Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*RS*)-Benzyl mandelate

Robila K. Mughal,[a]* Robin G. Pritchard[b] and Roger J. Davey[a]

[a]Colloids, Crystals and Interfaces Group, Department of Chemical Engineering, UMIST, PO Box 88, Manchester M60 1QD, England, and [b]Department of Chemistry, UMIST, PO Box 88, Manchester M60 1QD, England

Correspondence e-mail: robila.mughal@postgrad.umist.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.089
Data-to-parameter ratio = 11.0

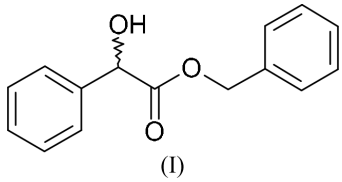
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 20 September 2004
Accepted 4 October 2004
Online 9 October 2004

A benzyl ester of mandelic acid, $C_{15}H_{14}O_3$, was obtained by the crystallization of racemic mandelic acid from benzyl alcohol followed by vacuum drying at 363 K. The structure is composed of two hydrogen-bonded chains of *S* or *R* configuration, running along the shortest crystallographic *b* axis. There is one molecule in the asymmetric unit and each molecule forms four intermolecular hydrogen bonds with two other molecules of the same chirality.

Comment

During the crystallization of racemic mandelic acid from benzyl alcohol and drying off the solvent in a vacuum oven, colourless needle-shaped crystals of (*RS*)-benzyl mandelate (BM), (I), were obtained. The crystal structure of this compound was not found in the Cambridge Structural Database (CSD, Version 1.6; Allen, 2002) and hence its structure was determined by single-crystal X-ray diffraction at 150 K.



(I)

The compound BM has one molecule in the asymmetric unit. Fig. 1 shows the structure and the atom labelling. The bond lengths and angles are unexceptional. Each molecule forms four intermolecular hydrogen bonds to two neighbouring molecules, as shown in Fig. 2. The unit-cell contents of BM are shown in Fig. 3.

The crystal structure is composed of two types of chains that run along the shortest crystallographic axis, *b*, which is the needle axis. The $C_1^1(5)$ chain runs through the hydroxyl and carbonyl groups *via* —C═O···H—O— hydrogen bonding.

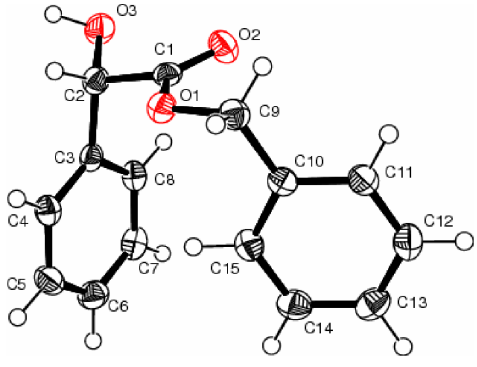


Figure 1
The crystallographically independent molecule in the asymmetric unit of BM; displacement ellipsoids are drawn at the 50% probability level.

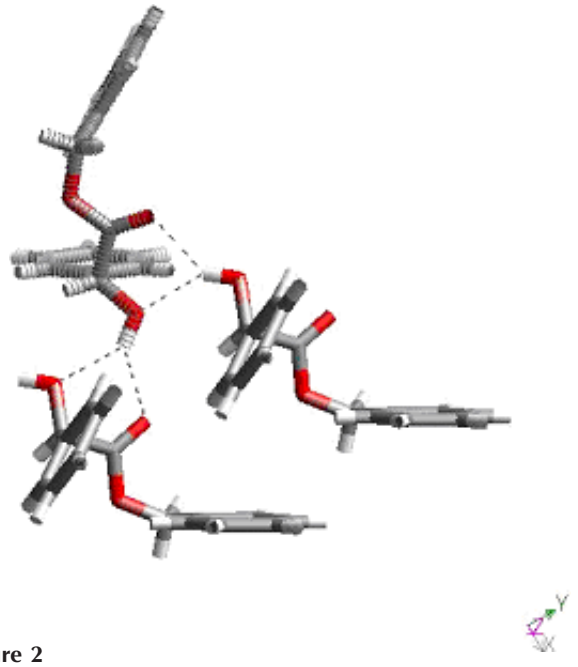


Figure 2
Hydrogen bonds (dashed lines) formed by each independent molecule with the neighbouring two molecules.

