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2′-(2-Hydroxyethoxy)-1,1′-biphenyl-2-ol

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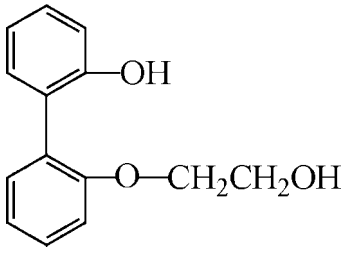
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.145; data-to-parameter ratio = 13.5.

The title compound, $C_{14}H_{14}O_3$, was obtained by the Williamson method using 2,2′-dihydroxy-1,1′-biphenyl with chlorohydrin. The asymmetric unit contains two crystallographically independent molecules which differ slightly in the orientations of the hydroxyethoxy side chains. In each independent molecule, an intramolecular O—H···O hydrogen bond is observed. In the solid state, each of the two independent molecules forms an O—H···O hydrogen-bonded centrosymmetric dimer. The crystal packing is further stabilized by C—H···π interactions.

Related literature

For the general role of biphenyl ethers, see: Martinez-Gomez *et al.* (2006); Shishkina *et al.* (2007). For related hydrogen bonds, see: Dabrowska *et al.* (2007). For the synthesis of related compounds, see: Niu *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{14}O_3$
M_r = 230.25
Triclinic, $P\overline{1}$
a = 7.2804 (15) Å
b = 12.8846 (18) Å
c = 14.106 (2) Å
α = 108.870 (3)°
β = 101.160 (2)°
γ = 99.516 (2)°
V = 1190.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.59 × 0.53 × 0.44 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.962
6226 measured reflections
4133 independent reflections
2562 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.145
S = 1.02
4133 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected torsion angles (°).

C3—O2—C2—C1	159.09 (19)	C17—O5—C16—C15	75.7 (3)
O1—C1—C2—O2	−59.1 (3)	O4—C15—C16—O5	50.4 (4)
C2—O2—C3—C4	27.2 (3)	C16—O5—C17—C18	15.8 (3)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 denote the centroids of the C23–C28, C17–C22 and C3–C8 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3	0.82	2.02	2.821 (3)	164
O3—H3···O1^{i}	0.82	1.87	2.660 (3)	160
O4—H4···O6	0.82	1.99	2.797 (3)	169
O6—H6···O4^{ii}	0.82	1.87	2.661 (3)	161
C1—H1*B*···*Cg*1^{iii}	0.97	2.75	3.584 (3)	144
C5—H5···*Cg*2^{iv}	0.93	2.71	3.602 (3)	160
C11—H11···*Cg*3^{v}	0.93	2.93	3.742 (3)	146

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x-1, y, z$; (v) $x+1, y, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2446).

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supplementary materials

Acta Cryst. (2007). E**63**, o4089 [**doi:10.1107/S1600536807044029**]

2'-(2-Hydroxyethoxy)-1,1'-biphenyl-2-ol

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Comment

Biphenyl ethers are used extensively as important chemical materials in the field of liquid crystal chemistry and crown ether chemistry (Martinez-Gomez *et al.*, 2006; Shishkina *et al.*, 2007). We report here the crystal structure of the title compound.

The asymmetric unit of the title compound contains two crystallographically independent molecules (Fig. 1). These molecules differ slightly in the orientations of the hydroxyethoxy side chains (Table 1). In one of the independent molecules the two benzene rings (C3—C8 and C9—C14) are twisted away from one another by 59.02 (13)° while in the other molecule the rings are twisted by 63.24 (16)°.

The conformation of each independent molecule is influenced by an intramolecular O—H···O hydrogen bond (Table 2), similar to that observed by Dabrowska *et al.* (2007). In the solid state, each of the two independent molecules exists as an O—H···O hydrogen-bonded centrosymmetric dimer, and one such dimer is shown in Fig.2. In addition, the crystal packing is stabilized by C—H···π interactions (Table 2). In Table 2, *Cg*1, *Cg*2 and *Cg*3 denote the centroids of C23—C28, C17—C22 and C3—C8 rings, respectively.

