

## 2-Ethyl 3,4-dimethyl 4'-bromobiphenyl-2,3,4-tricarboxylate

S. Thenmozhi,<sup>a</sup> A. Subbiah Pandi,<sup>a</sup> D. Velmurugan,<sup>b\*</sup> C. Prakash<sup>c</sup> and K. Ravikumar<sup>d</sup>

<sup>a</sup>Department of Physics, Presidency College (Autonomous), Chennai 600 005, India,

<sup>b</sup>Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, <sup>c</sup>Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and <sup>d</sup>Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India  
Correspondence e-mail: d\_velu@yahoo.com

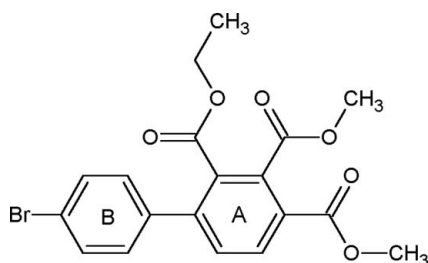
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.109; data-to-parameter ratio = 17.8.

In the title compound,  $\text{C}_{19}\text{H}_{17}\text{BrO}_6$ , the biphenyl twist angle is  $43.6$  (1)°. All three ester groups are planar and make dihedral angles of  $61.0$  (1),  $70.6$  (1) and  $14.1$  (1)° with the attached benzene ring.

### Related literature

For related literature, see: Bondi (1964); Kovacic & Jones (1987); Pedersen (1975); Subbiah Pandi, Velmurugan, Raghukumar *et al.* (2002); Subbiah Pandi, Velmurugan, Shanmuga Sundara Raj *et al.* (2002); Sundari Bhaskaran *et al.* (2005); Tour (1996).



### Experimental

#### Crystal data

$\text{C}_{19}\text{H}_{17}\text{BrO}_6$	$\gamma = 85.01$ (1)°
$M_r = 421.24$	$V = 930.21$ (11) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.0122$ (5) Å	Mo $K\alpha$ radiation
$b = 8.9766$ (6) Å	$\mu = 2.24$ mm <sup>-1</sup>
$c = 15.3539$ (10) Å	$T = 293$ (2) K
$\alpha = 75.073$ (10)°	$0.21 \times 0.19 \times 0.17$ mm
$\beta = 89.51$ (1)°	

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer	10647 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	4228 independent reflections
$T_{\min} = 0.631$ , $T_{\max} = 0.683$	3380 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.022$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	238 parameters
$wR(F^2) = 0.110$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.66$ e Å <sup>-3</sup>
4228 reflections	$\Delta\rho_{\text{min}} = -0.55$ e Å <sup>-3</sup>

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ZORTEP (Zsolnai, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PARST (Nardelli, 1995).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2466).

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**supplementary materials**

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## 2-Ethyl 3,4-dimethyl 4'-bromobiphenyl-2,3,4-tricarboxylate

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### Comment

Compounds with a bond between two aromatic rings and their derivatives with extended structures (Oligomers and polymers) have received considerable interest owing to their intriguing structural motifs and unique electroconductive, nonlinear optical and luminescence properties (Kovacic & Jones, 1987; Tour, 1996). Interestingly, after growth with biphenyl, many bacteria can oxidize polychlorinated biphenyl (PCBs). Compounds composed of biphenyl unities and containing from 1 to 10 chlorines are toxic in biosphere. Biphenyl dioxygenase plays a critical role in PCB degradation by catalyzing the first step. Its activity varies depending on the number of halogens and their positions on the aromatic ring. The study of brominated biphenyl is of importance both in terms of structure and function.

The angles in the phenyl rings range from 118.2 (2) to 121.5 (2)° in ring A and 118.3 (2) to 121.6 (2)° in ring B, differing significantly from 120°, a feature similar to that observed in polychlorinated biphenyls (Pedersen, 1975). The dihedral angle between the two rings comprising the biphenyl core, the biphenyl twist angle, is 43.6 (1)°. This biphenyl twist angle agrees well with chlorinated biphenyl [45.4 (2)°, Sundari Bhaskaran *et al.*, 2005]. In this structure inter ring bond distance C1—C1' is 1.491 (3) Å. This value agrees well with those of related structures found in chloro substituted biphenyl [1.491 (2) Å; Sundari Bhaskaran *et al.*, 2005]. The deviation from orthogonality can be attributed to the absence of a hydrogen bonding substituent in the *ortho* position of the second benzene ring. The twist angle of the present compound is comparable to that of the two polymorphic structures lacking an *ortho* substitution in the second ring (Subbiah Pandi, Velmurugan, Shanmuga Sundara Raj *et al.*, 2002; Subbiah Pandi, Velmurugan, Raghukumar *et al.*, 2002).

