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Intermolecularly associated carboxylic acid dimers in the supramolecular assembly of 2-(2-phenylethyl)benzoic acid

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The molecular structure of the title acid, $C_{15}H_{14}O_2$, exhibits a *trans*-planar arrangement of the aromatic rings. The carboxyl group is inclined at an angle of 6.4 (1)° with respect to the attached benzene ring. The classical hydrogen-bonded carboxylic acid dimers (O$\cdots$O = 2.7 Å), characterized by an $R_2^2(8)$ pattern, predominantly stabilize the supramolecular assembly.

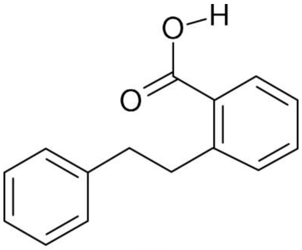
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.114
Data-to-parameter ratio = 11.1

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

Comment

Benzoic acid was among the first organic crystal structures to be examined by the application of the X-ray crystallography (Bragg, 1921, 1922). Since then, numerous structures of benzoic acid and its derivatives have been reported (Sim *et al.*, 1955; Parkin *et al.*, 2005), owing to their importance in synthetic medicinal chemistry.



(I)

In the present report, we discuss the structure of one of these derivatives and the intermolecular interactions which govern its supramolecular assembly. The title acid, (I), is an intermediate in the preparation of dibenzosuberone (Ramesha & Roy, 2001) and the tricyclic antidepressant amitriptyline (Barbui *et al.*, 2004; Maizels & McCarberg, 2005).

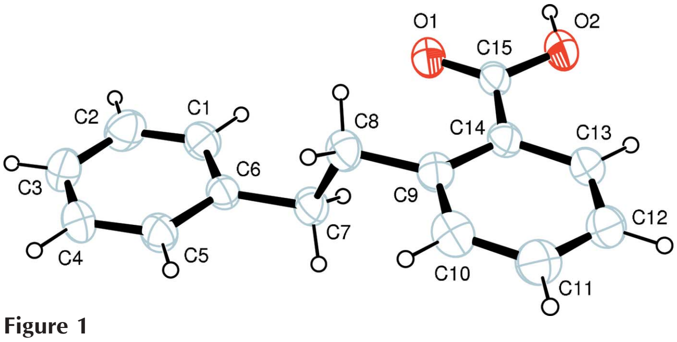


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

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The molecule, shown in Fig. 1, assumes an overall *trans* conformation; ω(C6—C7—C8—C9) = 175.8 (1)°. The aromatic rings, linked by an ethylene bridge, are nearly parallel, with a dihedral angle of 4.3 (1)°. The plane of the carboxyl group is twisted by 6.4 (1)° out of the plane of the attached benzene ring (C9–C14).

The characteristic feature of the molecular packing is the formation of classical hydrogen-bonded carboxylic acid dimers (Fig. 2). The O2—H2*A*···O1^{i} hydrogen-bond interaction involving centrosymmetrically related molecules is very strong (Table 1). The carboxylic acid dimers are characterized by an $R_2^2(8)$ ring pattern (Bernstein *et al.*, 1995). There are no significant overlaps of aromatic rings.

Experimental

The title acid was obtained from Arvee Pharma Mysore, India. Crystals were grown by slow evaporation of an ethanol solution.

Crystal data

$C_{15}H_{14}O_2$
M_r = 226.26
Monoclinic, $P2_1/c$
a = 13.7005 (2) Å
b = 6.0509 (1) Å
c = 15.1789 (1) Å
β = 103.155 (1)°
V = 1225.32 (3) Å^3
Z = 4
D_x = 1.227 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 1036 reflections
θ = 5–35°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colorless
0.14 × 0.12 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
4864 measured reflections
1761 independent reflections
1421 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.024
$\theta_{\rm max}$ = 23.3°
h = −15 → 14
k = −6 → 6
l = −16 → 14

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.114
S = 1.08
1761 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 0.18 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.030 (4)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O1^{i}	1.03 (2)	1.63 (2)	2.657 (2)	174 (2)

Symmetry codes: (i) $-x+2, -y, -z+2$.

All C-bound H atoms were positioned geometrically and refined as riding on their carrier atoms, with C—H = 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom). The carboxy H atom was located in a difference electron-density map and refined isotropically. The small crystal used in the analysis diffracted rather poorly. The data set was limited to a maximum θ angle of 23.3°, since only very weak diffraction was observed at higher angles.

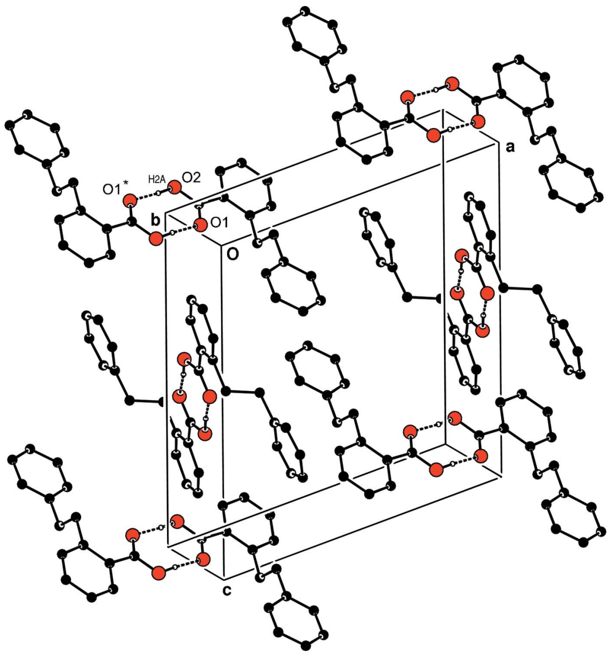

Figure 2
The crystal packing in (I), showing the strong O—H···O hydrogen bond between facing carboxylic acid groups of molecules related by an inversion center (dashed lines). The asterisk (*) indicates the symmetry operation ($-x, 2-y, -z$). H atoms not involved in the interactions have been omitted.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

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