

Hexacyclo[7.5.1.0^{1,6}.0^{6,13}.0^{8,12}.0^{10,14}]pentadecane-7,15-dione

Sambasivarao Kotha,* Vijayalakshmi Bandi, Rama Gunta and Sreevani Gaddamedi

Department of Chemistry, Indian Institute of Technology-Bombay, Powai, Mumbai 400 076, India. *Correspondence e-mail: srk@chem.iitb.ac.in

Received 1 June 2016

Accepted 19 July 2016

Edited by G. Smith, Queensland University of Technology, Australia

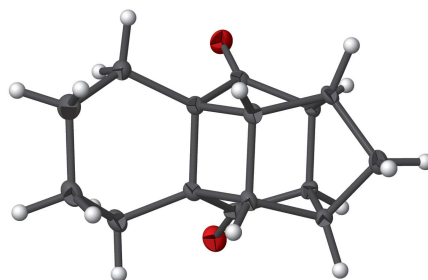
Keywords: Cage molecule; crystal structure; hexacyclic dione; unusual C—C bond length.

CCDC reference: 1014204

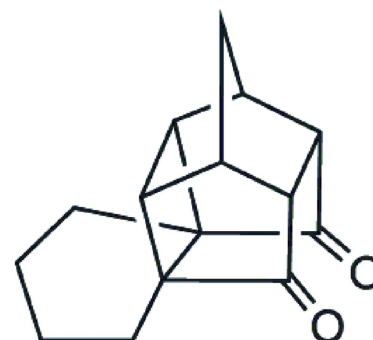
Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title cage compound, C₁₅H₁₆O₂, comprises eight fused rings, *viz.* one four-membered, four five-membered and three six-membered. One of the internal C—C bonds is unusually long for a cyclobutane bond length [1.607 (3) Å] and is comparable with the equivalent value of 1.598 (4) Å in the unsaturated homolog hexacyclo[7.4.2.0^{1,9}.0^{3,7}.0^{4,14}.0^{6,15}]pentadeca-10,12-diene-2,8-dione.

3D view



Chemical scheme



Structure description

Cage molecules are useful synthons for the design of natural and non-natural products. Several cage systems can undergo rearrangements to generate intricate polycycles (Hopf, 2000; Osawa & Yonemitsu, 1992). Polycyclic cage compounds have applications in medicinal chemistry for drug discovery research (Oliver & Malan, 2008; Geldenhuis *et al.* 2005).

The carbon framework of the title compound, C₁₅H₁₆O₂ (I), (Fig. 1), comprises one four-membered, four five-membered and three six-membered rings which are fused into a closed cage structure. All of the five-membered rings adopt envelope conformations, whereas the six-membered rings have boat conformations. The molecule appears as a 'cage' with one edge and the dione side is open.

The C—C bond lengths of the cyclobutane ring in the unsaturated hexacyclic system hexacyclo[7.4.2.0^{1,9}.0^{3,7}.0^{4,14}.0^{6,15}]pentadeca-10,12-diene-2,8-dione (II) (Fig. 2) range from 1.559 (4) to 1.598 (4) Å (Dhaneshwar *et al.*, 1988). However, in the saturated hexacyclic system of (I), the C4—C5 bond is longer, with a value of 1.607 (3) Å, which is unusual among cyclobutane bond lengths but is comparable with the corresponding bond in the related cage molecule 1,7-diallylpentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-8,11-dione [1.612 Å; Kotha *et al.*, 2014]. This may be because the hexacyclic dione system attached to the cyclobutane ring influences the bond length of the fused carbon atoms (C4—C5).