The non-H atoms of each ester group lie nearly in a plane. The ester plane O1/C7/O2/C8/C9, O3/C10/O4/C11 and O5/C12/O6/C13 are inclined at angles 61.0 (1)° and 70.6 (1)° and 14.1 (1)° to the phenyl ring to which they are attached. The ester plane O5/C12/O6/C13 is nearly orthogonal to the other two ester planes [73.2 (1)° and 73.6 (1)°] and is nearly parallel [14.1 (1)°] to the phenyl ring which is attached. The C—O—C angles [C7—O2—C8, C10—O4—C11 and C12—O6—C13] are around 116°.

The closest intermolecular distance is between H8B and H8B<sup>i</sup> [symmetry code: (i)  $-x + 2, -y + 2, -z$ ] and is shorter than the sum of the van der Waals radii sums (Bondi, 1964) by 0.29 Å. Another remarkable feature of the crystal structure of the title compound is the existence of a short intermolecular halogen...halogen contact Br1...Br1<sup>ii</sup> [3.474 (1) Å] [symmetry code: (ii)  $-x + 1, -y + 2, -z + 1$ ] between the bromine atoms.

### Experimental

The title compound was prepared involving a Diels-Alder reaction between insitu generated enamine [DMF-DMA,(2.5 mmol) and *p*-bromo unsaturated ester (1 mmol) and DMAD at 60° C. The usual workup followed by recrystallization using 1:1 ethyl acetate-hexane afforded excellent crystals.

## Refinement

All H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.93–0.97 Å and with  $U_{\text{iso}}(\text{H})$  values of  $1.5U_{\text{eq}}(\text{C})$  for methyl H and  $1.2U_{\text{eq}}(\text{C})$  for other H atoms.

## Figures

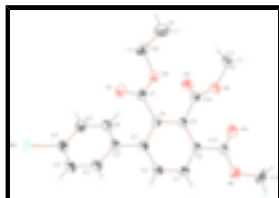


Fig. 1. The molecular configuration and atom-numbering scheme for the title compound. Displacement ellipsoids are drawn at the 40% probability level and H atoms are shown as small spheres of arbitrary radii.

## 2-Ethyl 3,4-dimethyl 4'-bromobiphenyl-2,3,4-tricarboxylate

### Crystal data

$\text{C}_{19}\text{H}_{17}\text{BrO}_6$

$M_r = 421.24$

Triclinic,  $P\bar{1}$

Hall symbol: -p 1

$a = 7.0122(5) \text{ \AA}$

$b = 8.9766(6) \text{ \AA}$

$c = 15.3539(10) \text{ \AA}$

$\alpha = 75.073(10)^\circ$

$\beta = 89.510(10)^\circ$

$\gamma = 85.010(10)^\circ$

$V = 930.21(11) \text{ \AA}^3$

$Z = 2$

$F_{000} = 428$

$D_x = 1.504 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2120 reflections

$\theta = 2.4\text{--}28.0^\circ$

$\mu = 2.24 \text{ mm}^{-1}$

$T = 293(2) \text{ K}$

Block, colourless

$0.21 \times 0.19 \times 0.17 \text{ mm}$

### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2) \text{ K}$

$\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2001)

$T_{\text{min}} = 0.631$ ,  $T_{\text{max}} = 0.683$

10647 measured reflections

4228 independent reflections

3380 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\text{max}} = 28.0^\circ$

$\theta_{\text{min}} = 2.4^\circ$

$h = -9 \rightarrow 9$

$k = -11 \rightarrow 11$

$l = -20 \rightarrow 19$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.3096P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
4228 reflections	$(\Delta/\sigma)_{\max} = 0.001$
238 parameters	$\Delta\rho_{\max} = 0.66 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.55 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	-0.37088 (4)	0.90355 (3)	0.43084 (2)	0.07536 (14)
O1	0.3586 (3)	0.90736 (19)	0.18374 (12)	0.0613 (4)
O2	0.3180 (2)	0.76398 (17)	0.08639 (10)	0.0477 (4)
O3	0.7671 (2)	0.74492 (18)	0.09710 (10)	0.0505 (4)
O4	0.6697 (2)	0.54018 (19)	0.05724 (10)	0.0481 (4)
O5	0.9818 (3)	0.4143 (2)	0.18441 (12)	0.0640 (5)
O6	0.9334 (3)	0.2182 (2)	0.30234 (12)	0.0640 (5)
C1	0.3577 (3)	0.5793 (2)	0.31186 (13)	0.0411 (4)
C2	0.4405 (3)	0.4438 (3)	0.36956 (14)	0.0503 (5)
H2	0.3833	0.4037	0.4245	0.060*
C3	0.6051 (3)	0.3678 (3)	0.34720 (14)	0.0482 (5)
H3	0.6581	0.2779	0.3874	0.058*
C4	0.6932 (3)	0.4239 (2)	0.26515 (13)	0.0398 (4)
C5	0.6081 (3)	0.5563 (2)	0.20462 (12)	0.0370 (4)
C6	0.4436 (3)	0.6351 (2)	0.22834 (13)	0.0382 (4)
C1'	0.1801 (3)	0.6579 (2)	0.33965 (13)	0.0427 (4)
C2'	0.1654 (4)	0.6749 (3)	0.42695 (15)	0.0567 (6)
H2'	0.2670	0.6372	0.4674	0.068*

