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# (4-Hydroxyphenoxy)acetic acid

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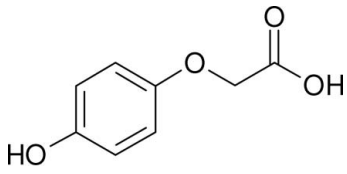
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.001 Å; $R$ factor = 0.034; $wR$ factor = 0.099; data-to-parameter ratio = 14.9.

The carboxyl groups in molecules of the title compound, $C_8H_8O_4$, are held together by $R_2^2(8)$ hydrogen bonding. The –OH groups at postion 4 on the aryl rings are linked by continuous hydrogen-bonded chains. The supramolecular structure is further defined by the formation of $R_6^6(44)$ rings.

## Related literature

For related literature, see: Birner (1972); Cox & Hickey (2004); Hodgson & Asplund (1991); Kumar & Rao (1982).




## Experimental

### Crystal data

$C_8H_8O_4$
$M_r$ = 168.14
Monoclinic, $P2_1/c$
$a$ = 8.6550 (2) Å
$b$ = 5.2531 (1) Å
$c$ = 16.2401 (4) Å
$\beta$ = 98.983 (1)°
$V$ = 729.31 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 120 (2) K
0.6 × 0.45 × 0.38 mm

### Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min}$ = 0.844, $T_{max}$ = 0.954
9200 measured reflections
1666 independent reflections
1518 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.099
$S$ = 1.07
1666 reflections
112 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

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

*Cg* is the centroid of the benzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O1$^{i}$ | 0.84 | 2.07 | 2.8878 (6) | 165 |
| O3—H31···O4$^{ii}$ | 0.84 | 1.78 | 2.6201 (10) | 173 |
| C5—H5···O3$^{iii}$ | 0.95 | 2.49 | 3.4318 (12) | 174 |
| C2—H2···*Cg*$^{iv}$ | 0.95 | 2.87 | 3.6190 (11) | 136 |

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

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2013).

## References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Birner, J. (1972). *J. Pharm. Sci.* **61**, 933–935.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Cox, P. J. & Hickey, G. (2004). *Acta Cryst.* E**60**, o771–o773.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hodgson, D. J. & Asplund, R. O. (1991). *Acta Cryst.* C**47**, 1986–1987.
Kumar, S. V. & Rao, L. M. (1982). *Z. Kristallogr.* **161**, 45–51.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o2931 [ **doi:10.1107/S1600536807022714** ]

# (4-Hydroxyphenoxy)acetic acid

**M. Byres and P. J. Cox**

## Comment

4-hydroxyphenoxyacetic acid has been found in phenoxymethyl penicillin fermentations (Birner, 1972) and its molecular structure was determined to establish the hydrogen bonding patterns in the crystal. Apart from the methylene H atoms the molecule is essentially planar and the torsion angle with the greatest deviation from zero or ±180° is C7—O2—C1—C2 = 6.62 (14)°. The molecular structure is shown in Figure 1, a partial packing diagram is given in Figure 2 and selected geometric parameters are listed in Table 1. Details of the hydrogen bonding are shown in Table 2.

As is often the case for monocarboxylic acids the carboxylate groups are linked by intermolecular hydrogen bonding to form a $R^2_2(8)$ ring across a centre of symmetry. Weaker hydrogen bonding is also present between the 4-hydroxy groups that link an infinite chain of molecules. Taken in combination the two hydrogen motifs also form $R^6_6(44)$ rings involving four molecules.

Other interactions involve a C5—H5···O3 contact and one C—H···π bonding distance (Table 2) less than 3 Å (where *Cg* is the centre of the aryl ring).

Related structures include phenylacetic acid (Hodgson & Asplund, 1991), 4-methoxyphenoxyacetic acid (Kumar & Rao, 1982) and 2-methylphenoxyacetic acid (Cox & Hickey, 2004).

## Experimental

The sample was purchased from Aldrich and was recrystallized from ethanol.

## Refinement

All non-hydrogen atoms were refined by full-matrix least squares calculations with anisotropic displacement parameters. All the hydrogen atoms were allowed to ride on their attached atoms with isotropic displacement parameters 1.2 times those of the $U_{eq}$ of their attached atoms. The constrained C—H distances were 0.95 Å (aromatic), 0.99 Å (methylene) and 0.84 Å (hydroxy).