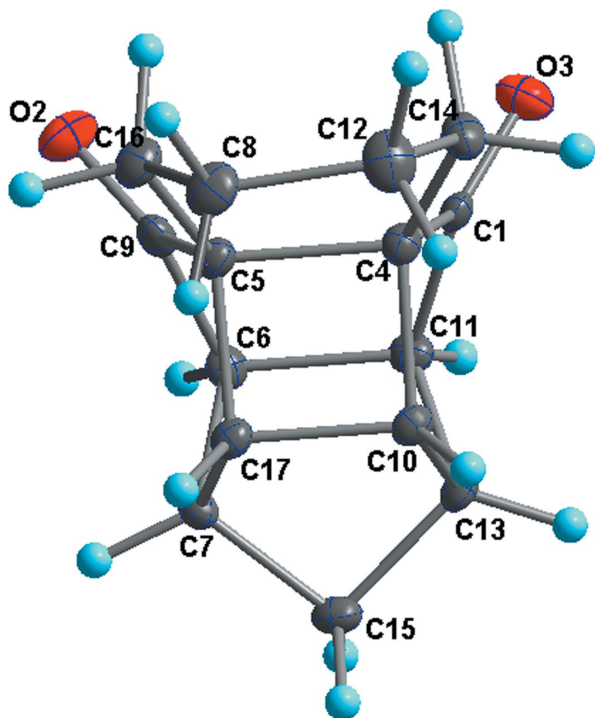


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

In the crystal, only one very weak intermolecular C6–H6···O3ⁱ hydrogen-bonding interaction is present (Table 1).

Synthesis and crystallization

The title compound can be prepared according to Kushner (1971) *via* a Diels–Alder reaction of cyclopentadiene with either naphthaquinone followed by [2 + 2] photo-cycloaddition and hydrogenation or 1,2,3,4-tetrahydro-5,8-naphthoquinone followed by [2 + 2] photo-cycloaddition (Kotha & Dipak, 2006). After recrystallization from a 3:2 mixture of dichloromethane–methanol, monoclinic crystals of the hexacyclic dione (I) were obtained, m.p. 360–362 K (lit. m.p. 360–361 K; Kotha, 1984).

Melting points were recorded on Veego melting point apparatus and are uncorrected. Nuclear Magnetic Resonance (NMR) spectra were recorded on a Varian VXR 400 spectrometer operated at 400 and 100 MHz for ¹H and ¹³C nuclei respectively.

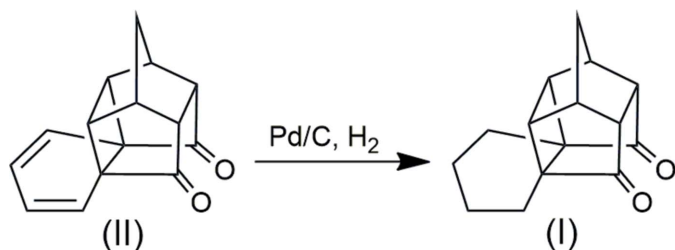


Figure 2
The reduction of (II), giving the title compound (I)

Table 1
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>
C6–H6···O3 ⁱ	1.00	2.58	3.547 (3)	163

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

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₆ O ₂
<i>M_r</i>	228.29
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.199 (2), 7.653 (2), 8.986 (3)
β (°)	104.005 (3)
<i>V</i> (Å ³)	547.1 (3)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.60 × 0.38 × 0.18
Data collection	
Diffractometer	Rigaku Saturn724 CCD
Absorption correction	Numerical (NUMABS; Rigaku, 1999)
<i>T</i> _{min} , <i>T</i> _{max}	0.954, 0.982
No. of measured, independent and observed [<i>F</i> ² > 2.0σ(<i>F</i> ²)] reflections	5855, 2877, 1935
<i>R</i> _{int}	0.067
(sin θ/λ) _{max} (Å ⁻¹)	0.686
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.086, 0.85
No. of reflections	2877
No. of parameters	154
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.27, -0.27

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *CrystalStructure* (Rigaku, 2010).

¹H NMR (400 MHz, CDCl₃): δ (p.p.m.) = 2.87 (*s*, 4H), 2.75 (*s*, 2H), 2.06 (*d*, *J* = 10.7 Hz, 2H), 1.94 (*t*, *J* = 12.6 Hz, 2H), 1.60–1.53 (*m*, 4H), 1.34 (*t*, *J* = 7.1 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃): δ (p.p.m.) = 213.8, 55.1, 49.7, 44.2, 43.7, 41.3, 22.8, 19.3.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The absolute structure was not determined in this analysis but the configuration for the eight arbitrarily numbered chiral centres of the molecule are C4(*R*), C5(*S*), C6(*R*), C7(*S*), C10(*R*), C11(*S*), C13(*R*), C17(*S*).