## supplementary materials

C3'	0.0018 (4)	0.7471 (3)	0.45488 (16)	0.0609 (6)
H3'	-0.0064	0.7586	0.5133	0.073*
C4'	-0.1480 (3)	0.8014 (3)	0.39456 (16)	0.0500 (5)
C5'	-0.1396 (3)	0.7849 (3)	0.30811 (16)	0.0491 (5)
H5'	-0.2424	0.8214	0.2683	0.059*
C6'	0.0253 (3)	0.7125 (3)	0.28117 (15)	0.0456 (5)
H6'	0.0320	0.7005	0.2228	0.055*
C7	0.3685 (3)	0.7860 (2)	0.16512 (14)	0.0420 (4)
C8	0.2483 (5)	0.9014 (3)	0.01784 (19)	0.0765 (9)
H8A	0.3369	0.9804	0.0122	0.092*
H8B	0.1250	0.9418	0.0351	0.092*
C9	0.2297 (6)	0.8634 (4)	-0.0678 (2)	0.0856 (10)
H9A	0.3530	0.8280	-0.0860	0.128*
H9B	0.1792	0.9537	-0.1125	0.128*
H9C	0.1445	0.7833	-0.0615	0.128*
C10	0.6951 (3)	0.6246 (2)	0.11437 (13)	0.0384 (4)
C11	0.7451 (4)	0.5970 (4)	-0.03205 (16)	0.0622 (7)
H11A	0.6755	0.6935	-0.0616	0.093*
H11B	0.7318	0.5229	-0.0664	0.093*
H11C	0.8780	0.6125	-0.0274	0.093*
C12	0.8826 (3)	0.3531 (2)	0.24429 (14)	0.0434 (5)
C13	1.1191 (4)	0.1446 (4)	0.2883 (2)	0.0771 (9)
H13A	1.1171	0.1152	0.2325	0.116*
H13B	1.1483	0.0542	0.3370	0.116*
H13C	1.2148	0.2156	0.2860	0.116*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0654 (2)	0.0704 (2)	0.0811 (2)	0.01665 (13)	0.03414 (15)	-0.01137 (14)
O1	0.0836 (13)	0.0411 (9)	0.0594 (10)	0.0062 (8)	0.0057 (9)	-0.0171 (7)
O2	0.0550 (9)	0.0430 (8)	0.0404 (8)	0.0092 (6)	-0.0041 (6)	-0.0061 (6)
O3	0.0604 (10)	0.0460 (9)	0.0437 (8)	-0.0089 (7)	0.0088 (7)	-0.0080 (6)
O4	0.0573 (9)	0.0542 (9)	0.0368 (7)	-0.0081 (7)	0.0146 (6)	-0.0181 (6)
O5	0.0575 (10)	0.0638 (10)	0.0584 (10)	0.0135 (8)	0.0233 (8)	-0.0007 (8)
O6	0.0591 (10)	0.0499 (9)	0.0684 (11)	0.0178 (8)	0.0185 (8)	0.0034 (8)
C1	0.0415 (11)	0.0465 (11)	0.0356 (10)	0.0016 (8)	0.0058 (8)	-0.0132 (8)
C2	0.0524 (12)	0.0555 (13)	0.0365 (10)	0.0040 (10)	0.0138 (9)	-0.0033 (9)
C3	0.0527 (12)	0.0455 (11)	0.0387 (10)	0.0074 (9)	0.0064 (9)	-0.0013 (9)
C4	0.0429 (10)	0.0387 (10)	0.0364 (9)	0.0031 (8)	0.0070 (8)	-0.0097 (8)
C5	0.0417 (10)	0.0370 (9)	0.0328 (9)	-0.0007 (8)	0.0059 (7)	-0.0109 (7)
C6	0.0408 (10)	0.0384 (10)	0.0353 (9)	0.0004 (8)	0.0039 (8)	-0.0111 (8)
C1'	0.0422 (11)	0.0475 (11)	0.0387 (10)	0.0004 (9)	0.0096 (8)	-0.0131 (9)
C2'	0.0513 (13)	0.0782 (17)	0.0381 (11)	0.0128 (12)	0.0036 (9)	-0.0166 (11)
C3'	0.0624 (15)	0.0784 (17)	0.0421 (12)	0.0090 (13)	0.0139 (11)	-0.0211 (12)
C4'	0.0453 (11)	0.0492 (12)	0.0539 (13)	0.0024 (9)	0.0195 (10)	-0.0130 (10)
C5'	0.0387 (11)	0.0551 (13)	0.0530 (12)	-0.0008 (9)	0.0040 (9)	-0.0142 (10)
C6'	0.0441 (11)	0.0539 (12)	0.0423 (11)	-0.0024 (9)	0.0051 (9)	-0.0193 (9)

