—C16—H16C	109.5
C8—C9—C14	119.5 (2)	H16A—C16—H16C	109.5
C9—C10—C11	123.3 (2)	H16B—C16—H16C	109.5
C9—C10—H10	118.3	O2—C17—H17A	109.5
C11—C10—H10	118.3	O2—C17—H17B	109.5
O1—C11—C10	121.1 (3)	H17A—C17—H17B	109.5
O1—C11—C12	121.6 (3)	O2—C17—H17C	109.5
C10—C11—C12	117.3 (2)	H17A—C17—H17C	109.5
C11—C12—C13	113.0 (2)	H17B—C17—H17C	109.5
C11—C12—H12A	109.0	C3—O2—C17	118.2 (2)

C6—C1—C2—C3	−0.1 (5)	C8—C9—C10—C11	−177.4 (2)
C1—C2—C3—O2	−179.2 (3)	C14—C9—C10—C11	0.6 (4)
C1—C2—C3—C4	1.4 (4)	C9—C10—C11—O1	−176.8 (3)
O2—C3—C4—C5	179.1 (2)	C9—C10—C11—C12	3.7 (4)
C2—C3—C4—C5	−1.6 (4)	O1—C11—C12—C13	148.6 (3)
O2—C3—C4—C7	−1.5 (4)	C10—C11—C12—C13	−31.9 (3)
C2—C3—C4—C7	177.9 (3)	C11—C12—C13—C14	53.3 (3)
C3—C4—C5—C6	0.4 (4)	C11—C12—C13—C15	−67.5 (3)
C7—C4—C5—C6	−179.2 (3)	C11—C12—C13—C16	172.7 (2)
C4—C5—C6—C1	1.0 (4)	C10—C9—C14—C13	24.0 (3)
C2—C1—C6—C5	−1.1 (5)	C8—C9—C14—C13	−158.0 (2)
C5—C4—C7—C8	179.3 (3)	C15—C13—C14—C9	70.0 (3)
C3—C4—C7—C8	−0.2 (5)	C12—C13—C14—C9	−49.6 (3)
C4—C7—C8—C9	−177.6 (3)	C16—C13—C14—C9	−169.5 (2)
C7—C8—C9—C10	177.9 (3)	C2—C3—O2—C17	4.8 (4)
C7—C8—C9—C14	0.0 (4)	C4—C3—O2—C17	−175.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*B*···O1^{i}	0.97	2.62	3.554 (4)	161

Symmetry code: (i) *x*+1, *y*, *z*.