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# 2-Methoxy-2-phenylacetic acid

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**Key indicators**

Single-crystal X-ray study
*T* = 299 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.055
*wR* factor = 0.174
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.



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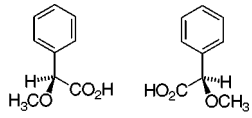
2-Methoxy-2-phenylacetic acid, $C_9H_{10}O_3$, forms helical columns of single enantiomers linked by hydrogen bonding between the acidic proton of one molecule and the methoxy O atom of a neighbouring molecule, to give an overall racemic structure.

## Comment

2-Methoxy-2-phenylacetic acid, (1), is a chiral compound with one stereogenic center. The racemate of (1) has been crystallized. It forms helical columns of single enantiomers linked by hydrogen bonding between the acidic proton of one molecule and the methoxy O atom of a neighbouring molecule in the solid state [O1···O3$^{i}$ = 2.725 (2) Å, O1—H1O···O3$^{i}$ = 162 (3) Å; symmetry code as in Table 1] (Figs. 1 and 2). Atom H1O is located in the plane defined by atoms O1, O2$^{i}$, and O3$^{i}$ [the deviation is only 0.05 (3) Å]. This arrangement leads to a packing of molecules of (1) (Fig. 3) similar to the structure that has been reported for its acidic sodium acid salt (Moore *et al.*, 1980).




(*S*)-(1) (*R*)-(1)

## Experimental

The racemate of 2-methoxy-2-phenylacetic acid, (1), is commercially available. The crystal analyzed in this study was grown from a solution of *rac*-2-(2-methoxy-2-phenylacetylsulfanyl)pyridine (Gottwald *et al.*, 2004) in $CH_2Cl_2$/*n*-hexane (3:1 *v*/*v*), which was kept in the dark for 7 d at 293 K.

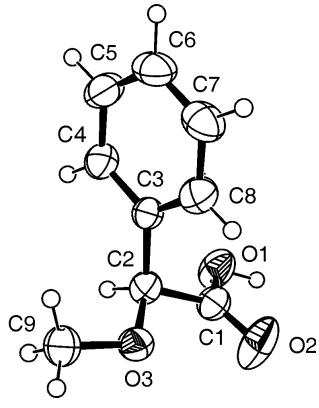



**Figure 1**
The molecular structure of (*S*)-(1) which was arbitrarily selected from the racemate that is present in the unit cell of (1). Displacement ellipsoids are drawn at the 50% probability level.

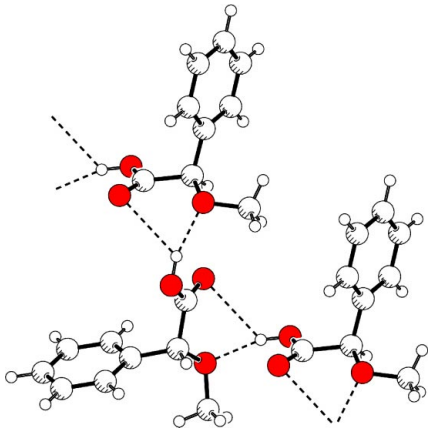


**Figure 2**
Hydrogen bonding of (1) in the solid state.

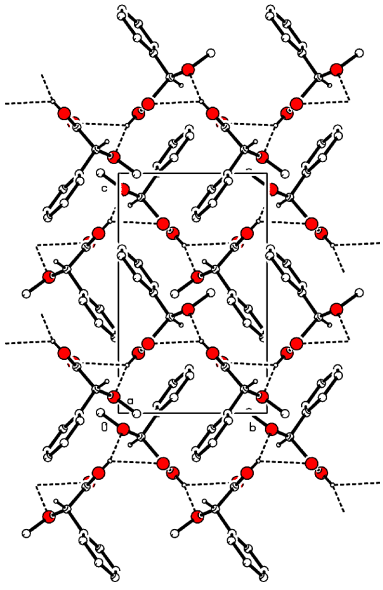


**Figure 3**
(*P*)-helical packing of (*S*)-(1) and (*M*)-helical arrangement of (*R*)-(1) in the unit cell. View along [100].

*Crystal data*

$C_9H_{10}O_3$
$M_r$ = 166.17
Monoclinic, $P2_1/n$
$a$ = 10.093 (3) Å
$b$ = 7.123 (2) Å
$c$ = 12.270 (3) Å
$\beta$ = 110.40 (1)°
$V$ = 826.8 (4) Å$^3$
$Z$ = 4
$D_x$ = 1.335 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 877 reflections
$\theta$ = 3.3–20.9°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 299 (2) K
Prism, colorless
0.60 × 0.48 × 0.16 mm

*Data collection*

Oxford Diffraction Xcalibur CCD diffractometer
$\omega$ rotation scans
Absorption correction: none
4076 measured reflections
1665 independent reflections
994 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 26.4°
$h = -12 \rightarrow 12$
$k = -8 \rightarrow 8$
$l = -15 \rightarrow 8$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.174
$S$ = 0.88
1665 reflections
128 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1149P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.045
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$
Extinction correction: *SHELXL*97 and Larson (1970)
Extinction coefficient: 0.051 (11)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—O2 | 1.187 (3) | C2—C3 | 1.502 (3) |
| C1—O1 | 1.306 (3) | C9—O3 | 1.422 (3) |
| C1—C2 | 1.512 (3) | O1—H1O | 0.90 (3) |
| C2—O3 | 1.408 (3) | | |
| O2—C1—O1 | 124.6 (2) | O3—C2—C1 | 106.16 (18) |
| O2—C1—C2 | 123.8 (2) | C1—O1—H1O | 104.9 (18) |
| O1—C1—C2 | 111.6 (2) | C2—O3—C9 | 112.89 (17) |
| O2—C1—C2—O3 | −16.5 (3) | O1—C1—C2—C3 | −74.3 (3) |
| O1—C1—C2—O3 | 163.59 (19) | C3—C2—O3—C9 | 70.6 (2) |
| O2—C1—C2—C3 | 105.6 (3) | C1—C2—O3—C9 | −168.23 (18) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1O···O3$^{i}$ | 0.90 (3) | 1.85 (3) | 2.725 (2) | 162 (3) |
| O1—H1O···O2$^{i}$ | 0.90 (3) | 2.57 (3) | 3.190 (3) | 127 (2) |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2001); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2001); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *PLATON*2002 (Spek, 2002); software used to prepare material for publication: *SHELXL*97.

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## References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gottwald, T., Hartung, J., Heubes, M. & Špehar, K. (2004). In preparation.
Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall and C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.
Moore, P. B., Pluth, J. J., Mollin-Norris, J. A., Weinstein, D. A. & Compere, E. L. Jr (1980). *Acta Cryst.* B**36**, 47–50.
Oxford Diffraction (2001). *CrysAlis RED* and *CrysAlis CCD*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2002) *PLATON*. Version 160902. Utrecht University, The Netherlands.