

James L. Wardell,^a John N. Low^b
and Christopher Glidewell^{c*}

^aInstituto de Química, Departamento de Química Inorgânica, Universidade Federal do Rio de Janeiro, CP 68563, 21945-970 Rio de Janeiro, RJ, Brazil, ^bDepartment of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and ^cSchool of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland

Correspondence e-mail: cg@st-andrews.ac.uk

Key indicators

Single-crystal X-ray study
 T = 120 K
 Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
 R factor = 0.036
 wR factor = 0.108
 Data-to-parameter ratio = 15.2

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

2-Nitrophenylacetic acid: hydrogen-bonded sheets of $R_2^2(8)$ and $R_4^4(18)$ rings

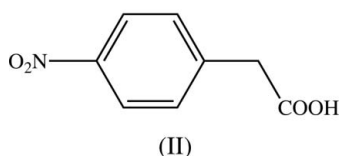
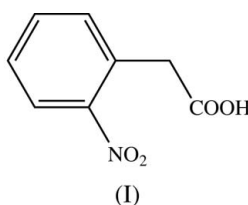
Molecules of the title compound, $\text{C}_8\text{H}_7\text{NO}_4$, are linked into centrosymmetric $R_2^2(8)$ dimers by paired $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, and these dimers are linked by two $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds into sheets of $R_2^2(8)$ and $R_4^4(18)$ rings.

Received 11 April 2006

Accepted 11 April 2006

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).

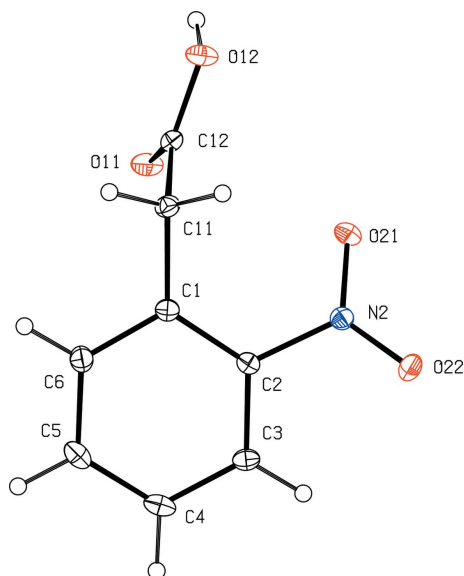


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

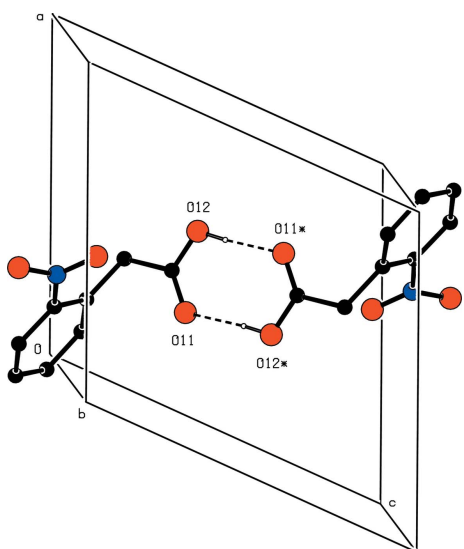


Figure 2
Part of the crystal structure of (I), showing the formation of a centrosymmetric $R_2^2(8)$ dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(1 - x, 1 - y, 1 - z)$.

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 |
| $\beta = 114.7990(17)^\circ$ | $0.52 \times 0.26 \times 0.10 \text{ mm}$ |
| $V = 796.95(4) \text{ \AA}^3$ | |

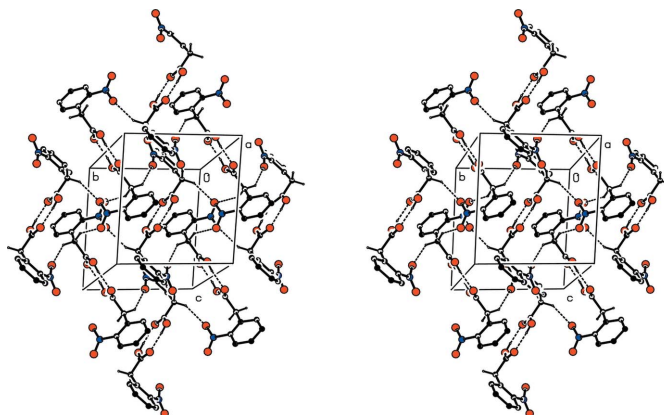


Figure 3
A stereoview of part of the crystal structure of (I), showing the formation of a (100) sheet of $R_2^2(8)$ and $R_4^4(18)$ rings. For the sake of clarity, H atoms bonded to aromatic C atoms have been omitted.

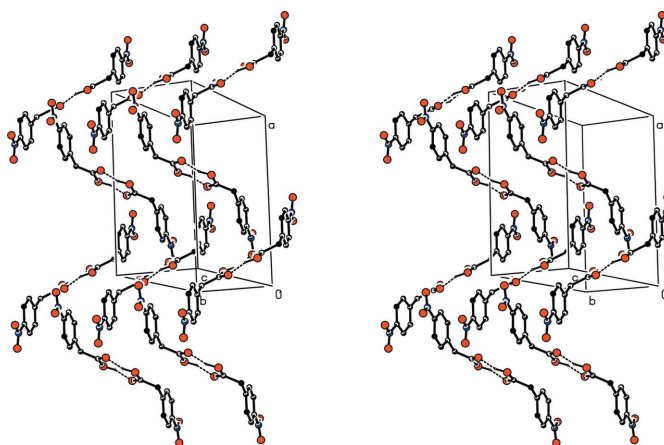


Figure 4
A stereoview of part of the crystal structure of (II), showing the formation of a sheet of π -stacked hydrogen-bonded dimers. The original atomic coordinates (Grabowski *et al.*, 1990) have been used. For the sake of clarity, H atoms bonded to C atoms have been omitted.

Data collection

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

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 $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.108$ | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| $S = 1.16$ | $\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$ |
| 1829 reflections | $\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$ |
| 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 ⁱ | 0.84 | 1.83 | 2.6622 (14) | 173 |
| C11—H11A...O21 ⁱⁱ | 0.99 | 2.35 | 3.1758 (16) | 140 |
| C11—H11B...O22 ⁱⁱⁱ | 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 (CH₂), 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).

The X-ray data were collected at the EPSRC X-Ray Crystallographic Service, University of Southampton, UK; the authors thank the staff of the Service for all their help and advice. JLW thanks CNPq and FAPERJ for financial support.

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