Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

(2S)-[(2S)-2-Hydroxy-2-phenylethanoyloxy]phenylacetic acid

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The novel title compound, $C_{16}H_{14}O_5$, forms four intermolecular hydrogen bonds and takes part in two chains running along the shortest crystallographic *b* axis.

Received 22 December 2003
Accepted 9 January 2004
Online 17 January 2004

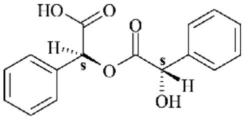
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.098
Data-to-parameter ratio = 9.1

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

Comment

During structural studies of *S*-(+)-mandelic acid [*S*-(+)-MA], needle-like crystals of an unknown compound were isolated. The compound was shown to be the unusual 'ester' with the assumed stereochemistry (2*S*)-[(2*S*)-2-hydroxy-2-phenylethanoyloxy]phenylacetic acid, (I). The molecular structure of (I) is shown in Fig. 1 and the unit-cell contents in Fig. 2.



(I)

Each molecule is involved in four intermolecular hydrogen bonds to four symmetry-related molecules, as shown in Fig. 3. These hydrogen bonds form a network comprising two distinct $C_1^1(5)$ and $C_1^1(4)$ catemeric chains along the shortest crystallographic *b* axis. The $C_1^1(5)$ chain connects the 'ester' carbonyl of one molecule to the alcohol hydroxyl group of the next molecule. The $C_1^1(4)$ chain arises from $-C{=}O\cdots H-O-$ hydrogen bonding through adjacent carboxylic acid groups. Fig. 4 shows the hydrogen-bonding scheme giving rise to the two chains, and details are given in Table 1.

Experimental

Saturated solutions of *S*-(+)-MA (supplied by Sigma Aldrich, 99+%) in distilled water were prepared and rhombic crystals of *S*-(+)-MA were obtained. The mother liquors were allowed to evaporate slowly under ambient conditions. After several weeks, needle-like crystals of the title compound were isolated as the minor product.

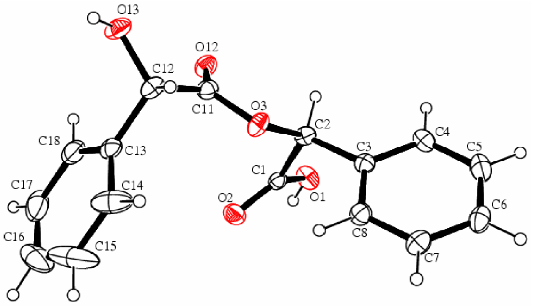


Figure 1
The molecular structure of the title compound, (I), showing the labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

DOI: 10.1107/S1600536804000741

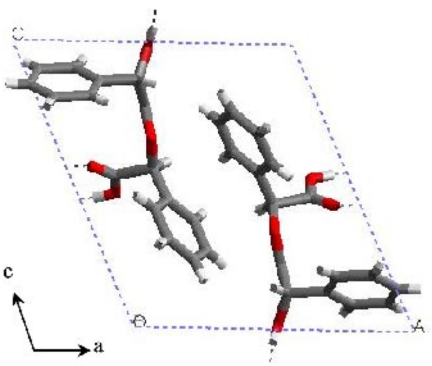


Figure 2
The unit-cell contents of (I), viewed along *b*.

Crystal data

$C_{16}H_{14}O_5$
$M_r = 286.27$
Monoclinic, $P2_1$
$a = 10.5196$ (4) Å
$b = 6.4129$ (3) Å
$c = 11.7201$ (7) Å
$\beta = 114.107$ (2)°
$V = 721.69$ (6) Å^3
$Z = 2$
$D_x = 1.317$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4075 reflections
$\theta = 1.0$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 150$ K
Needle, colourless
0.30 × 0.15 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Thick-slice ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.916$, $T_{\max} = 0.990$
4184 measured reflections
1760 independent reflections
1413 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 27.3°$
$h = -11 \rightarrow 13$
$k = -7 \rightarrow 8$
$l = -12 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.098$
$S = 1.03$
1760 reflections
193 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.1103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.115 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2$^{\rm i}$	0.82	1.94	2.715 (3)	157
O13—H13···O12$^{\rm ii}$	0.82	2.04	2.817 (3)	159

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

The Friedel pairs were merged and the $\Delta f''$ term was set to zero. [The calculated absolute structure parameter (Flack, 1983) of 0.23 (13) was meaningless in this analysis.] All H atoms attached to C atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.98 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The OH H atoms were positioned geometrically with torsion angles selected so as to maximise electron density and were refined as rotating groups, with O—H = 0.82 Å, and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CERIUS*^{2} (Accelrys, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

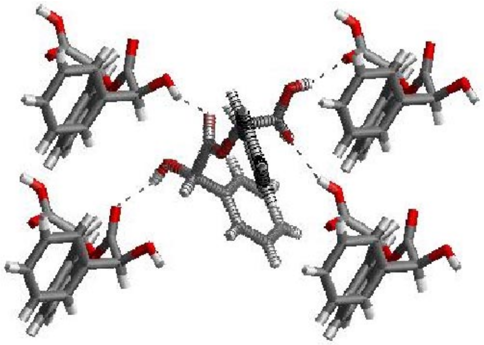


Figure 3
The hydrogen bonds (dashed lines) formed by each independent molecule with four neighbouring molecules.

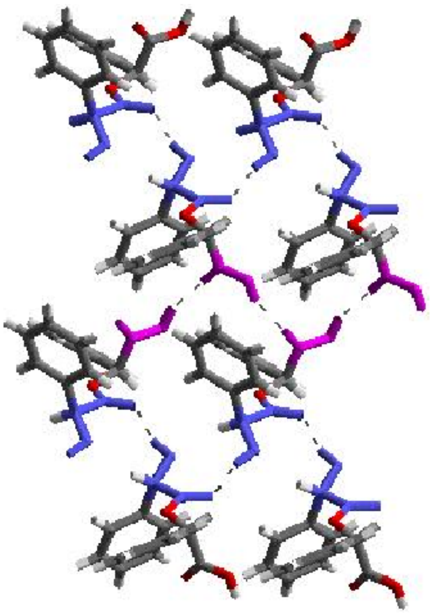


Figure 4
The $C_1^1(5)$ (blue) and $C_1^1(4)$ (pink) hydrogen-bonded chains of the acid, viewed along *c*. Hydrogen bonds are indicated by dashed lines.

The authors thank the EPSRC and Avecia Ltd for financial support, and Edwin A. Collier and Dr Amy L. Gillon for crystallographic discussions.

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