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(2*S**)-2-Hydroxy-2-[(2*S**,5*R**)-5-(1-hydroxy-1-methylethyl)tetrahydrofuran-2-yl]-1-phenylethanone

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Key indicators

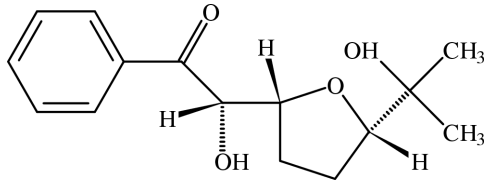
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.146
Data-to-parameter ratio = 13.0

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

The molecules of the title compound, $C_{15}H_{20}O_4$, link *via* a single intermolecular hydrogen bond to form chains running along the *b* axis.

Comment

During the development of chiral phase-transfer catalysed permanganate oxidations of 1,5-dienes, the title compound, (I), was prepared (Brown & Keily, 2001).



(I)

An intermolecular hydrogen bond links the molecules into chains extending along the *b* axis. Also present are three intramolecular hydrogen bonds (Table 1).

Experimental

(*E*)-7-Methyl-1-phenylocta-2,6-dien-1-one was oxidized by potassium permanganate under solid–liquid phase-transfer conditions using a chiral quaternary ammonium salt. Following a standard work-up and column chromatography, the product was recrystallized from ethanol/hexane to give colourless crystals of the title compound.

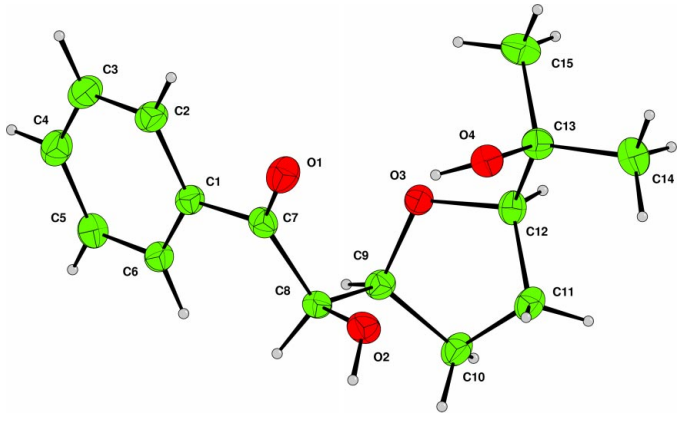


Figure 1
A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

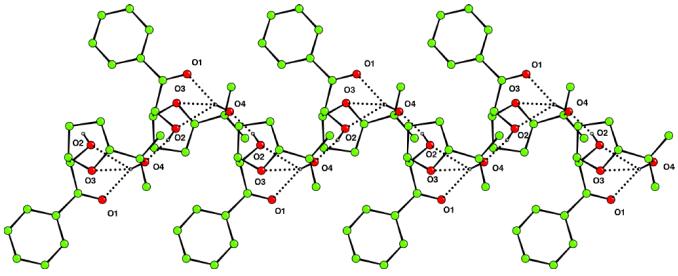


Figure 2
A view looking down the *a* axis showing the hydrogen-bonded chains extending along the *b* direction.

Crystal data

$C_{15}H_{20}O_4$
$M_r = 264.31$
Orthorhombic, $P2_12_12_1$
$a = 7.5556\ (3)$ Å
$b = 8.0446\ (3)$ Å
$c = 22.9549\ (8)$ Å
$V = 1395.24\ (9)$ Å^3
$Z = 4$
$D_x = 1.258$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4487 reflections
$\theta = 3.2$–$25.0°$
$\mu = 0.09$ mm^{-1}
$T = 150\ (2)$ K
Block, colourless
0.25 × 0.10 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans to fill the Ewald sphere
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{min} = 0.978$, $T_{max} = 0.993$
4487 measured reflections
2254 independent reflections
1917 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 25.0°$
$h = -7 \rightarrow 8$
$k = -9 \rightarrow 7$
$l = -26 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.146$
$S = 1.03$
2254 reflections
174 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0959P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O4^{i}	0.84	1.88	2.707 (3)	170
O4—H4A···O3	0.84	2.31	2.756 (3)	113
O4—H4A···O1	0.84	2.33	3.131 (3)	161
O4—H4A···O2	0.84	2.58	3.186 (3)	130

Symmetry code: (i) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$.

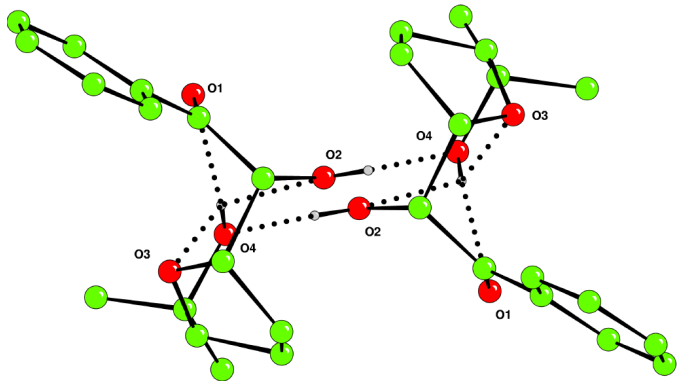


Figure 3
A view looking down the *b* axis showing both the inter- and intramolecular hydrogen bonds.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* (Otwinowski & Minor, 1997), *COLLECT* and *MAXUS* (Mackay *et al.*, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WINGX* (Farrugia, 1998).

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