

2-Nitrophenylacetic acid: hydrogen-bonded sheets of  $R_2^2(8)$  and  $R_4^4(18)$  ringsJames L. Wardell,<sup>a</sup> John N. Low<sup>b</sup>  
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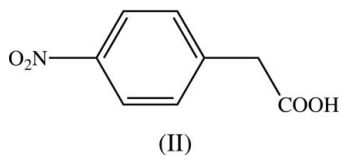
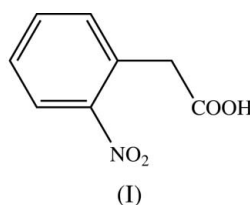
## Key indicators

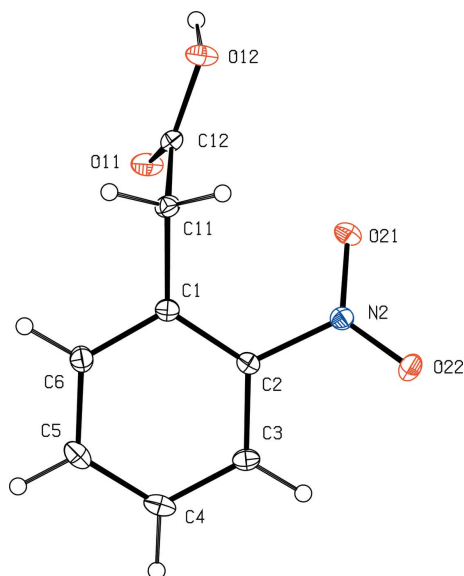
Single-crystal X-ray study  
 $T = 120$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.108  
Data-to-parameter ratio = 15.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Molecules of the title compound,  $\text{C}_8\text{H}_7\text{NO}_4$ , are linked into centrosymmetric  $R_2^2(8)$  dimers by paired  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, and these dimers are linked by two  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds into sheets of  $R_2^2(8)$  and  $R_4^4(18)$  rings.

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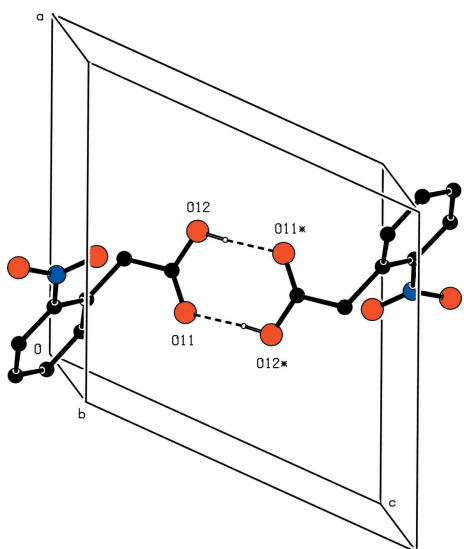
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## Comment

As part of our investigations of compounds containing nitro and carboxylic acid groups (Glidewell *et al.*, 2003*a,b*, 2004, 2006; Wardell *et al.*, 2005), we now report the molecular and supramolecular structure of 2-nitrophenylacetic acid, (I) (Fig. 1).The plane of atoms C1/C11/C12 is almost orthogonal to the plane of the aryl ring (Fig. 1, Table 1), while the  $\text{C}-\text{NO}_2$  plane makes a dihedral angle of  $30.1(2)^\circ$  with the ring.The molecules of (I) are linked into sheets by a combination of  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2). Paired  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into centrosymmetric  $R_2^2(8)$  (Bernstein *et al.*, 1995) dimers (Fig. 2). Two  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the dimers, so forming a (100) sheet built from  $R_2^2(8)$  and  $R_4^4(18)$  rings. The resulting net is of type (4,4) (Batten & Robson, 1998). There are no direction-specific interactions between adjacent sheets. In particular,  $\text{C}-\text{H}\cdots\pi(\text{arene})$  hydrogen bonds and aromatic  $\pi-\pi$  stacking interactions are both absent.The structure of the isomeric 4-nitrophenylacetic acid, (II), was reported some years ago [Cambridge Structural Database (Version of November 2005; Allen, 2002) refcode SEMTAF; Grabowski *et al.*, 1990]. The authors reported the formation of a centrosymmetric hydrogen-bonded dimer, but further aggregation of the dimers was not reported. In the event, the dimers are linked into sheets by a single aromatic  $\pi-\pi$  stacking interaction (Fig. 4).