Acknowledgements

We would like to thank the DST for financial support. SK thanks the DST for the award of a J. C. Bose fellowship. SG and RG thank the CSIR–New Delhi and UGC–New Delhi, respectively, for the award of research fellowships. We thank Mr Darshan Mhatre for collecting the X-ray data.

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full crystallographic data

IUCrData (2016). **1**, x161173 [https://doi.org/10.1107/S2414314616011731]

Hexacyclo[7.5.1.0^{1,6}.0^{6,13}.0^{8,12}.0^{10,14}]pentadecane-7,15-dione

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Hexacyclo[7.5.1.0^{1,6}.0^{6,13}.0^{8,12}.0^{10,14}]pentadecane-7,15-dione*Crystal data*

$C_{15}H_{16}O_2$	$F(000) = 244.00$
$M_r = 228.29$	$D_x = 1.386 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Melting point = 360.1–362.1 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$
$a = 8.199 (2) \text{ \AA}$	Cell parameters from 1809 reflections
$b = 7.653 (2) \text{ \AA}$	$\theta = 3.5\text{--}29.2^\circ$
$c = 8.986 (3) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$\beta = 104.005 (3)^\circ$	$T = 100 \text{ K}$
$V = 547.1 (3) \text{ \AA}^3$	Prism, colourless
$Z = 2$	$0.60 \times 0.38 \times 0.18 \text{ mm}$

Data collection

Rigaku Saturn724 CCD diffractometer	2877 independent reflections
Detector resolution: 7.111 pixels mm^{-1}	1935 reflections with $F^2 > 2.0\sigma(F^2)$
ω scans	$R_{\text{int}} = 0.067$
Absorption correction: numerical (NUMABS; Rigaku, 1999)	$\theta_{\text{max}} = 29.2^\circ$
$T_{\text{min}} = 0.954$, $T_{\text{max}} = 0.982$	$h = -11 \rightarrow 11$
5855 measured reflections	$k = -10 \rightarrow 10$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.086$	H-atom parameters constrained
$S = 0.85$	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2]$
2877 reflections	where $P = (F_o^2 + 2F_c^2)/3$
154 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
1 restraint	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$