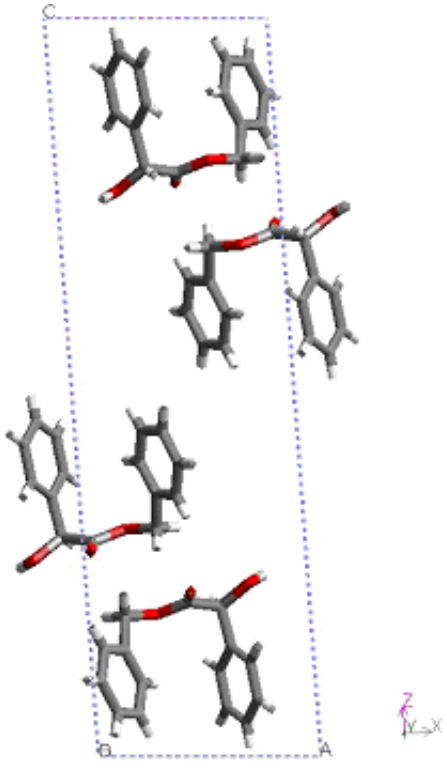


Figure 3
The unit-cell contents of BM, viewed along *b*.

The $C_1^1(2)$ chain arises from the linking of OH in one molecule to OH of another molecule. Fig. 4 shows the packing of the two chains and the resulting bilayer sandwich. Layers of hydrogen-bonded chains are sandwiched between bilayers of phenyl rings. There is face–edge interaction between the phenyl rings of each molecule, and also between the phenyl rings of adjacent molecules in the same chain. Each $C_1^1(5)$ and

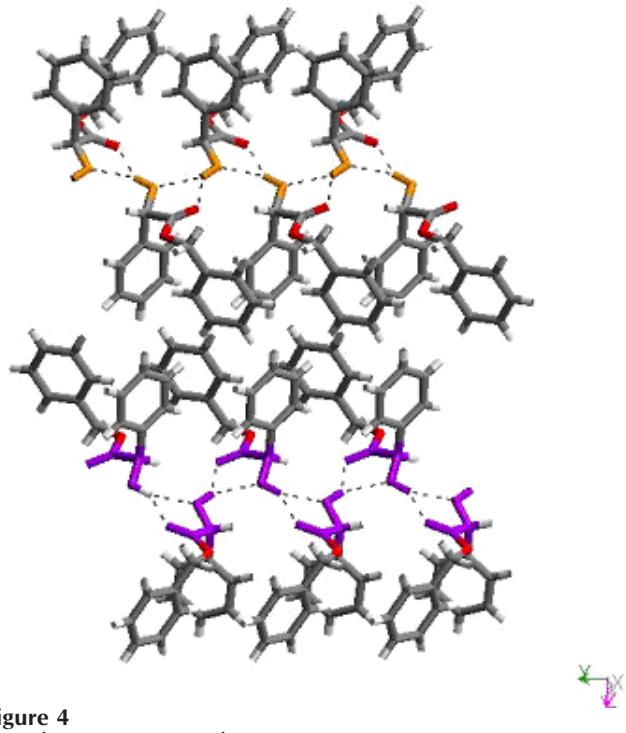


Figure 4
The $C_1^1(5)$ (purple) and $C_1^1(2)$ (orange) hydrogen-bonded chains (dashed lines) of BM, viewed along *c*.

$C_1^1(2)$ chain is composed of either all-*S* configuration molecules or all-*R* molecules, and the chains pack such that there are alternating *R* and *S* chains, as shown in Fig. 5. There are no hydrogen-bonding interactions between *R* and *S* molecules. The hydrogen bonds are listed in Table 1.