Experimental

The reaction was carried out under nitrogen atmosphere (Niu *et al.*, 2006). 2,2'-Dihydroxy-1,1'-biphenyl (7.44 g, 0.04 mol), sodium hydroxide (1.6 g, 0.04 mol) and chlorohydrin (2.68 ml, 0.04 mol) were added to a solution of ethanol (40 ml). The mixture was heated at reflux for 7 h to ensure completion of the reaction. After cooling to room temperature, the solid product obtained was filtered off and was recrystallized from n-heptane. Single crystals of the title compound suitable for X-ray analysis were grown from ethanol by slow evaporation at room temperature over a period of about one week. Analysis $C_{14}H_{14}O_3$: C 72.76, H 6.43%; found: C 72.71, H 6.53%.

Refinement

All H atoms were placed in geometrically idealized positions (O—H = 0.82 Å and C—H 0.93 or 0.97 Å) and treated as riding on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}(O)$ or $1.2U_{eq}(C)$.

Figures

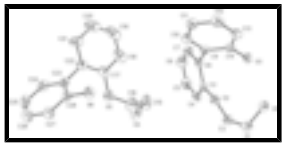


Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering. H atoms have been omitted for clarity.

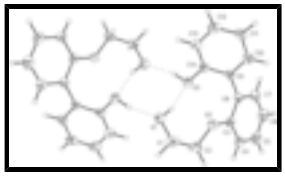


Fig. 2. A view of an O—H···O hydrogen-bonded (dashed lines) dimer in the title compound.

2'-(2-Hydroxyethoxy)-1,1'-biphenyl-2-ol

Crystal data

$C_{14}H_{14}O_3$	$Z = 4$
$M_r = 230.25$	$F_{000} = 488$
Triclinic, $P\overline{1}$	$D_x = 1.284$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.2804$ (15) Å	Cell parameters from 1864 reflections
$b = 12.8846$ (18) Å	$\theta = 2.7$–23.7º
$c = 14.106$ (2) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 108.870$ (3)º	$T = 298$ (2) K
$\beta = 101.160$ (2)º	Block, colourless
$\gamma = 99.516$ (2)º	0.59 × 0.53 × 0.44 mm
$V = 1190.8$ (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4133 independent reflections
Radiation source: fine-focus sealed tube	2562 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.949$, $T_{max} = 0.962$	$k = -15 \rightarrow 14$
6226 measured reflections	$l = -16 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.145$	$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.2314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
4133 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
307 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.0453 (3)	0.04937 (14)	0.14343 (14)	0.0736 (6)
H1	0.0755	0.0910	0.1127	0.110*
O2	0.2256 (2)	0.27719 (12)	0.22548 (12)	0.0469 (4)
O3	0.1344 (2)	0.15170 (13)	0.00340 (12)	0.0506 (4)
H3	0.0992	0.0844	−0.0338	0.076*
O4	0.7641 (3)	0.52204 (15)	0.45876 (17)	0.0794 (6)
H4	0.8674	0.5627	0.4634	0.119*
O5	0.7889 (3)	0.74097 (15)	0.46791 (14)	0.0628 (5)
O6	1.1385 (2)	0.64946 (13)	0.49509 (13)	0.0564 (5)
H6	1.1735	0.6069	0.5234	0.085*
C1	0.0777 (4)	0.1153 (2)	0.25096 (19)	0.0559 (7)
H1A	0.2016	0.1127	0.2895	0.067*
H1B	−0.0217	0.0834	0.2776	0.067*
C2	0.0755 (4)	0.2349 (2)	0.2665 (2)	0.0549 (7)
H2A	−0.0491	0.2389	0.2302	0.066*
H2B	0.0998	0.2793	0.3398	0.066*
C3	0.2114 (3)	0.36991 (18)	0.19976 (17)	0.0422 (6)
C4	0.1180 (4)	0.4490 (2)	0.24718 (19)	0.0525 (6)
H4A	0.0594	0.4395	0.2978	0.063*
C5	0.1116 (4)	0.5422 (2)	0.2196 (2)	0.0642 (8)
H5	0.0474	0.5949	0.2510	0.077*
C6	0.1997 (5)	0.5569 (2)	0.1459 (2)	0.0708 (8)
H6A	0.1954	0.6196	0.1272	0.085*
C7	0.2950 (4)	0.4788 (2)	0.0994 (2)	0.0599 (7)
H7	0.3545	0.4900	0.0496	0.072*
C8	0.3046 (3)	0.38399 (18)	0.12474 (17)	0.0419 (6)
C9	0.4140 (3)	0.30379 (19)	0.07534 (17)	0.0413 (6)
C10	0.6086 (4)	0.3426 (2)	0.08374 (19)	0.0550 (7)
H10	0.6697	0.4182	0.1229	0.066*
C11	0.7144 (4)	0.2715 (3)	0.0352 (2)	0.0614 (7)
H11	0.8441	0.2995	0.0413	0.074*