C7	0.0404 (10)	0.0415 (11)	0.0418 (11)	0.0034 (8)	0.0081 (8)	-0.0091 (8)
C8	0.095 (2)	0.0599 (16)	0.0597 (16)	0.0268 (15)	-0.0185 (15)	0.0009 (13)
C9	0.124 (3)	0.0666 (18)	0.0573 (16)	-0.0003 (19)	-0.0186 (17)	-0.0021 (14)
C10	0.0391 (10)	0.0399 (10)	0.0340 (9)	0.0040 (8)	0.0041 (8)	-0.0080 (8)
C11	0.0658 (16)	0.0857 (19)	0.0390 (12)	-0.0132 (13)	0.0184 (11)	-0.0217 (12)
C12	0.0472 (11)	0.0416 (11)	0.0408 (10)	0.0046 (9)	0.0057 (9)	-0.0124 (8)
C13	0.0622 (16)	0.0595 (16)	0.097 (2)	0.0239 (13)	0.0155 (15)	-0.0077 (15)

*Geometric parameters (Å, °)*

Br1—C4'	1.895 (2)	C1'—C6'	1.386 (3)
O1—C7	1.192 (3)	C1'—C2'	1.390 (3)
O2—C7	1.330 (3)	C2'—C3'	1.388 (3)
O2—C8	1.450 (3)	C2'—H2'	0.9300
O3—C10	1.199 (3)	C3'—C4'	1.376 (4)
O4—C10	1.320 (3)	C3'—H3'	0.9300
O4—C11	1.447 (3)	C4'—C5'	1.373 (3)
O5—C12	1.194 (3)	C5'—C6'	1.389 (3)
O6—C12	1.327 (3)	C5'—H5'	0.9300
O6—C13	1.448 (3)	C6'—H6'	0.9300
C1—C2	1.390 (3)	C8—C9	1.450 (4)
C1—C6	1.402 (3)	C8—H8A	0.9700
C1—C1'	1.491 (3)	C8—H8B	0.9700
C2—C3	1.376 (3)	C9—H9A	0.9600
C2—H2	0.9300	C9—H9B	0.9600
C3—C4	1.391 (3)	C9—H9C	0.9600
C3—H3	0.9300	C11—H11A	0.9600
C4—C5	1.396 (3)	C11—H11B	0.9600
C4—C12	1.491 (3)	C11—H11C	0.9600
C5—C6	1.395 (3)	C13—H13A	0.9600
C5—C10	1.510 (3)	C13—H13B	0.9600
C6—C7	1.503 (3)	C13—H13C	0.9600
C7—O2—C8	116.2 (2)	C5'—C6'—C1'	121.2 (2)
C10—O4—C11	115.7 (2)	C5'—C6'—H6'	119.4
C12—O6—C13	115.8 (2)	C1'—C6'—H6'	119.4
C2—C1—C6	118.17 (19)	O1—C7—O2	125.6 (2)
C2—C1—C1'	119.34 (18)	O1—C7—C6	124.0 (2)
C6—C1—C1'	122.48 (18)	O2—C7—C6	110.38 (17)
C3—C2—C1	121.47 (19)	O2—C8—C9	109.7 (3)
C3—C2—H2	119.3	O2—C8—H8A	109.7
C1—C2—H2	119.3	C9—C8—H8A	109.7
C2—C3—C4	120.70 (19)	O2—C8—H8B	109.7
C2—C3—H3	119.7	C9—C8—H8B	109.7
C4—C3—H3	119.7	H8A—C8—H8B	108.2
C3—C4—C5	118.76 (19)	C8—C9—H9A	109.5
C3—C4—C12	121.23 (18)	C8—C9—H9B	109.5
C5—C4—C12	119.83 (17)	H9A—C9—H9B	109.5
C4—C5—C6	120.33 (17)	C8—C9—H9C	109.5
C4—C5—C10	121.90 (17)	H9A—C9—H9C	109.5