Experimental

A saturated solution of racemic mandelic acid (supplied by Sigma–Aldrich, 99%) in benzyl alcohol was prepared at 323 K and stirred at 343 K for 2 h. On cooling to 298–303 K, needle-shaped crystals of racemic mandelic acid formed; these were vacuum-filtered and then dried in a vacuum oven at 363 K to remove benzyl alcohol mother liquor. After a few weeks in the vacuum oven, crystals of (*RS*)-benzyl mandelate were found alongside an orange–yellow amorphous glass-like residue.

Crystal data

$C_{15}H_{14}O_3$
$M_r = 242.15$
Monoclinic, $P2_1/n$
$a = 8.0627\ (3)$ Å
$b = 5.6494\ (2)$ Å
$c = 26.7944\ (11)$ Å
$\beta = 94.130\ (1)^\circ$
$V = 1217.30\ (8)$ Å^3
$Z = 4$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7192 reflections
$\theta = 1$–26°
$\mu = 0.09$ mm^{-1}
$T = 150\ (2)$ K
Needle, colourless
0.25 × 0.10 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.978$, $T_{max} = 0.994$
7192 measured reflections
2425 independent reflections
1732 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 26.5^\circ$
$h = -7 \rightarrow 10$
$k = -5 \rightarrow 7$
$l = -32 \rightarrow 33$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 0.1653P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.089$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
2425 reflections	Extinction correction: *SHELXL*97
220 parameters	Extinction coefficient: 0.026 (4)
All H-atom parameters refined	

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.94 (2)	2.08 (2)	2.8711 (15)	141.2 (18)
O3—H3···O3^{i}	0.94 (2)	2.17 (2)	2.9522 (6)	140.1 (19)

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

All H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); 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); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

The authors thank the EPSRC and Avecia Ltd for financial support.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Nonius (1997–2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

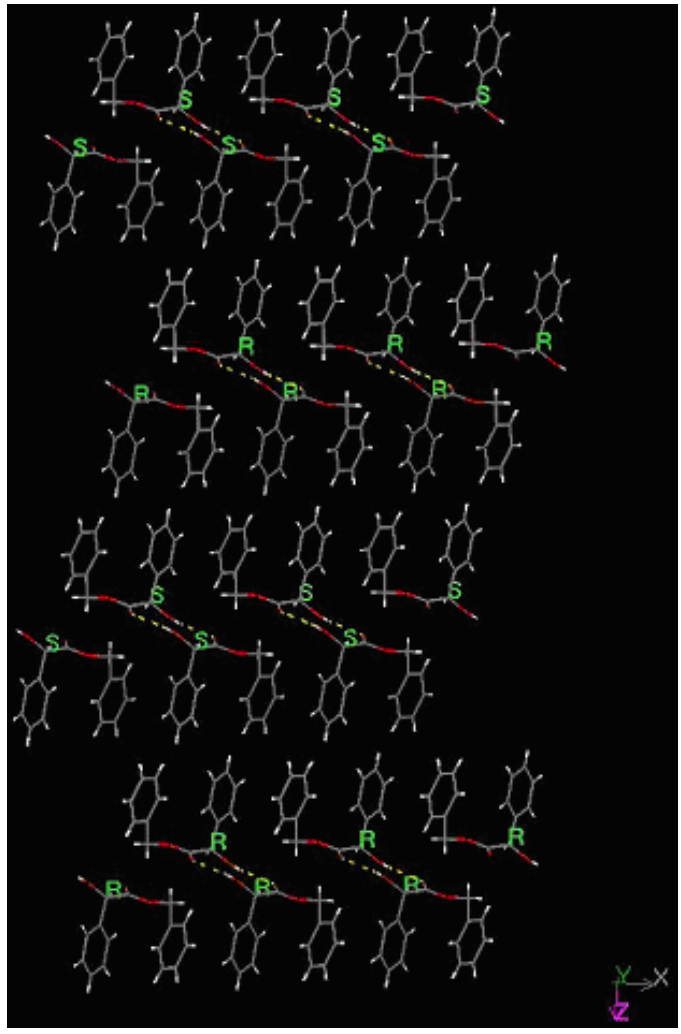


Figure 5
Packing of alternating *R* and *S* chains, together with the phenyl bilayer and the sandwiched hydrogen-bonded chains.