## Figures

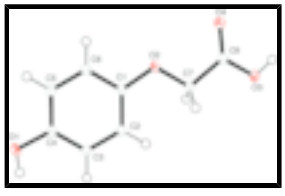

Fig. 1. View of (I) (50% probability displacement ellipsoids)

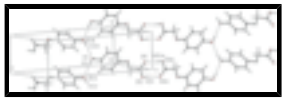

Fig. 2. A partial packing diagram of (I) showing $R^2_2(8)$ and $R^6_6(44)$ ring formations. Symbols used to denote symmetry positions of atom coordinates are: asterisk (*) = 2 − *x*, −*y*, −*z*; dollar ($) = −*x*, 1/2 + *y*, 0.5 − *z* and hash (#) = −*x*, −1/2 + *y*, 0.5 − *z*.

### (4-Hydroxyphenoxy)acetic acid

*Crystal data*

| | |
|---|---|
| $C_8H_8O_4$ | $F_{000}$ = 352 |
| $M_r$ = 168.14 | $D_x$ = 1.531 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 1796 reflections |
| *a* = 8.6550 (2) Å | θ = 2.9–27.5º |
| *b* = 5.25310 (10) Å | μ = 0.12 mm$^{-1}$ |
| *c* = 16.2401 (4) Å | *T* = 120 (2) K |
| β = 98.9830 (10)º | Block, colourless |
| *V* = 729.31 (3) Å$^3$ | 0.6 × 0.45 × 0.38 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker Nonius KappaCCD area-detector diffractometer | 1518 reflections with $I > 2\sigma(I)$ |
| *T* = 150(2) K | $R_{int}$ = 0.022 |
| φ and ω scans to fill Ewald sphere | $\theta_{max}$ = 27.5º |
| Absorption correction: multi-scan (SORTAV; Blessing, 1995) | $\theta_{min}$ = 3.2º |
| $T_{min}$ = 0.844, $T_{max}$ = 0.954 | *h* = −10→11 |
| 9200 measured reflections | *k* = −5→6 |
| 1666 independent reflections | *l* = −20→18 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 0.1898P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.034 | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2)$ = 0.099 | $\Delta\rho_{max}$ = 0.35 e Å$^{-3}$ |
| *S* = 1.07 | $\Delta\rho_{min}$ = −0.23 e Å$^{-3}$ |
| 1666 reflections | Extinction correction: none |
| 112 parameters | |

