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(3-Methoxyphenyl)acetic acid

A. R Choudhury and T. N. Guru Row*

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India

Correspondence e-mail: ssctng@sscu.iisc.ernet.in

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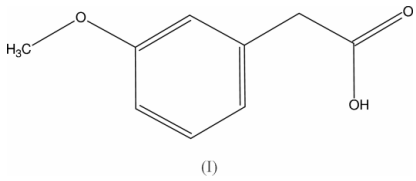
The title compound, $C_9H_{10}O_3$, also known as (*m*-methoxyphenyl)acetic acid, has been found to crystallize in the monoclinic space group $P2_1/c$ at room temperature. It is the starting material for the synthesis of a large number of 1,2,3,4-tetrahydroisoquinoline compounds [Nagarajan *et al.* (1985). *Indian J. Chem. Sect. B*, **24**, 83–97]. The compound forms dimers in the crystalline state, with O—H···O hydrogen bonds between the carboxyl groups, across a crystallographic centre of symmetry.



(I)

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.117
Data-to-parameter ratio = 11.5

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

Experimental

The 98% pure compound was bought from Sigma Aldrich. Single crystals were grown from a mixture of ethyl acetate and hexane at room temperature, by slow evaporation. The compound crystallizes as prisms.

Crystal data

$C_9H_{10}O_3$
M_r = 166.17
Monoclinic, $P2_1/c$
a = 16.266 (3) Å
b = 5.1024 (11) Å
c = 10.095 (2) Å
β = 90.73 (1)°
V = 837.8 (3) Å^3
Z = 4
D_x = 1.317 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3478 reflections
θ = 2.4–21.3°
μ = 0.10 mm^{-1}
T = 293 (2) K
Prism, colourless
0.40 × 0.35 × 0.20 mm

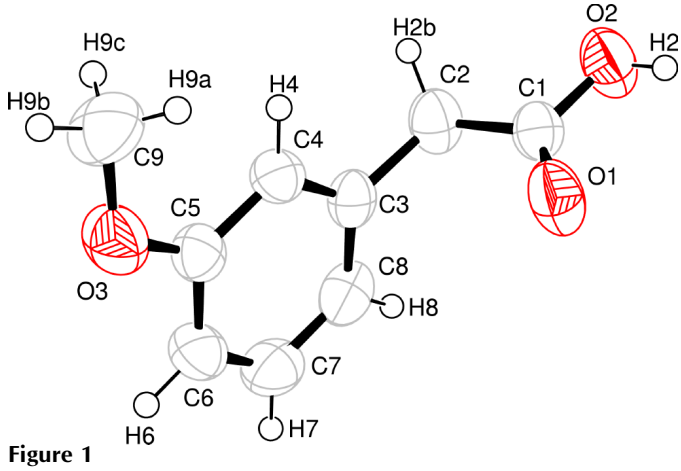


Figure 1
The molecular structure of the title compound, drawn with 50% probability displacement ellipsoids.

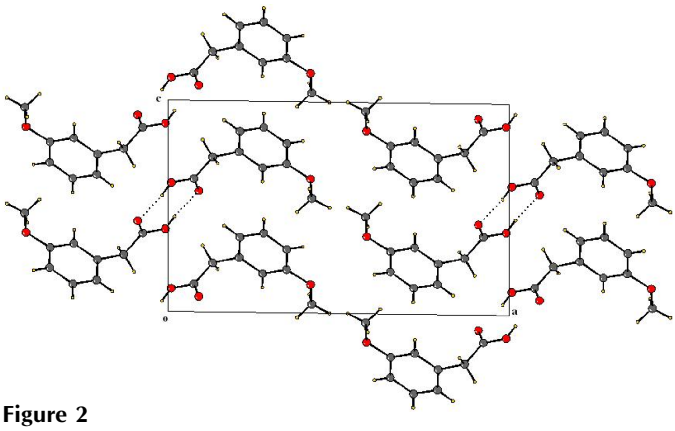


Figure 2
Packing diagram of the title compound, viewed down the *b* axis, showing O—H···O hydrogen-bonded dimers.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6276 measured reflections
1714 independent reflections
1310 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.4^\circ$
$h = -20 \rightarrow 20$
$k = -6 \rightarrow 6$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.117$
$S = 1.03$
1714 reflections
149 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 0.0041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.87	2.687 (2)	173

Symmetry code: (i) $-x, 1-y, 1-z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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 *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 1990).

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