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.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2 . R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R-factor (gt).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O2	−0.15236 (18)	0.65835 (18)	0.14997 (17)	0.0245 (4)
O3	0.21822 (19)	0.35607 (16)	0.36795 (16)	0.0227 (4)
C1	0.2308 (3)	0.5131 (3)	0.3578 (3)	0.0129 (4)
C4	0.2893 (3)	0.6133 (3)	0.2348 (3)	0.0132 (5)
C5	0.1366 (3)	0.7346 (3)	0.1461 (2)	0.0138 (4)
C6	0.0443 (3)	0.7697 (3)	0.3796 (3)	0.0139 (5)
C7	0.1357 (3)	0.9434 (3)	0.3630 (2)	0.0138 (4)
C8	0.2653 (3)	0.7375 (3)	−0.0798 (3)	0.0212 (5)
C9	−0.0133 (3)	0.7099 (3)	0.2146 (3)	0.0155 (5)
C10	0.3755 (3)	0.7783 (3)	0.3226 (3)	0.0131 (4)
C11	0.1960 (3)	0.6497 (3)	0.4671 (3)	0.0144 (5)
C12	0.4054 (3)	0.6088 (3)	−0.0035 (3)	0.0231 (5)
C13	0.3488 (3)	0.7736 (3)	0.4888 (2)	0.0139 (4)
C14	0.3686 (3)	0.5051 (3)	0.1302 (3)	0.0178 (5)
C15	0.2773 (3)	0.9543 (3)	0.5073 (2)	0.0159 (5)
C16	0.1044 (3)	0.7194 (3)	−0.0258 (2)	0.0193 (5)
C17	0.2274 (3)	0.8958 (3)	0.2354 (2)	0.0130 (5)
H6	−0.0485	0.7817	0.4335	0.0166*
H7	0.0615	1.0488	0.3414	0.0166*
H8A	0.3081	0.8582	−0.0590	0.0255*
H8B	0.2389	0.7195	−0.1922	0.0255*
H10	0.4906	0.8081	0.3113	0.0157*
H11	0.1796	0.6001	0.5654	0.0173*
H12A	0.4240	0.5256	−0.0821	0.0277*
H12B	0.5110	0.6752	0.0343	0.0277*
H13	0.4494	0.7390	0.5708	0.0166*
H14A	0.2924	0.4070	0.0885	0.0213*
H14B	0.4750	0.4545	0.1912	0.0213*
H15A	0.2359	0.9646	0.6017	0.0191*
H15B	0.3577	1.0495	0.5030	0.0191*
H16A	0.0242	0.8114	−0.0744	0.0231*
H16B	0.0524	0.6045	−0.0586	0.0231*
H17	0.2561	0.9943	0.1731	0.0155*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0176 (8)	0.0300 (8)	0.0243 (9)	−0.0060 (7)	0.0021 (7)	−0.0043 (7)
O3	0.0299 (9)	0.0148 (8)	0.0241 (9)	−0.0015 (7)	0.0081 (8)	−0.0011 (7)
C1	0.0097 (10)	0.0150 (10)	0.0120 (11)	−0.0003 (9)	−0.0013 (9)	0.0004 (8)
C4	0.0125 (10)	0.0154 (10)	0.0119 (10)	0.0007 (9)	0.0031 (9)	−0.0003 (8)

C5	0.0140 (10)	0.0151 (10)	0.0115 (10)	-0.0009 (9)	0.0015 (8)	0.0006 (9)
C6	0.0127 (10)	0.0158 (10)	0.0147 (10)	0.0014 (9)	0.0064 (9)	-0.0006 (9)
C7	0.0172 (10)	0.0119 (10)	0.0120 (10)	0.0021 (10)	0.0029 (9)	-0.0005 (8)
C8	0.0234 (11)	0.0272 (12)	0.0133 (11)	-0.0008 (10)	0.0047 (10)	0.0015 (10)
C9	0.0155 (10)	0.0103 (10)	0.0203 (11)	0.0010 (9)	0.0033 (9)	0.0025 (9)
C10	0.0108 (10)	0.0162 (10)	0.0125 (10)	-0.0016 (9)	0.0032 (8)	-0.0005 (9)
C11	0.0185 (11)	0.0145 (10)	0.0104 (10)	-0.0010 (9)	0.0038 (9)	0.0000 (9)
C12	0.0243 (12)	0.0289 (12)	0.0191 (12)	0.0046 (11)	0.0111 (11)	0.0029 (10)
C13	0.0135 (10)	0.0176 (10)	0.0088 (10)	0.0002 (9)	-0.0005 (8)	0.0001 (9)
C14	0.0215 (11)	0.0182 (10)	0.0136 (11)	0.0046 (10)	0.0041 (10)	-0.0002 (9)
C15	0.0194 (11)	0.0148 (10)	0.0135 (10)	-0.0043 (9)	0.0040 (9)	-0.0023 (9)
C16	0.0187 (11)	0.0245 (11)	0.0132 (11)	-0.0002 (10)	0.0012 (9)	-0.0006 (10)
C17	0.0141 (10)	0.0157 (11)	0.0092 (10)	-0.0011 (9)	0.0028 (8)	0.0004 (8)

Geometric parameters (Å, °)

