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4′-Methylbiphenyl-2-carboxylic acid

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.077
Data-to-parameter ratio = 14.1

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

The title compound, $C_{14}H_{12}O_2$, is used as an intermediate for the synthesis of various biologically active and pharmaceutical compounds. Bond lengths and angles adopt usual values. The dihedral angles between the two aromatic rings [53.39 (3)°] and between the carboxyl group and adjacent ring [42.37 (10)°] lie in the expected ranges. The crystal structure is characterized by centrosymmetric hydrogen-bonded dimers.

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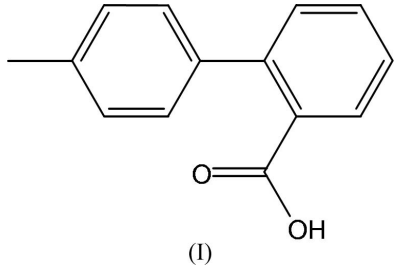
Comment

The title compound, (I), is used as an intermediate for the synthesis of various biologically active and pharmaceutical compounds (Gillis & Markham, 1997; Markham & Goa, 1997). In view of its importance and in order to determine the conformation of this molecule, a crystal structure determination has been carried out.



(I)

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles (Table 1) can be regarded as normal [Cambridge Structural Database (CSD), Version 1.7; *MOGUL* Version 1.0.1; Allen, 2002]. The dihedral angle between the two

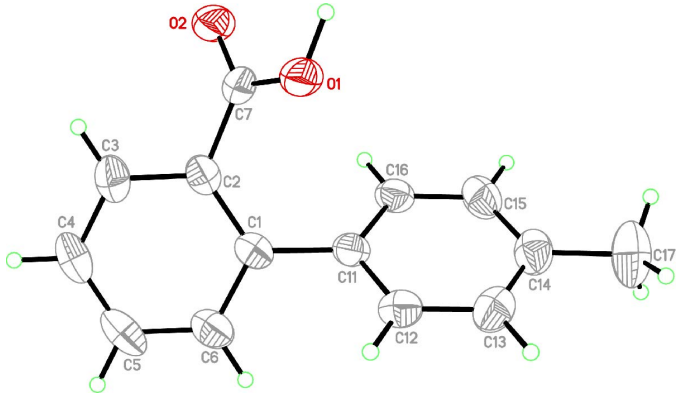


Figure 1
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

aromatic rings is 53.39 (3)°. The carboxyl group subtends an angle of 42.37 (10)° with the ring to which it is attached. In seven comparable structures retrieved from the CSD containing the biphenyl-2-carboxylic acid moiety, the dihedral angles between the aromatic rings are in the range 44.9–62.9°, whereas the dihedral angles between the carboxyl group and the adjacent aromatic plane shows a significantly wider range of 32.5–85.9°. The molecules form hydrogen-bonded centrosymmetric dimers in the crystal structure (Table 2).

Experimental

4′-Methylbiphenyl-2-carbonitrile (1.93 g, 10 mmol) was refluxed with methanol (10 ml) and 30% NaOH solution (10 ml) for 3 h to yield the title compound, which was recrystallized from dichloromethane (m.p. 419 K).

Crystal data

$C_{14}H_{12}O_2$
M_r = 212.24
Monoclinic, $P2_1/c$
a = 7.5953 (15) Å
b = 14.582 (3) Å
c = 10.616 (2) Å
β = 90.610 (16)°
V = 1175.7 (4) Å^3
Z = 4
D_x = 1.199 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8476 reflections
θ = 3.6–25.5°
μ = 0.08 mm^{-1}
T = 173 (2) K
Block, colourless
0.30 × 0.21 × 0.11 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
5269 measured reflections
2073 independent reflections
1528 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = -10 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.077
S = 0.88
2073 reflections
147 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C11	1.5011 (18)	C7—O2	1.2287 (15)
C2—C7	1.4920 (17)	C7—O1	1.3225 (14)
O2—C7—O1	122.50 (10)	O1—C7—C2	115.78 (11)
O2—C7—C2	121.65 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.84	1.83	2.6604 (13)	170

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

All H atoms were located in a difference map, but were then positioned geometrically and refined with fixed individual displacement parameters (set at 1.2 times U_{eq} of the parent atom, but 1.5U_{eq} for hydroxyl and methyl groups) using a riding model, with O—H = 0.84 Å and C—H = 0.95 and 0.98 Å for aromatic and methyl H atoms, respectively. In addition, the torsion angles of the hydroxyl group and the methyl group were refined.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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