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3-(4-Carboxyphenoxy)propionic acid

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Key indicators

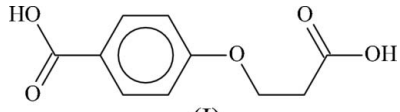
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.153
Data-to-parameter ratio = 15.2

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

The molecules of the title compound, $C_{10}H_{10}O_5$, are linked by O—H···O hydrogen bonds into a linear chain along [20$\bar{1}$].

Comment

The crystal structures of 2- and 3-carboxyphenoxyacetic acid have been reported previously. The 2-isomer exists as a zigzag chain polymer hydrogen-bonded through a pair of hydrogen bonds (Byriel *et al.*, 1991), whereas the 3-isomer exists as a monohydrate that displays a three-dimensional hydrogen-bonded network (Gu *et al.*, 2004). The structure of the 4-isomer has not been reported to date, as the compound does not furnish single crystals. Interest in the 4-isomer is extended to the title compound, (I), which has an extra methylene linkage.



(I)

The title compound is anhydrous (Fig. 1). A pair of hydrogen bonds (Table 1) links adjacent molecules into a linear chain along [20$\bar{1}$] (Fig. 2).

Experimental

4-Carboxyphenoxyacetic acid was synthesized in a manner analogous to that used for synthesizing 3-carboxyphenoxyacetic acid (Gu *et al.*, 2004), but with 4-hydroxybenzoic acid in place of 3-hydroxybenzoic acid and 3-chloropropionic acid in place of chloroacetic acid. Colourless crystals of (I) separated from the aqueous solution after several days.

Crystal data

$C_{10}H_{10}O_5$
M_r = 210.18
Monoclinic, $P2_1/c$
a = 7.813 (4) Å
b = 9.032 (6) Å
c = 13.631 (9) Å
β = 94.92 (2)°
V = 958 (1) Å^3
Z = 4
D_x = 1.457 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 (2) K
Plate, colourless
0.42 × 0.17 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.722, T_{max} = 0.937
(expected range = 0.763–0.991)
9176 measured reflections
2188 independent reflections
1359 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°

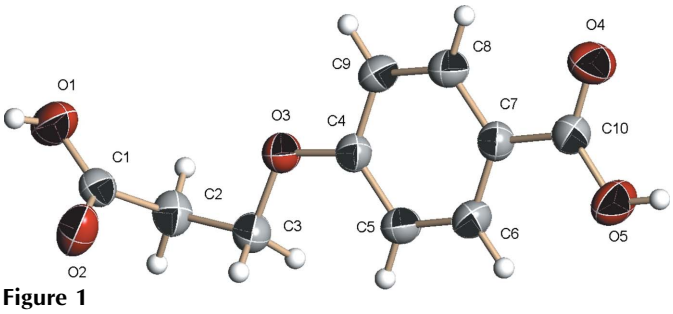


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.153$
$S = 1.00$
2188 reflections
144 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0912P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O4^{i}	0.83 (1)	1.82 (2)	2.618 (2)	162 (5)
O5—H5O···O2^{ii}	0.84 (1)	1.85 (1)	2.676 (2)	173 (5)

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

Carbon-bound H atoms were positioned geometrically, with C—H = 0.93 or 0.97 Å, and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The acid H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.82 (1) Å; their displacement parameters were freely refined.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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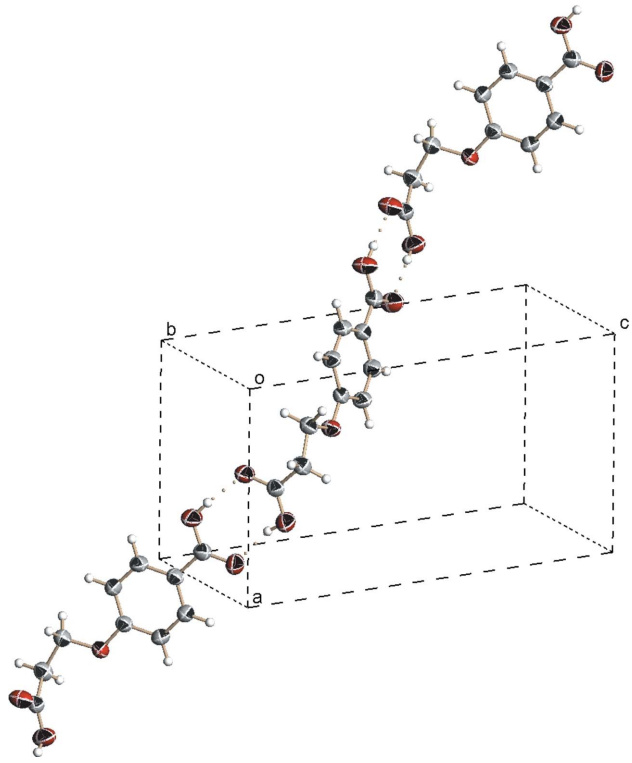

Figure 2
The hydrogen-bonded (dotted lines) chain structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

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