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4-Aminophenylacetic acid

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.133
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.

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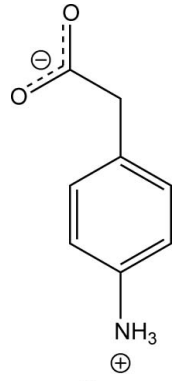
Crystals of the title compound, $C_8H_9NO_2$, were obtained from ethyl acetate. The structure consists of the acid in its zwitterionic form. In the crystal structure, each molecule interacts through strong N—H···O hydrogen bonds with six adjacent molecules, yielding a three-dimensional network.

Comment

The crystal structure of 4-aminophenylacetic acid, (I), has, to our knowledge, not been determined so far. Since we were interested in surface phenomena and interactions of solution species, knowledge of the crystal structure is crucial. We decided, therefore, to grow crystals suitable for a structure determination, the results of which are presented here.



(I)

The geometry of the molecule is unexceptional; remarkable, however, is the fact that it is present as a zwitterion, containing an ammonium group and a carboxylate group (Fig. 1). The former acts as a donor for three hydrogen bonds, the latter as an acceptor. Each molecule is thus bonded to six neighbours *via* six hydrogen bonds, yielding a rather complex three-dimensional network, as shown in Fig. 2. The formation of zwitterions is common for amino acids, although in the case of aromatic amino acids it is not commonly observed. The crucial structural feature is apparently the CH_2 group, which separates the COOH group from the π system of the benzene ring, thus facilitating the formation of the zwitterion.

Experimental

Crystals were grown from ethyl acetate solutions by dissolving the purchased material (Sigma–Aldrich, purity >98%) in the solvent (Merck, p.a.) at room temperature. The clear solutions were slowly evaporated to dryness over a couple of weeks. The rate of evaporation was reduced by covering the solution with perforated Parafilm.

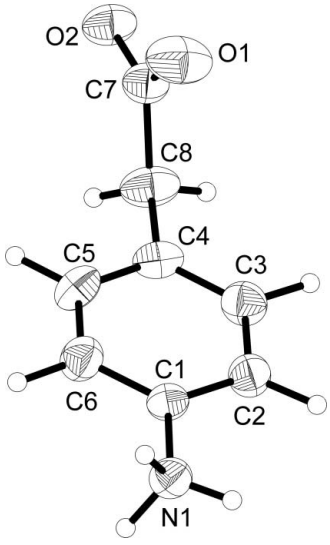


Figure 1
The molecule of 4-aminophenylacetic acid in the crystal structure. Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$C_8H_9NO_2$
M_r = 151.17
Orthorhombic, *Pbca*
a = 11.3184 (10) Å
b = 7.6823 (7) Å
c = 16.8656 (12) Å
V = 1466.5 (2) Å^3
Z = 8
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 72 reflections
θ = 5.1–20.5°
μ = 0.10 mm^{-1}
T = 298 K
Fragment, colourless
0.39 × 0.32 × 0.21 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
11 376 measured reflections
1425 independent reflections
1027 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 26.0°
$h = -13 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$= 0.059
$wR(F^2)$ = 0.133
S = 1.16
1425 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 1.286P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0093 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.92	1.84	2.753 (3)	170
N1—H1B···O2^{ii}	0.94	1.79	2.723 (3)	175
N1—H1C···O2^{iii}	0.97	1.79	2.756 (3)	179

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

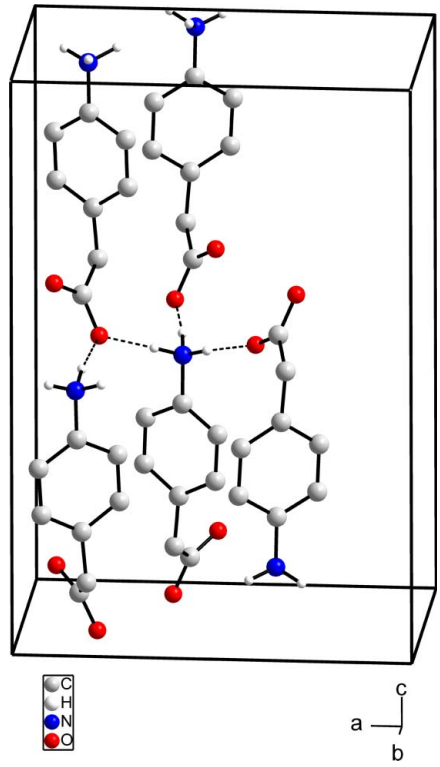


Figure 2
The network formed by hydrogen bonds in the crystal structure of 4-aminophenylacetic acid. Hydrogen bonds are indicated by dashed lines.

All H atoms were located in a difference Fourier map and were refined using a riding model in their as-found relative positions, with C—H and N—H distances in the range 0.93–1.07 and 0.91–0.97 Å, respectively, and with the constraint U_{iso}(H) = 1.2U_{eq}(carrier atom) applied in all cases.

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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