## supplementary materials

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C6—C5—C10	117.67 (17)	H9B—C9—H9C	109.5
C5—C6—C1	120.48 (18)	O3—C10—O4	125.60 (18)
C5—C6—C7	118.51 (17)	O3—C10—C5	123.02 (18)
C1—C6—C7	120.89 (18)	O4—C10—C5	111.24 (17)
C6'—C1'—C2'	118.3 (2)	O4—C11—H11A	109.5
C6'—C1'—C1	121.85 (18)	O4—C11—H11B	109.5
C2'—C1'—C1	119.83 (19)	H11A—C11—H11B	109.5
C1'—C2'—C3'	121.2 (2)	O4—C11—H11C	109.5
C1'—C2'—H2'	119.4	H11A—C11—H11C	109.5
C3'—C2'—H2'	119.4	H11B—C11—H11C	109.5
C4'—C3'—C2'	118.8 (2)	O5—C12—O6	123.6 (2)
C4'—C3'—H3'	120.6	O5—C12—C4	123.66 (19)
C2'—C3'—H3'	120.6	O6—C12—C4	112.61 (18)
C3'—C4'—C5'	121.6 (2)	O6—C13—H13A	109.5
C3'—C4'—Br1	119.43 (17)	O6—C13—H13B	109.5
C5'—C4'—Br1	118.95 (18)	H13A—C13—H13B	109.5
C4'—C5'—C6'	118.8 (2)	O6—C13—H13C	109.5
C4'—C5'—H5'	120.6	H13A—C13—H13C	109.5
C6'—C5'—H5'	120.6	H13B—C13—H13C	109.5
C6—C1—C2—C3	1.7 (3)	C2'—C3'—C4'—Br1	-178.9 (2)
C1'—C1—C2—C3	-179.5 (2)	C3'—C4'—C5'—C6'	-0.5 (4)
C1—C2—C3—C4	-0.6 (4)	Br1—C4'—C5'—C6'	178.81 (17)
C2—C3—C4—C5	-2.0 (3)	C4'—C5'—C6'—C1'	-0.2 (3)
C2—C3—C4—C12	173.1 (2)	C2'—C1'—C6'—C5'	1.1 (3)
C3—C4—C5—C6	3.4 (3)	C1—C1'—C6'—C5'	179.7 (2)
C12—C4—C5—C6	-171.74 (19)	C8—O2—C7—O1	1.1 (3)
C3—C4—C5—C10	179.8 (2)	C8—O2—C7—C6	-178.1 (2)
C12—C4—C5—C10	4.7 (3)	C5—C6—C7—O1	-116.9 (2)
C4—C5—C6—C1	-2.4 (3)	C1—C6—C7—O1	59.2 (3)
C10—C5—C6—C1	-178.90 (19)	C5—C6—C7—O2	62.3 (2)
C4—C5—C6—C7	173.77 (19)	C1—C6—C7—O2	-121.6 (2)
C10—C5—C6—C7	-2.8 (3)	C7—O2—C8—C9	170.5 (3)
C2—C1—C6—C5	-0.3 (3)	C11—O4—C10—O3	3.2 (3)
C1'—C1—C6—C5	-178.98 (19)	C11—O4—C10—C5	179.0 (2)
C2—C1—C6—C7	-176.3 (2)	C4—C5—C10—O3	-109.6 (2)
C1'—C1—C6—C7	5.0 (3)	C6—C5—C10—O3	66.9 (3)
C2—C1—C1'—C6'	-134.7 (2)	C4—C5—C10—O4	74.4 (2)
C6—C1—C1'—C6'	44.0 (3)	C6—C5—C10—O4	-109.1 (2)
C2—C1—C1'—C2'	43.9 (3)	C13—O6—C12—O5	-1.2 (4)
C6—C1—C1'—C2'	-137.4 (2)	C13—O6—C12—C4	-178.0 (2)
C6'—C1'—C2'—C3'	-1.2 (4)	C3—C4—C12—O5	-164.0 (2)
C1—C1'—C2'—C3'	-179.8 (2)	C5—C4—C12—O5	11.0 (3)
C1'—C2'—C3'—C4'	0.4 (4)	C3—C4—C12—O6	12.7 (3)
C2'—C3'—C4'—C5'	0.4 (4)	C5—C4—C12—O6	-172.2 (2)



Fig. 1

