diffractometer was purchased with funds provided in part by an NIH grant.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1226). Services for accessing these data are described at the back of the journal.

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# 3-(2-Methylphenyl)propanoic acid

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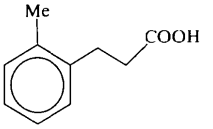
## Abstract

The title acid, $C_{10}H_{12}O_2$, crystallized in the centrosymmetric space group $P2_1/c$ with one molecule in the asymmetric unit. There is a single hydrogen bond with $O_D\cdots O_A$ = 2.639 (2) Å and $O_D$—H$\cdots O_A$ = 175 (3)°. This bond forms an $R_2^2(8)$ cyclic dimer about a center of symmetry. The non-H atoms of the molecule lie nearly in a plane. The molecules in this structure are oriented such that their best-fit planes are either strictly parallel or make dihedral angles of 88.9 (1)°. The structure comprises double layers of aromatic rings separated by double layers of hydrogen-bonded aliphatic strings and is analogous to the structures of other terminally aryl-substituted *n*-aliphatic carboxylic acids.


## Comment

This report on the title acid, (I), is one of a series on hydrogen bonding in carboxylic acids. It follows reports on the analogous 'terminal aromatic ring–*n*-aliphatic string–carboxyl group' acids 4-(2-naphthyl)-butanoic acid [(II); Dobson & Gerkin, 1996] and 4-(3-phenanthryl)butanoic acid [(III); Gerkin, 1997], as well as 4-(1-pyrenyl)butanoic acid [(IV); Olszak *et al.*, 1989], 4-(2-anthryl)butanoic acid [(V); Durfee *et al.*, 1989] and (2-naphthyl)ethanoic acid [(VI); Barrett & Gellman, 1993]. Of particular interest is the packing of the rings, the strings and the carboxyl groups in such solids.




(I)

Compound (I) crystallized in the centrosymmetric space group $P2_1/c$ with one molecule in the asymmetric unit. The refined molecule and the labeling scheme are shown in Fig. 1. There is a single hydrogen bond in this structure involving O1, H1 and O2$^i$ [symmetry code: (i) $1-x$, $1-y$, $1-z$], in which the $O_D$—H distance is 0.97 (3), H$\cdots O_A$ is 1.67 (3), $O_D\cdots O_A$ = 2.639 (2) Å and $O_D$—H$\cdots O_A$ is 175 (3)°. The H atom and O atoms are ordered. This bond forms a first-level (Bernstein *et al.*, 1995) cyclic dimer with descriptor $R_2^2(8)$ about a center of symmetry; there are of course no higher-level graphs. Three of the cyclic dimers are shown in the packing diagram, Fig. 2. As is apparent there, this structure can be viewed as consisting of double layers of aromatic rings separated by double layers of hydrogen-bonded aliphatic strings. In this respect, it is similar to the other 'ring–string–carboxyl group' structures cited above. Further, in (I) and (II)–(IV) cited above, there is a small dihedral angle between the best-fit string plane and the carboxyl-group plane [(V) and (VI) are not compared since (V) has reported O-atom disorder, and (VI) has too short a string to define a string plane]. However, (I) is unlike (II)–(IV) in having its carboxyl group coplanar with its ring, as described below, rather than almost perpendicular to it [in (II) and (III), for example, the relevant dihedral angles are 80.5 (2) and 83.2 (3)°].

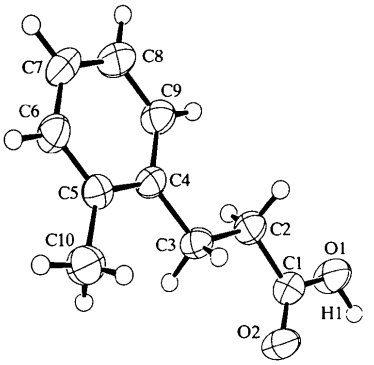



Fig. 1. *ORTEP*II (Johnson, 1976) drawing of (I), showing the labeling scheme. Displacement ellipsoids are drawn for 50% probability for non-H atoms; circles of arbitrary small radius depict H atoms.