C12	0.6259 (4)	0.1602 (2)	−0.0215 (2)	0.0606 (7)
H12	0.6958	0.1120	−0.0540	0.073*
C13	0.4345 (4)	0.1191 (2)	−0.03062 (18)	0.0508 (6)
H13	0.3757	0.0429	−0.0685	0.061*
C14	0.3284 (3)	0.19018 (19)	0.01615 (17)	0.0410 (5)
C15	0.6137 (5)	0.5472 (3)	0.3989 (3)	0.0881 (11)
H15A	0.4921	0.4983	0.3930	0.106*
H15B	0.6307	0.5317	0.3296	0.106*
C16	0.6050 (4)	0.6646 (3)	0.4432 (3)	0.0827 (10)
H16A	0.5120	0.6807	0.3940	0.099*
H16B	0.5612	0.6762	0.5057	0.099*
C17	0.8592 (5)	0.7621 (2)	0.3902 (2)	0.0602 (7)
C18	0.7459 (6)	0.7352 (2)	0.2908 (2)	0.0853 (11)
H18	0.6161	0.6977	0.2717	0.102*
C19	0.8302 (8)	0.7657 (3)	0.2196 (3)	0.1014 (14)
H19	0.7558	0.7468	0.1522	0.122*
C20	1.0166 (8)	0.8217 (3)	0.2467 (3)	0.0997 (13)
H20	1.0695	0.8424	0.1986	0.120*
C21	1.1299 (6)	0.8487 (2)	0.3464 (3)	0.0802 (10)
H21	1.2583	0.8883	0.3648	0.096*
C22	1.0549 (4)	0.8175 (2)	0.4192 (2)	0.0568 (7)
C23	1.1798 (4)	0.84402 (19)	0.52450 (19)	0.0495 (6)
C24	1.2675 (4)	0.9555 (2)	0.5899 (2)	0.0637 (7)
H24	1.2429	1.0138	0.5680	0.076*
C25	1.3902 (4)	0.9814 (3)	0.6867 (3)	0.0731 (9)
H25	1.4473	1.0566	0.7292	0.088*
C26	1.4279 (4)	0.8967 (3)	0.7198 (2)	0.0700 (8)
H26	1.5103	0.9144	0.7851	0.084*
C27	1.3445 (4)	0.7853 (2)	0.6571 (2)	0.0588 (7)
H27	1.3703	0.7277	0.6798	0.071*
C28	1.2219 (3)	0.75958 (19)	0.56005 (19)	0.0471 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0995 (15)	0.0516 (11)	0.0570 (12)	−0.0078 (10)	0.0310 (11)	0.0106 (9)
O2	0.0470 (10)	0.0498 (9)	0.0476 (10)	0.0121 (7)	0.0190 (8)	0.0190 (8)
O3	0.0447 (10)	0.0479 (9)	0.0491 (10)	0.0026 (7)	0.0147 (8)	0.0079 (8)
O4	0.0594 (12)	0.0650 (12)	0.1080 (16)	0.0071 (10)	−0.0061 (12)	0.0444 (12)
O5	0.0576 (12)	0.0642 (11)	0.0653 (12)	0.0134 (9)	0.0122 (10)	0.0253 (10)
O6	0.0612 (11)	0.0449 (10)	0.0614 (11)	0.0136 (8)	0.0100 (9)	0.0205 (9)
C1	0.0592 (17)	0.0593 (16)	0.0518 (16)	0.0098 (13)	0.0225 (13)	0.0217 (13)
C2	0.0526 (16)	0.0650 (17)	0.0493 (15)	0.0121 (13)	0.0221 (13)	0.0200 (13)
C3	0.0383 (13)	0.0395 (13)	0.0392 (13)	0.0050 (10)	0.0036 (11)	0.0078 (10)
C4	0.0495 (15)	0.0521 (15)	0.0483 (15)	0.0118 (12)	0.0164 (12)	0.0069 (12)
C5	0.0654 (19)	0.0471 (15)	0.0738 (19)	0.0219 (13)	0.0188 (16)	0.0099 (14)
C6	0.087 (2)	0.0508 (16)	0.082 (2)	0.0236 (15)	0.0246 (18)	0.0288 (16)
C7	0.0723 (19)	0.0528 (16)	0.0603 (17)	0.0145 (14)	0.0246 (15)	0.0244 (14)