O2—C9	1.213 (3)	C11—C13	1.545 (3)
O3—C1	1.212 (3)	C12—C14	1.529 (3)
C1—C4	1.515 (3)	C13—C15	1.527 (3)
C1—C11	1.508 (3)	C6—H6	1.000
C4—C5	1.607 (3)	C7—H7	1.000
C4—C10	1.563 (3)	C8—H8A	0.990
C4—C14	1.513 (3)	C8—H8B	0.990
C5—C9	1.514 (3)	C10—H10	1.000
C5—C16	1.507 (3)	C11—H11	1.000
C5—C17	1.559 (3)	C12—H12A	0.990
C6—C7	1.551 (3)	C12—H12B	0.990
C6—C9	1.514 (3)	C13—H13	1.000
C6—C11	1.592 (3)	C14—H14A	0.990
C7—C15	1.519 (3)	C14—H14B	0.990
C7—C17	1.559 (3)	C15—H15A	0.990
C8—C12	1.542 (3)	C15—H15B	0.990
C8—C16	1.518 (4)	C16—H16A	0.990
C10—C13	1.562 (3)	C16—H16B	0.990
C10—C17	1.561 (3)	C17—H17	1.000
O3—C1—C4	127.23 (19)	C9—C6—H6	114.135
O3—C1—C11	127.2 (2)	C11—C6—H6	114.135
C4—C1—C11	105.51 (16)	C6—C7—H7	115.119
C1—C4—C5	107.96 (17)	C15—C7—H7	115.118
C1—C4—C10	103.01 (16)	C17—C7—H7	115.120
C1—C4—C14	115.82 (16)	C12—C8—H8A	108.685
C5—C4—C10	89.22 (13)	C12—C8—H8B	108.683
C5—C4—C14	114.08 (16)	C16—C8—H8A	108.691
C10—C4—C14	123.09 (18)	C16—C8—H8B	108.689
C4—C5—C9	109.73 (16)	H8A—C8—H8B	107.606
C4—C5—C16	112.73 (17)	C4—C10—H10	117.129
C4—C5—C17	89.09 (13)	C13—C10—H10	117.131

C9—C5—C16	116.65 (16)	C17—C10—H10	117.131
C9—C5—C17	102.89 (16)	C1—C11—H11	113.539
C16—C5—C17	122.17 (17)	C6—C11—H11	113.536
C7—C6—C9	102.03 (16)	C13—C11—H11	113.541
C7—C6—C11	101.77 (15)	C8—C12—H12A	108.656
C9—C6—C11	109.32 (16)	C8—C12—H12B	108.657
C6—C7—C15	104.62 (15)	C14—C12—H12A	108.658
C6—C7—C17	101.58 (15)	C14—C12—H12B	108.656
C15—C7—C17	103.62 (16)	H12A—C12—H12B	107.600
C12—C8—C16	114.29 (18)	C10—C13—H13	115.440
O2—C9—C5	127.41 (19)	C11—C13—H13	115.441
O2—C9—C6	127.0 (2)	C15—C13—H13	115.439
C5—C9—C6	105.60 (16)	C4—C14—H14A	108.851
C4—C10—C13	108.25 (16)	C4—C14—H14B	108.853
C4—C10—C17	90.62 (13)	C12—C14—H14A	108.847
C13—C10—C17	102.79 (16)	C12—C14—H14B	108.851
C1—C11—C6	109.06 (15)	H14A—C14—H14B	107.705
C1—C11—C13	103.40 (17)	C7—C15—H15A	112.692
C6—C11—C13	102.78 (14)	C7—C15—H15B	112.693
C8—C12—C14	114.41 (19)	C13—C15—H15A	112.688
C10—C13—C11	100.97 (14)	C13—C15—H15B	112.691
C10—C13—C15	103.29 (15)	H15A—C15—H15B	110.171
C11—C13—C15	104.40 (16)	C5—C16—H16A	109.278
C4—C14—C12	113.57 (17)	C5—C16—H16B	109.284
C7—C15—C13	95.25 (14)	C8—C16—H16A	109.283
C5—C16—C8	111.68 (15)	C8—C16—H16B	109.289
C5—C17—C7	107.95 (16)	H16A—C16—H16B	107.945
C5—C17—C10	91.07 (13)	C5—C17—H17	117.132
C7—C17—C10	102.72 (15)	C7—C17—H17	117.128
C7—C6—H6	114.136	C10—C17—H17	117.125
O3—C1—C4—C5	117.82 (19)	C17—C5—C9—C6	-31.56 (16)
O3—C1—C4—C10	-148.72 (17)	C16—C5—C17—C7	139.41 (16)
O3—C1—C4—C14	-11.5 (3)	C16—C5—C17—C10	-116.85 (17)
O3—C1—C11—C6	-116.94 (19)	C17—C5—C16—C8	55.3 (3)
O3—C1—C11—C13	134.22 (18)	C7—C6—C9—O2	-132.44 (18)
C4—C1—C11—C6	64.50 (17)	C7—C6—C9—C5	45.45 (16)
C4—C1—C11—C13	-44.33 (16)	C9—C6—C7—C15	-146.90 (14)
C11—C1—C4—C5	-63.62 (16)	C9—C6—C7—C17	-39.33 (16)
C11—C1—C4—C10	29.83 (16)	C7—C6—C11—C1	-108.45 (15)
C11—C1—C4—C14	167.07 (13)	C7—C6—C11—C13	0.80 (18)
C1—C4—C5—C9	0.38 (18)	C11—C6—C7—C15	-33.95 (18)
C1—C4—C5—C16	-131.45 (15)	C11—C6—C7—C17	73.62 (15)
C1—C4—C5—C17	103.75 (14)	C9—C6—C11—C1	-1.1 (2)
C1—C4—C10—C13	-4.89 (17)	C9—C6—C11—C13	108.17 (16)
C1—C4—C10—C17	-108.59 (14)	C11—C6—C9—O2	120.36 (19)
C1—C4—C14—C12	172.87 (13)	C11—C6—C9—C5	-61.75 (18)
C5—C4—C10—C13	103.37 (14)	C6—C7—C15—C13	52.83 (17)