*Special details*

**Experimental**. Please note cell_measurement_ fields are not relevant to area detector data, the entire data set is used to refine the cell, which is indexed from all observed reflections in a 10 degree phi range.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.03717 (8) | 0.18406 (14) | 0.22174 (5) | 0.0183 (2) |
| H1 | 0.0231 | 0.0486 | 0.247 | 0.022* |
| O2 | 0.58461 (8) | 0.16604 (13) | 0.08499 (4) | 0.0169 (2) |
| O3 | 0.92145 (8) | −0.20002 (14) | 0.07019 (5) | 0.0184 (2) |
| H31 | 0.9935 | −0.1832 | 0.0414 | 0.022* |
| O4 | 0.84072 (8) | 0.17346 (14) | 0.01142 (4) | 0.0188 (2) |
| C1 | 0.45139 (11) | 0.15605 (18) | 0.12213 (6) | 0.0132 (2) |
| C2 | 0.42258 (11) | −0.03065 (19) | 0.17835 (6) | 0.0150 (2) |
| H2 | 0.4964 | −0.163 | 0.1934 | 0.018* |
| C3 | 0.28426 (11) | −0.02249 (19) | 0.21258 (6) | 0.0152 (2) |
| H3 | 0.2645 | −0.1483 | 0.2516 | 0.018* |
| C4 | 0.17624 (11) | 0.16823 (18) | 0.18973 (6) | 0.0139 (2) |
| C5 | 0.20589 (11) | 0.35600 (19) | 0.13400 (6) | 0.0158 (2) |
| H5 | 0.1319 | 0.4881 | 0.119 | 0.019* |
| C6 | 0.34355 (12) | 0.35056 (18) | 0.10027 (6) | 0.0152 (2) |
| H6 | 0.3642 | 0.4793 | 0.0624 | 0.018* |
| C7 | 0.68607 (11) | −0.04464 (19) | 0.10067 (6) | 0.0153 (2) |
| H7A | 0.6296 | −0.2028 | 0.0813 | 0.018* |
| H7B | 0.7228 | −0.0601 | 0.1613 | 0.018* |
| C8 | 0.82384 (11) | −0.00948 (19) | 0.05559 (6) | 0.0145 (2) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0148 (4) | 0.0192 (4) | 0.0228 (4) | 0.0023 (3) | 0.0094 (3) | 0.0016 (3) |
| O2 | 0.0130 (4) | 0.0179 (4) | 0.0213 (4) | 0.0040 (3) | 0.0076 (3) | 0.0050 (3) |
| O3 | 0.0150 (4) | 0.0204 (4) | 0.0212 (4) | 0.0059 (3) | 0.0071 (3) | 0.0051 (3) |
| O4 | 0.0168 (4) | 0.0185 (4) | 0.0223 (4) | 0.0031 (3) | 0.0069 (3) | 0.0047 (3) |
| C1 | 0.0108 (5) | 0.0154 (5) | 0.0138 (4) | −0.0012 (3) | 0.0029 (3) | −0.0022 (3) |
| C2 | 0.0134 (5) | 0.0146 (5) | 0.0171 (5) | 0.0019 (3) | 0.0023 (3) | 0.0008 (3) |
| C3 | 0.0156 (5) | 0.0151 (5) | 0.0157 (4) | −0.0008 (3) | 0.0044 (4) | 0.0017 (3) |
| C4 | 0.0113 (4) | 0.0163 (5) | 0.0147 (4) | −0.0010 (3) | 0.0034 (3) | −0.0030 (3) |
| C5 | 0.0146 (5) | 0.0152 (5) | 0.0177 (5) | 0.0032 (3) | 0.0028 (4) | 0.0004 (3) |
| C6 | 0.0162 (5) | 0.0141 (5) | 0.0156 (4) | 0.0004 (3) | 0.0032 (4) | 0.0015 (3) |
| C7 | 0.0127 (4) | 0.0167 (5) | 0.0173 (5) | 0.0026 (4) | 0.0042 (3) | 0.0023 (4) |
| C8 | 0.0126 (4) | 0.0173 (5) | 0.0136 (4) | 0.0004 (3) | 0.0020 (3) | −0.0013 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.3861 (11) | C2—H2 | 0.95 |

| | | | |
|---|---|---|---|
| O1—H1 | 0.84 | C3—C4 | 1.3810 (14) |
| O2—C1 | 1.3832 (11) | C3—H3 | 0.95 |
| O2—C7 | 1.4110 (12) | C4—C5 | 1.3894 (14) |
| O3—C8 | 1.3074 (12) | C5—C6 | 1.3871 (13) |
| O3—H31 | 0.84 | C5—H5 | 0.95 |
| O4—C8 | 1.2215 (12) | C6—H6 | 0.95 |
| C1—C2 | 1.3887 (14) | C7—C8 | 1.5048 (13) |
| C1—C6 | 1.3920 (14) | C7—H7A | 0.99 |
| C2—C3 | 1.3971 (13) | C7—H7B | 0.99 |
| C4—O1—H1 | 109.5 | C6—C5—C4 | 120.00 (9) |
| C1—O2—C7 | 115.42 (7) | C6—C5—H5 | 120 |
| C8—O3—H31 | 109.5 | C4—C5—H5 | 120 |
| O2—C1—C2 | 124.12 (9) | C5—C6—C1 | 119.83 (9) |
| O2—C1—C6 | 115.61 (8) | C5—C6—H6 | 120.1 |
| C2—C1—C6 | 120.27 (9) | C1—C6—H6 | 120.1 |
| C1—C2—C3 | 119.53 (9) | O2—C7—C8 | 109.51 (8) |
| C1—C2—H2 | 120.2 | O2—C7—H7A | 109.8 |
| C3—C2—H2 | 120.2 | C8—C7—H7A | 109.8 |
| C4—C3—C2 | 120.10 (9) | O2—C7—H7B | 109.8 |
| C4—C3—H3 | 119.9 | C8—C7—H7B | 109.8 |
| C2—C3—H3 | 119.9 | H7A—C7—H7B | 108.2 |
| C3—C4—O1 | 122.26 (9) | O4—C8—O3 | 125.14 (9) |
| C3—C4—C5 | 120.26 (9) | O4—C8—C7 | 123.97 (9) |
| O1—C4—C5 | 117.47 (8) | O3—C8—C7 | 110.89 (8) |
| C7—O2—C1—C2 | 6.62 (14) | O1—C4—C5—C6 | 179.69 (8) |
| C7—O2—C1—C6 | −173.88 (8) | C4—C5—C6—C1 | 0.27 (15) |
| O2—C1—C2—C3 | 179.73 (8) | O2—C1—C6—C5 | 179.67 (8) |
| C6—C1—C2—C3 | 0.25 (14) | C2—C1—C6—C5 | −0.81 (15) |
| C1—C2—C3—C4 | 0.84 (14) | C1—O2—C7—C8 | 179.19 (7) |
| C2—C3—C4—O1 | 179.81 (8) | O2—C7—C8—O4 | −1.16 (13) |
| C2—C3—C4—C5 | −1.38 (15) | O2—C7—C8—O3 | 178.87 (8) |
| C3—C4—C5—C6 | 0.82 (15) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O1$^{i}$ | 0.84 | 2.07 | 2.8878 (6) | 165 |
| O3—H31···O4$^{ii}$ | 0.84 | 1.78 | 2.6201 (10) | 173 |
| C5—H5···O3$^{iii}$ | 0.95 | 2.49 | 3.4318 (12) | 174 |
| C2—H2···Cg$^{iv}$ | 0.95 | 2.87 | 3.6190 (11) | 136 |