C8	0.0367 (13)	0.0420 (13)	0.0404 (13)	0.0040 (10)	0.0081 (11)	0.0106 (11)
C9	0.0410 (14)	0.0480 (14)	0.0347 (12)	0.0062 (11)	0.0108 (11)	0.0165 (11)
C10	0.0448 (16)	0.0615 (16)	0.0503 (15)	0.0009 (13)	0.0113 (13)	0.0164 (13)
C11	0.0361 (14)	0.091 (2)	0.0560 (17)	0.0121 (14)	0.0159 (13)	0.0244 (16)
C12	0.0534 (17)	0.077 (2)	0.0546 (16)	0.0274 (15)	0.0190 (14)	0.0200 (15)
C13	0.0548 (17)	0.0523 (14)	0.0456 (14)	0.0167 (12)	0.0168 (12)	0.0147 (12)
C14	0.0395 (14)	0.0501 (14)	0.0361 (12)	0.0105 (11)	0.0117 (11)	0.0184 (11)
C15	0.066 (2)	0.077 (2)	0.106 (3)	0.0042 (17)	−0.0099 (19)	0.038 (2)
C16	0.0533 (19)	0.083 (2)	0.110 (3)	0.0160 (16)	0.0113 (18)	0.038 (2)
C17	0.086 (2)	0.0436 (14)	0.0533 (17)	0.0297 (14)	0.0099 (16)	0.0193 (13)
C18	0.122 (3)	0.0630 (19)	0.066 (2)	0.0372 (19)	−0.003 (2)	0.0255 (17)
C19	0.167 (4)	0.080 (2)	0.058 (2)	0.054 (3)	0.003 (3)	0.031 (2)
C20	0.175 (4)	0.080 (2)	0.072 (3)	0.049 (3)	0.048 (3)	0.048 (2)
C21	0.129 (3)	0.0599 (18)	0.074 (2)	0.0314 (18)	0.047 (2)	0.0384 (16)
C22	0.084 (2)	0.0393 (13)	0.0572 (17)	0.0232 (14)	0.0291 (16)	0.0212 (13)
C23	0.0540 (15)	0.0460 (14)	0.0515 (15)	0.0119 (12)	0.0261 (13)	0.0150 (12)
C24	0.0678 (19)	0.0490 (16)	0.075 (2)	0.0118 (14)	0.0310 (17)	0.0173 (15)
C25	0.0573 (18)	0.0591 (18)	0.077 (2)	0.0004 (15)	0.0205 (17)	−0.0027 (16)
C26	0.0497 (17)	0.083 (2)	0.0596 (18)	0.0192 (15)	0.0131 (14)	0.0032 (17)
C27	0.0483 (16)	0.0710 (18)	0.0564 (17)	0.0211 (14)	0.0159 (14)	0.0179 (15)
C28	0.0430 (14)	0.0458 (14)	0.0515 (15)	0.0103 (11)	0.0201 (12)	0.0126 (12)