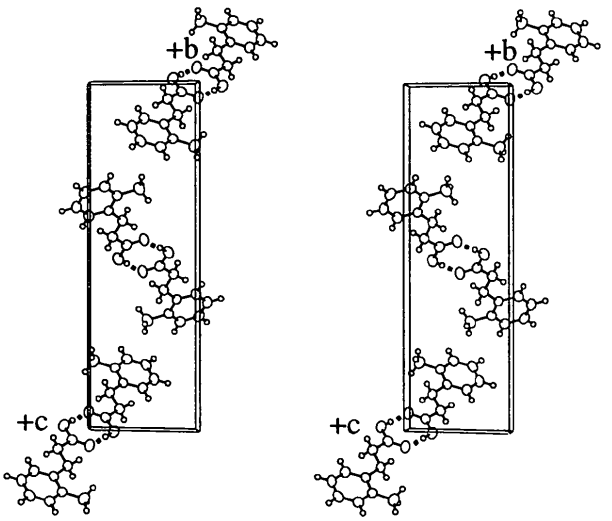



Fig. 2. *ORTEP*II (Johnson, 1976) packing stereodiagram of (I) viewed down the *a* axis. Displacement ellipsoids are drawn for 50% probability for non-H atoms; circles of arbitrary small radius depict H atoms. Hydrogen bonds are depicted by single bold dashes.

The benzene ring in (I) is very nearly planar, the maximum deviation of any of its atoms from the best-fit plane describing them being 0.007 (2) Å, while the average deviation is 0.005 (2) Å. Indeed, all of the non-H atoms of (I) lie nearly in a plane: the greatest deviation of any of these atoms from the best-fit plane describing them is 0.034 (2) Å, while the average deviation is 0.012 (10) Å. In (I) the dihedral angle between the sets of molecular best-fit planes not required to be parallel by symmetry is 88.9 (1)°. Thus, the structure consists of nearly planar molecules which are either strictly parallel or virtually perpendicular to each other.

Selected distances and angles are given in Table 1. All distances and angles fall within normal ranges. Excluding pairs of atoms in hydrogen-bonded carboxyl groups, the closest intermolecular approaches are between C6 and H10C$^{ii}$ [symmetry code: (ii) $x$, $\frac{1}{2}-y$, $-\frac{1}{2}+z$], and are 0.04 Å less than the corresponding Bondi (1964) van der Waals radius sum.

## Experimental

The title acid was obtained as a white, flocculent powder from a sample in Dr M. S. Newman's chemical collection. Evaporation at room temperature of a solution of this powder in acetonitrile produced colorless plates, one of which was cut to provide the experimental sample. A synthesis has been described by Jacobs & Harvey (1981).

*Crystal data*

$C_{10}H_{12}O_2$
$M_r$ = 164.20
Monoclinic
$P2_1/c$
$a$ = 5.318 (1) Å
$b$ = 23.100 (1) Å
$c$ = 7.619 (2) Å
$\beta$ = 109.92 (1)°
$V$ = 879.9 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.239 Mg m$^{-3}$
$D_m$ not measured
Mo $K\alpha$ radiation
$\lambda$ = 0.71073 Å
Cell parameters from 25 reflections
$\theta$ = 14.5–17.3°
$\mu$ = 0.085 mm$^{-1}$
$T$ = 296 K
Cut plate
0.38 × 0.23 × 0.08 mm
Colorless

*Data collection*

AFC-5*S* diffractometer
$\omega$ scans
Absorption correction: none
2220 measured reflections
2014 independent reflections
956 reflections with $I > 2\sigma I$
$R_{int}$ = 0.038
$\theta_{max}$ = 27.56°
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 30$
$l = -9 \rightarrow 9$
6 standard reflections
every 150 reflections
intensity decay: 5.83%

*Refinement*

Refinement on $F^2$
$R(F)$ = 0.051
$wR(F^2)$ = 0.082
$S$ = 1.44
2014 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2_{cs} + (0.006I)^2]$
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$
Extinction correction: none
Scattering factors from Stewart *et al.* (1965) (H) and Creagh & McAuley (1992) (C, O)

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

| | | | |
|---|---|---|---|
| O1—C1 | 1.320 (3) | O2—C1 | 1.217 (2) |
| O1—C1—O2 | 122.6 (2) | O2—C1—C2 | 124.4 (2) |
| O1—C1—C2 | 113.0 (2) | | |

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1995). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *TEXSAN* and *PLATON* (Spek, 1990).

