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2-(2-Methyl-3-nitrophenyl)acetic acid

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.117
Data-to-parameter ratio = 13.9

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

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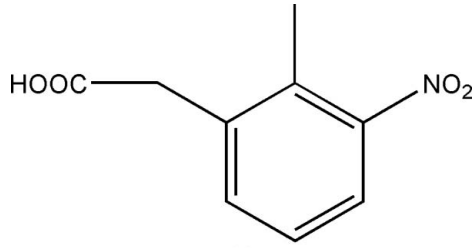
In the crystal structure of the title compound, $C_9H_9NO_4$, intermolecular O—H···O hydrogen bonds link the molecules into centrosymmetric dimers.

Comment

The title compound, (I), can be prepared by oxidizing methyl-3-nitrobenzaldehyde using a solution of potassium permanganate and sodium hydrogen carbonate in water (Askam & Deeks, 1969). The crystal structure determination of (I) has been carried out in order to elucidate the molecular conformation.



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

As can be seen from the packing diagram (Fig. 2), intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers; these hydrogen bonds may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

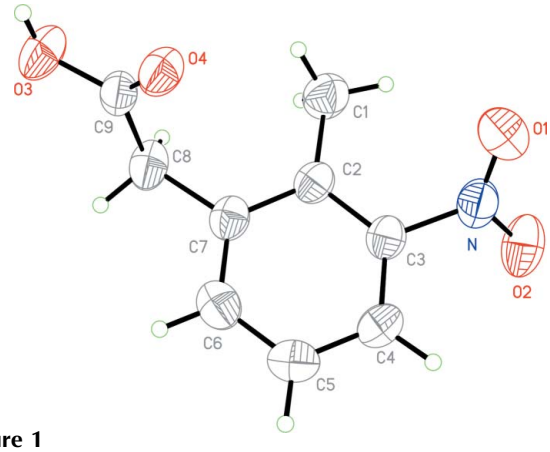


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The title compound, (I), was prepared by the literature method (Askam & Deeks, 1969). Crystals were obtained by dissolving (I) (0.2 g, 1.0 mmol) in methanol (30 ml) and evaporating the solvent slowly at room temperature for about 7 d (yield 2.1 g, 50%; m.p. 405 K).

Crystal data

$C_9H_9NO_4$
M_r = 195.17
Triclinic, $P\overline{1}$
a = 7.2250 (14) Å
b = 8.2220 (16) Å
c = 8.6470 (17) Å
α = 74.21 (3)°
β = 75.65 (3)°
γ = 67.96 (3)°
V = 452.01 (19) Å^3
Z = 2
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.944, T_{max} = 0.987
1767 measured reflections
1767 independent reflections
1263 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 26.0°
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.117
S = 1.08
1767 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.08P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O4^{i}	0.82	1.84	2.661 (2)	179

Symmetry code: (i) $-x+1, -y+2, -z$.

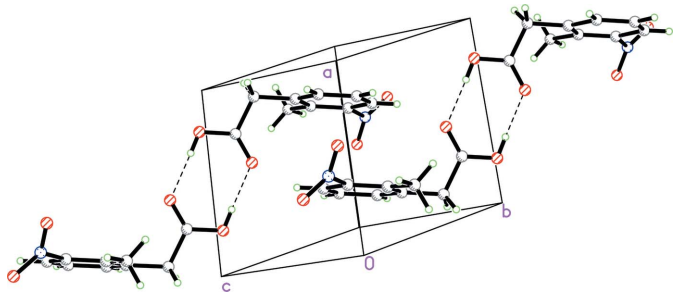


Figure 2
A packing diagram of (I). Intermolecular O—H···O hydrogen bonds are shown as dashed lines.

H atoms were positioned geometrically, with O—H = 0.82 Å, and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,O), where x = 1.2 for aromatic and methylene H, and x = 1.5 for all other H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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