Geometric parameters (Å, °)

O1—C1	1.428 (3)	C11—C12	1.365 (4)
O1—H1	0.82	C11—H11	0.93
O2—C3	1.370 (3)	C12—C13	1.372 (3)
O2—C2	1.442 (3)	C12—H12	0.93
O3—C14	1.374 (3)	C13—C14	1.383 (3)
O3—H3	0.82	C13—H13	0.93
O4—C15	1.398 (3)	C15—C16	1.455 (4)
O4—H4	0.82	C15—H15A	0.97
O5—C17	1.378 (3)	C15—H15B	0.97
O5—C16	1.430 (3)	C16—H16A	0.97
O6—C28	1.371 (3)	C16—H16B	0.97
O6—H6	0.82	C17—C18	1.382 (4)
C1—C2	1.488 (3)	C17—C22	1.399 (4)
C1—H1A	0.97	C18—C19	1.397 (5)
C1—H1B	0.97	C18—H18	0.93
C2—H2A	0.97	C19—C20	1.344 (5)
C2—H2B	0.97	C19—H19	0.93
C3—C4	1.383 (3)	C20—C21	1.385 (5)
C3—C8	1.405 (3)	C20—H20	0.93
C4—C5	1.382 (4)	C21—C22	1.388 (4)
C4—H4A	0.93	C21—H21	0.93
C5—C6	1.368 (4)	C22—C23	1.482 (4)
C5—H5	0.93	C23—C28	1.390 (3)
C6—C7	1.381 (4)	C23—C24	1.390 (3)
C6—H6A	0.93	C24—C25	1.381 (4)

C7—C8	1.387 (3)	C24—H24	0.93
C7—H7	0.93	C25—C26	1.366 (4)
C8—C9	1.486 (3)	C25—H25	0.93
C9—C10	1.391 (3)	C26—C27	1.376 (4)
C9—C14	1.391 (3)	C26—H26	0.93
C10—C11	1.390 (4)	C27—C28	1.385 (3)
C10—H10	0.93	C27—H27	0.93
C1—O1—H1	109.5	O3—C14—C13	121.1 (2)
C3—O2—C2	116.93 (18)	O3—C14—C9	117.9 (2)
C14—O3—H3	109.5	C13—C14—C9	120.9 (2)
C15—O4—H4	109.5	O4—C15—C16	112.6 (3)
C17—O5—C16	120.3 (2)	O4—C15—H15A	109.1
C28—O6—H6	109.5	C16—C15—H15A	109.1
O1—C1—C2	110.9 (2)	O4—C15—H15B	109.1
O1—C1—H1A	109.5	C16—C15—H15B	109.1
C2—C1—H1A	109.5	H15A—C15—H15B	107.8
O1—C1—H1B	109.5	O5—C16—C15	111.7 (3)
C2—C1—H1B	109.5	O5—C16—H16A	109.3
H1A—C1—H1B	108.0	C15—C16—H16A	109.3
O2—C2—C1	106.8 (2)	O5—C16—H16B	109.3
O2—C2—H2A	110.4	C15—C16—H16B	109.3
C1—C2—H2A	110.4	H16A—C16—H16B	107.9
O2—C2—H2B	110.4	O5—C17—C18	123.5 (3)
C1—C2—H2B	110.4	O5—C17—C22	115.5 (2)
H2A—C2—H2B	108.6	C18—C17—C22	121.0 (3)
O2—C3—C4	122.7 (2)	C17—C18—C19	118.7 (4)
O2—C3—C8	116.4 (2)	C17—C18—H18	120.7
C4—C3—C8	120.8 (2)	C19—C18—H18	120.7
C5—C4—C3	120.2 (2)	C20—C19—C18	121.3 (3)
C5—C4—H4A	119.9	C20—C19—H19	119.3
C3—C4—H4A	119.9	C18—C19—H19	119.3
C6—C5—C4	119.9 (3)	C19—C20—C21	120.0 (4)
C6—C5—H5	120.1	C19—C20—H20	120.0
C4—C5—H5	120.1	C21—C20—H20	120.0
C5—C6—C7	120.0 (2)	C20—C21—C22	121.1 (4)
C5—C6—H6A	120.0	C20—C21—H21	119.4
C7—C6—H6A	120.0	C22—C21—H21	119.4
C6—C7—C8	122.0 (2)	C21—C22—C17	117.9 (3)
C6—C7—H7	119.0	C21—C22—C23	120.4 (3)
C8—C7—H7	119.0	C17—C22—C23	121.7 (2)
C7—C8—C3	117.1 (2)	C28—C23—C24	117.3 (2)
C7—C8—C9	120.3 (2)	C28—C23—C22	121.9 (2)
C3—C8—C9	122.58 (19)	C24—C23—C22	120.7 (2)
C10—C9—C14	117.2 (2)	C25—C24—C23	121.4 (3)
C10—C9—C8	119.9 (2)	C25—C24—H24	119.3
C14—C9—C8	122.8 (2)	C23—C24—H24	119.3
C11—C10—C9	121.8 (2)	C26—C25—C24	120.0 (3)
C11—C10—H10	119.1	C26—C25—H25	120.0
C9—C10—H10	119.1	C24—C25—H25	120.0