I acknowledge with pleasure my use of the departmental X-ray crystallographic facility, which is supervised by Dr J. C. Gallucci. The diffractometer system was purchased with funds provided in part by an NIH grant.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1221). Services for accessing these data are described at the back of the journal.

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*Acta Cryst.* (1999). C**55**, 1859–1861

# 2′,5′-Dimethylbiphenyl-2-carboxylic acid

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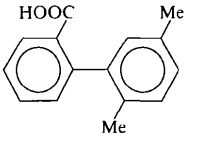
## Abstract

The title acid, $C_{15}H_{14}O_2$, crystallized in the centrosymmetric space group $P2_1/n$ with one molecule in the asymmetric unit. There is a single hydrogen bond with $O_D\cdots O_A$ = 2.627 (2) Å and $O_D$—H$\cdots O_A$ = 174 (2)°. This bond forms an $R_2^2(8)$ cyclic dimer about a center of symmetry. The dihedral angle between the best-fit planes of the benzene rings within a molecule (biphenyl twist angle) is 85.4 (1)°. The dihedral angle between the carboxyl-group plane and the best-fit plane of the ring to which it is attached is 31.1 (3)°.


## Comment

This report on 2′,5′-dimethylbiphenyl-2-carboxylic acid, (I), is one of a series on hydrogen bonding in carboxylic acids. It follows our reports on other biphenylcarboxylic acids, among which that on 6,6′-dimethylbiphenyl-2,2′-dicarboxylic acid (hereafter, DBDA; Gerkin, 1998) is of particular relevance here. Compound (I) crystallized in the centrosymmetric space group $P2_1/n$ with one molecule in the asymmetric unit. The refined molecule and the labeling scheme are shown in Fig. 1. There is a single hydrogen bond in this structure, in which $O_D$—H = 0.98 (3) Å, H$\cdots O_A$ = 1.65 (3) Å, $O_D\cdots O_A$ = 2.627 (2) Å and $O_D$—H$\cdots O_A$ = 174 (2)°. The H and O atoms are ordered. This bond forms a first-level (Bernstein *et al.*, 1995) cyclic dimer with descriptor $R_2^2(8)$ about a center of symmetry; there are of course no higher-level graphs. One of the cyclic dimers appears in the packing diagram (Fig. 2).




(I)

The benzene rings in (I) are nearly planar, the maximum deviation of any of their atoms from the best-fit planes describing them being 0.002 (2) and 0.010 (2) Å, while the average deviations are 0.001 (2) and 0.006 (2) Å. These values are quite similar to the corresponding maximum and average deviations found in DBDA; 0.012 (2) Å for both rings and 0.007 (3) Å for both rings, respectively. The dihedral angle between

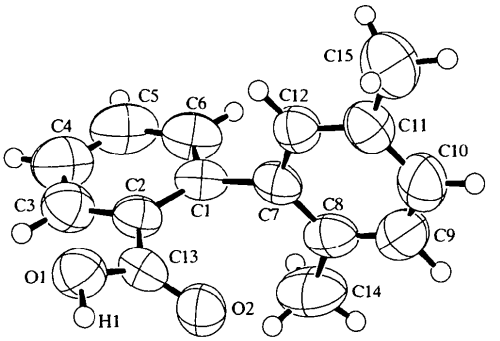



Fig. 1. *ORTEP*II (Johnson, 1976) drawing of (I), showing the labeling scheme. Displacement ellipsoids are drawn for 50% probability for non-H atoms; spheres of arbitrary small radii depict H atoms.