**Figure 1**  
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.



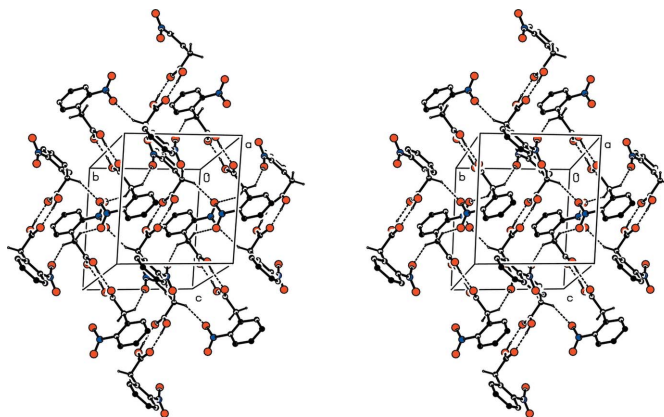
**Figure 2**  
Part of the crystal structure of (I), showing the formation of a centrosymmetric  $R_2^2(8)$  dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (\*) are at the symmetry position  $(1 - x, 1 - y, 1 - z)$ .

## Experimental

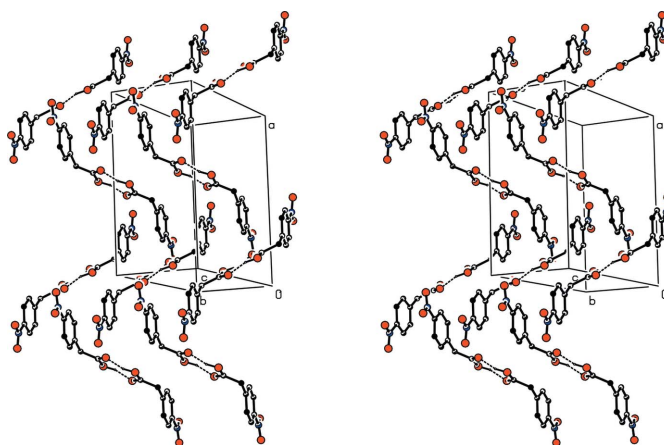
A commercial sample of (I) (Acros) was crystallized from ethanol (m.p. 412–413 K).

### Crystal data

$C_8H_7NO_4$	$Z = 4$
$M_r = 181.15$	$D_x = 1.510 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 9.3182(3) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$b = 9.4466(2) \text{ \AA}$	$T = 120(2) \text{ K}$
$c = 9.9733(3) \text{ \AA}$	Lath, colourless
$\beta = 114.7990(17)^\circ$	$0.52 \times 0.26 \times 0.10 \text{ mm}$
$V = 796.95(4) \text{ \AA}^3$	



**Figure 3**  
A stereoview of part of the crystal structure of (I), showing the formation of a (100) sheet of  $R_2^2(8)$  and  $R_4^4(18)$  rings. For the sake of clarity, H atoms bonded to aromatic C atoms have been omitted.



**Figure 4**  
A stereoview of part of the crystal structure of (II), showing the formation of a sheet of  $\pi$ -stacked hydrogen-bonded dimers. The original atomic coordinates (Grabowski *et al.*, 1990) have been used. For the sake of clarity, H atoms bonded to C atoms have been omitted.

### Data collection

Bruker Nonius KappaCCD area-detector diffractometer	8852 measured reflections
$\varphi$ and $\omega$ scans	1829 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	1682 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.949, T_{\max} = 0.988$	$R_{\text{int}} = 0.031$
	$\theta_{\max} = 27.7^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.341P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.16$	$\Delta\rho_{\max} = 0.34 \text{ e \AA}^{-3}$
1829 reflections	$\Delta\rho_{\min} = -0.27 \text{ e \AA}^{-3}$
120 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.103 (10)

**Table 1**

Selected torsion angles (°).

C2—C1—C11—C12	83.34 (16)	C1—C2—N2—O21	−29.64 (17)
C1—C11—C12—O12	−159.51 (11)		

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O12—H12...O11 <sup>i</sup>	0.84	1.83	2.6622 (14)	173
C11—H11A...O21 <sup>ii</sup>	0.99	2.35	3.1758 (16)	140
C11—H11B...O22 <sup>iii</sup>	0.99	2.54	3.4398 (19)	151

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

All H atoms were located in a difference map and then treated as riding, with C—H distances of 0.95 Å (aromatic) or 0.99 Å (CH<sub>2</sub>), and O—H distances of 0.84 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{O})$ .

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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