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4-Hydroxyphenylacetic acid

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.111
Data-to-parameter ratio = 8.6

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

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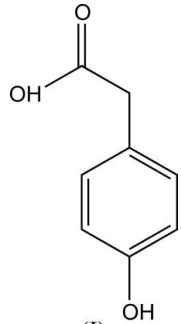
The crystal structure of commercially available 4-hydroxyphenylacetic acid, $C_8H_8O_3$, is non-centrosymmetric, with four hydrogen bonds between each molecule and adjacent molecules. The hydrogen bonds link the molecules in the crystal structure into an infinite three-dimensional framework.

Comment

We are currently studying surface phenomena and interactions between solid compounds and species in solution in contact with the solid phases. One of the compounds studied is 4-hydroxyphenylacetic acid, (I), the structure of which has not been determined so far. Since knowledge of structure, in particular hydrogen-bonding patterns, is crucial for an understanding of the above-mentioned phenomena, we decided to determine the crystal structure. The quality of the crystals in the sample of the commercially available compound was sufficient for collection of reasonable X-ray diffraction data. Therefore, we did not make any attempts to recrystallize the sample. The results of the structure determination are presented here.



(I)

The geometry of the 4-hydroxyphenylacetic acid molecule (Fig. 1) is unexceptional. Although the molecule is not chiral, the compound crystallizes in the non-centrosymmetric space group $P2_12_12_1$.

Unlike 4-aminophenylacetic acid, the structure of which has been determined recently (Gracin *et al.*, 2005) and which crystallizes as a zwitterion, 4-hydroxyphenylacetic acid is present as a neutral uncharged molecule, because of the much lower basicity of the OH group compared with that of the NH_2 group.

Both phenolic and carboxylic OH groups act as hydrogen-bond donors. Phenol atom O3 also serves as a hydrogen-bond acceptor; the second hydrogen bond uses carbonyl atom O2 as an acceptor (Table 1). The three-dimensional network thus formed is shown in Fig. 2.

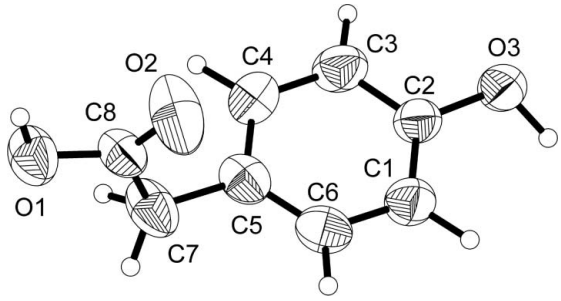


Figure 1
The molecule of *p*-hydroxyphenylacetic acid. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

A crystal of the purchased material (Sigma–Aldrich, catalogue No. H5,000-4) was used for the structure determination.

Crystal data

$C_8H_8O_3$
M_r = 152.15
Orthorhombic, $P2_12_12_1$
a = 5.3100 (3) Å
b = 9.0392 (4) Å
c = 15.3871 (8) Å
V = 738.55 (7) Å^3
Z = 4
D_x = 1.368 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 74 reflections
θ = 4.5–21.2°
μ = 0.10 mm^{-1}
T = 299 K
Block, colourless
0.49 × 0.18 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
6743 measured reflections
871 independent reflections
706 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 26.0°
$h = -5 \rightarrow 6$
$k = -10 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.111
S = 1.08
871 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.28P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.036 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{i}	0.98	1.71	2.676 (4)	166
O1—H1A···O3^{ii}	0.95	1.74	2.689 (3)	175

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

All H atoms were located in a difference Fourier map (C—H = 0.90–1.03 Å) and then included in the refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(carrier atoms). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

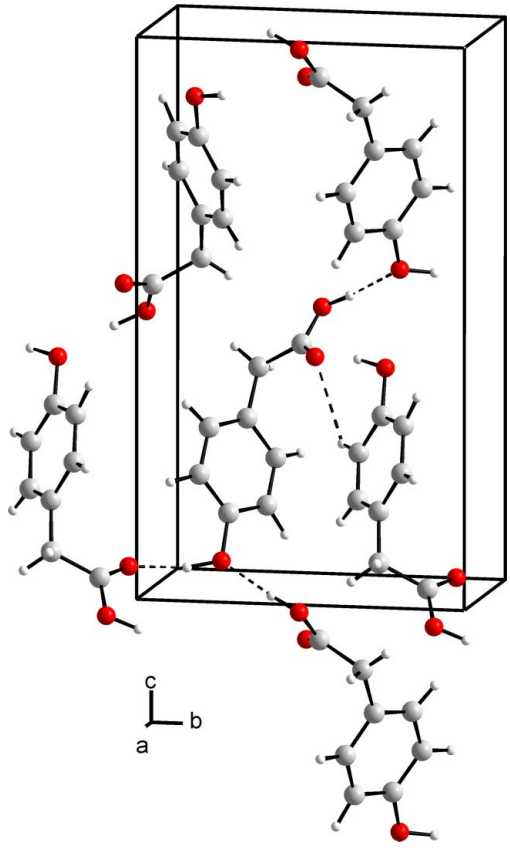


Figure 2
Packing diagram of *p*-hydroxyphenylacetic acid, showing the network formed by hydrogen-bonded acid molecules. The packing is viewed approximately along the *a* axis of the crystal. Hydrogen bonds are shown as dashed lines.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *MAXUS* (Mackay *et al.*, 1999).

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