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(R,R)-(+)-2-(2-Methacryloyloxy)-1,2-diphenylethanol

Cecilia Rodríguez de Barbarín,[a]* M. Judith Percino,[b] Victor M. Chapela[b] and Tony Alcantarilla[b]

[a]Facultad de Ciencias Químicas, División de Estudios de Posgrado, Guerrero y Progreso S/N, Col. Treviño, Universidad Autónoma de Nuevo León, 64570 Monterrey, N.L., Mexico, and [b]Centro de Química, Instituto de Ciencias, Universidad Autónoma de Puebla, Complejo de Ciencias, ICUAP, Edif. 76, 22 Sur y San Claudio, 72570, Puebla, Puebla, Mexico

Correspondence e-mail:
cecybarbarin@yahoo.com

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Key indicators

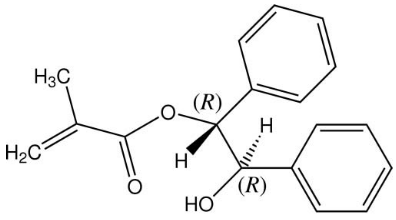
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.046
wR factor = 0.140
Data-to-parameter ratio = 7.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{18}H_{18}O_3$, was synthesized with pure optically active reagents. The molecules possess two chiral atoms and are linked through O—H···O hydrogen bonds in the crystal structure.

Comment

The title compound, (I), is one of a group of new monomers synthesized with the main purpose of exhibiting second harmonic generation of laser light. These monomers were then polymerized by free radical reactions (Percino *et al.*, 2004).



(I)

The title compound possesses two chiral atoms, C7 and C8, both with the same chirality (Fig. 1). The absolute cofiguration was assigned *R*,*R* from the synthesis, using pure optically active reactants.

The phenyl rings are in *cis* positions across the C—C single bond [C7—C8 = 1.514 (5) Å and C6—C7—C8—C9 = 61.2 (5)°]. The dihedral angle between the phenyl ring planes is 50.6 (2)°. The equivalent angle in related compounds with an —O—C(Ph)—C(Ph)—O— unit varies over a wide range: 60.5 (Liu *et al.*, 1987), 42.4 (Braun *et al.*, 1999) and 34.3° (Sacha *et al.*, 1994).

The crystal packing shows the formation of a network of intermolecular H bonds involving hydroxyl groups and ketone O atoms of symmetry-related molecules (Table 1). These weak contacts form a continuous zigzag molecular chain along the [010] axis (Fig. 2). In the title compound, the larger angle between phenyl groups is probably influenced not only by the steric hindrance of the rings, but also by the intermolecular hydrogen-bond formation along the [010] direction.

Experimental

The title compound was prepared according to the method of Percino *et al.* (2004). Single crystals suitable for X-ray crystallographic study were grown by slow evaporation of a hexane solution at room temperature over a period of 24 h. The absolute configuration (*R*,*R*) was corroborated by NMR spectroscopy (see archived CIF; Percino *et al.*, 2004). The optical activity was measured using a Perkin Elmer

Polarimeter, Model 341, with λ = 590 nm, T = 298 K using $CHCl_3$ as solvent, $[\alpha]_D^{25}$ = +37.5°.

Crystal data

$C_{18}H_{18}O_3$
M_r = 282.32
Monoclinic, $P2_1$
a = 12.094 (5) Å
b = 5.756 (3) Å
c = 12.503 (6) Å
β = 118.18 (2)°
V = 767.1 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.60 × 0.12 × 0.05 mm

Data collection

Siemens P4 diffractometer
Absorption correction: none
6004 measured reflections
1511 independent reflections
907 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.115
3 standard reflections
every 97 reflections
intensity decay: 3.8%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.140
S = 1.04
1511 reflections
192 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.16 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3$^{\rm i}$	0.87	2.20	2.965 (5)	147
O1—H1A···O1$^{\rm i}$	0.87	2.50	3.094 (7)	126

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

Diffraction data were limited to 2θ = 50° due to the habit of the available single crystals, which systematically crystallized as needles with small dimensions. C-bound H atoms were placed in idealized positions and refined using a riding model (constrained C—H distances: 0.93 Å for H atoms bonded to Csp^2 atoms, 0.96 Å for methyl CH_3 and 0.98 Å for methine CH). Isotropic displacement parameters were fixed at $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for the methyl group and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for all other H atoms. Hydroxyl atom H1 was found in a difference map and refined as riding on O1, with an O—H distance constrained to 0.87 Å and with $U_{\rm iso}$(H1) = 1.5$U_{\rm eq}$(O1). It was not possible to confirm the absolute configuration by X-ray diffraction, as no significant anomalous effects are present. Measured Friedel pairs (1214) were merged.

Data collection: *XSCANS* (Bruker, 1999); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and Mercury (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXTL-Plus*.

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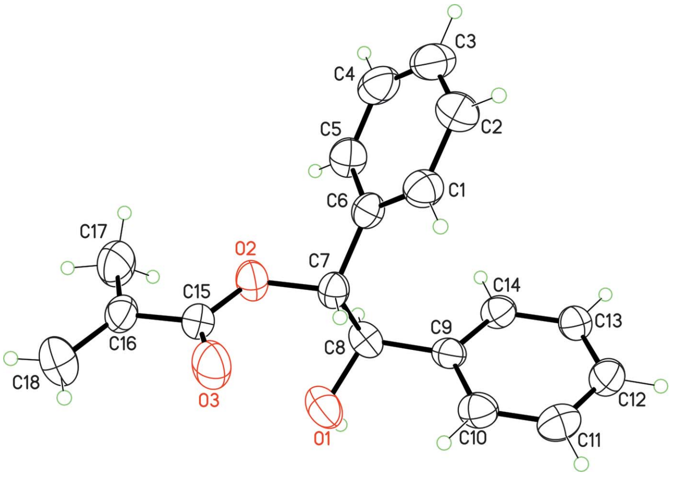

Figure 1
The molecular structure of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

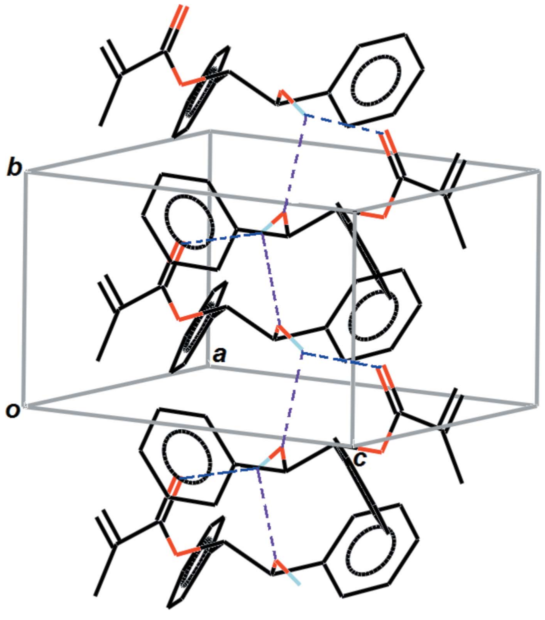

Figure 2
The packing, showing the hydrogen-bonded (dashed lines) zigzag molecular chain along the [010] direction.

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