C5—C4—C10—C17	-0.32 (14)	C6—C7—C17—C5	20.61 (15)
C10—C4—C5—C9	-103.05 (15)	C6—C7—C17—C10	-74.74 (14)
C10—C4—C5—C16	125.12 (15)	C15—C7—C17—C5	128.95 (13)
C10—C4—C5—C17	0.32 (14)	C15—C7—C17—C10	33.60 (16)
C5—C4—C14—C12	46.6 (2)	C17—C7—C15—C13	-53.23 (15)
C14—C4—C5—C9	130.65 (16)	C12—C8—C16—C5	55.0 (3)
C14—C4—C5—C16	-1.2 (2)	C16—C8—C12—C14	-8.9 (3)
C14—C4—C5—C17	-125.97 (16)	C4—C10—C13—C11	-20.73 (17)
C10—C4—C14—C12	-59.3 (2)	C4—C10—C13—C15	-128.55 (14)
C14—C4—C10—C13	-138.05 (16)	C4—C10—C17—C5	0.33 (14)
C14—C4—C10—C17	118.25 (17)	C4—C10—C17—C7	109.01 (14)
C4—C5—C9—O2	-119.97 (18)	C13—C10—C17—C5	-108.55 (13)
C4—C5—C9—C6	62.16 (16)	C13—C10—C17—C7	0.13 (15)
C4—C5—C16—C8	-48.8 (2)	C17—C10—C13—C11	74.24 (14)
C4—C5—C17—C7	-104.06 (14)	C17—C10—C13—C15	-33.59 (16)
C4—C5—C17—C10	-0.32 (14)	C1—C11—C13—C10	38.86 (15)
C9—C5—C16—C8	-177.11 (14)	C1—C11—C13—C15	145.81 (13)
C16—C5—C9—O2	9.8 (3)	C6—C11—C13—C10	-74.61 (16)
C16—C5—C9—C6	-168.10 (14)	C6—C11—C13—C15	32.34 (17)
C9—C5—C17—C7	5.98 (16)	C8—C12—C14—C4	-41.6 (2)
C9—C5—C17—C10	109.72 (13)	C10—C13—C15—C7	53.16 (16)
C17—C5—C9—O2	146.32 (17)	C11—C13—C15—C7	-52.06 (16)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C6—H6...O3 ⁱ	1.00	2.58	3.547 (3)	163

Symmetry code: (i) $-x, y+1/2, -z+1$.