C12—C11—C10	119.3 (2)	C25—C26—C27	120.3 (3)
C12—C11—H11	120.3	C25—C26—H26	119.8
C10—C11—H11	120.3	C27—C26—H26	119.8
C11—C12—C13	120.3 (3)	C26—C27—C28	119.5 (3)
C11—C12—H12	119.8	C26—C27—H27	120.2
C13—C12—H12	119.8	C28—C27—H27	120.2
C12—C13—C14	120.4 (2)	O6—C28—C27	121.0 (2)
C12—C13—H13	119.8	O6—C28—C23	117.6 (2)
C14—C13—H13	119.8	C27—C28—C23	121.4 (2)
C3—O2—C2—C1	159.09 (19)	C17—O5—C16—C15	75.7 (3)
O1—C1—C2—O2	−59.1 (3)	O4—C15—C16—O5	50.4 (4)
C2—O2—C3—C4	27.2 (3)	C16—O5—C17—C18	15.8 (3)
C2—O2—C3—C8	−155.41 (19)	C16—O5—C17—C22	−166.6 (2)
O2—C3—C4—C5	178.6 (2)	O5—C17—C18—C19	176.9 (3)
C8—C3—C4—C5	1.4 (3)	C22—C17—C18—C19	−0.5 (4)
C3—C4—C5—C6	−0.7 (4)	C17—C18—C19—C20	−1.6 (5)
C4—C5—C6—C7	−0.1 (4)	C18—C19—C20—C21	1.7 (6)
C5—C6—C7—C8	0.2 (4)	C19—C20—C21—C22	0.3 (5)
C6—C7—C8—C3	0.5 (4)	C20—C21—C22—C17	−2.4 (4)
C6—C7—C8—C9	−178.0 (2)	C20—C21—C22—C23	178.3 (3)
O2—C3—C8—C7	−178.7 (2)	O5—C17—C22—C21	−175.2 (2)
C4—C3—C8—C7	−1.3 (3)	C18—C17—C22—C21	2.4 (4)
O2—C3—C8—C9	−0.2 (3)	O5—C17—C22—C23	4.2 (3)
C4—C3—C8—C9	177.2 (2)	C18—C17—C22—C23	−178.2 (2)
C7—C8—C9—C10	57.1 (3)	C21—C22—C23—C28	−115.6 (3)
C3—C8—C9—C10	−121.3 (2)	C17—C22—C23—C28	65.0 (3)
C7—C8—C9—C14	−120.1 (2)	C21—C22—C23—C24	61.3 (3)
C3—C8—C9—C14	61.4 (3)	C17—C22—C23—C24	−118.1 (3)
C14—C9—C10—C11	0.0 (3)	C28—C23—C24—C25	−0.5 (4)
C8—C9—C10—C11	−177.4 (2)	C22—C23—C24—C25	−177.5 (2)
C9—C10—C11—C12	−0.7 (4)	C23—C24—C25—C26	0.1 (4)
C10—C11—C12—C13	0.2 (4)	C24—C25—C26—C27	0.2 (4)
C11—C12—C13—C14	0.9 (4)	C25—C26—C27—C28	−0.1 (4)
C12—C13—C14—O3	176.7 (2)	C26—C27—C28—O6	179.0 (2)
C12—C13—C14—C9	−1.5 (3)	C26—C27—C28—C23	−0.4 (4)
C10—C9—C14—O3	−177.20 (19)	C24—C23—C28—O6	−178.8 (2)
C8—C9—C14—O3	0.1 (3)	C22—C23—C28—O6	−1.8 (3)
C10—C9—C14—C13	1.1 (3)	C24—C23—C28—C27	0.6 (4)
C8—C9—C14—C13	178.4 (2)	C22—C23—C28—C27	177.6 (2)