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) −*x*+2, −*y*, −*z*; (iii) *x*−1, *y*+1, *z*; (iv) −*x*+1, *y*−1/2, −*z*+1/2.

**Fig. 1**

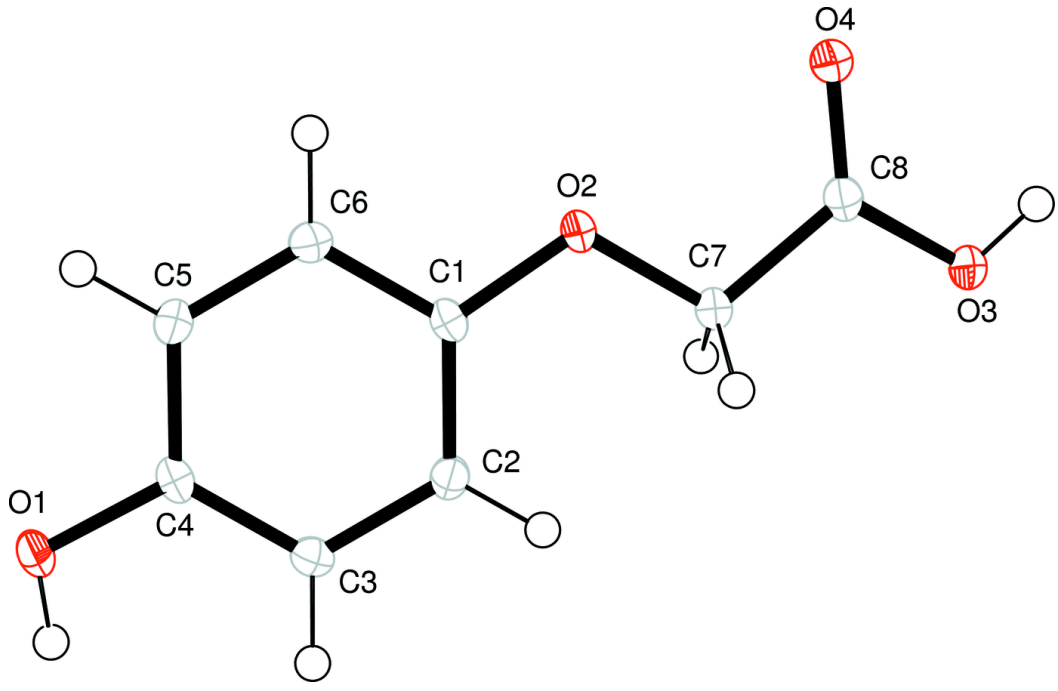

**Fig. 2**