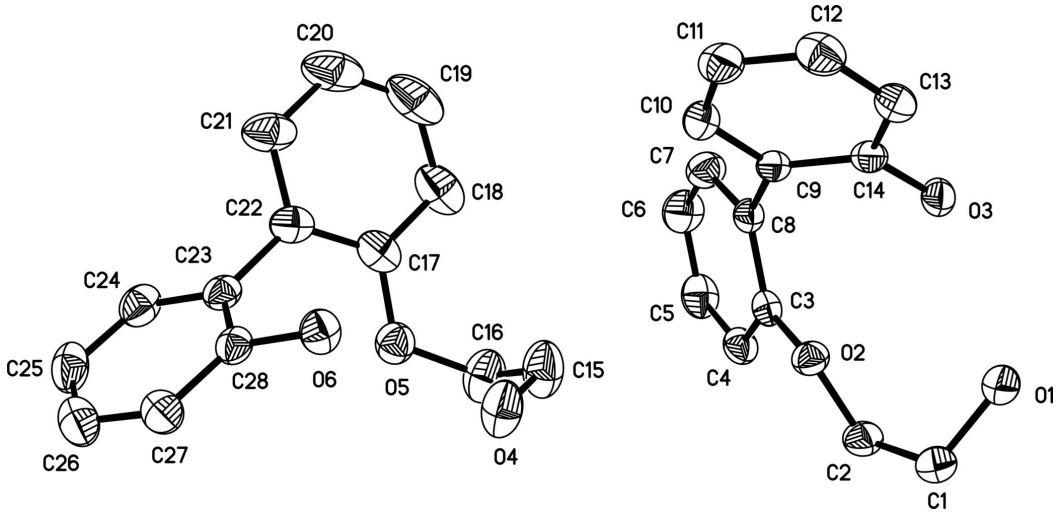
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3	0.82	2.02	2.821 (3)	164
O3—H3···O1^{i}	0.82	1.87	2.660 (3)	160
O4—H4···O6	0.82	1.99	2.797 (3)	169
O6—H6···O4^{ii}	0.82	1.87	2.661 (3)	161
C1—H1B···Cg1^{iii}	0.97	2.75	3.584 (3)	144

C5—H5···Cg2^{iv}	0.93	2.71	3.602 (3)	160
C11—H11···Cg3^{v}	0.93	2.93	3.742 (3)	146

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

Fig. 1


C20
C19
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O4
C11
C12
C13
C10
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C9
C14
O3
C6
C8
C5
C3
C4
O2
O1
C2
C1

Fig. 2