

2-Methyl-3-(4-nitrophenyl)acrylic acid

Niaz Muhammad,^a M. Nawaz Tahir,^{b*} Zia-ur-Rehman^a and Saqib Ali^a^aDepartment of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and ^bUniversity of Sargodha, Department of Physics, Sargodha, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

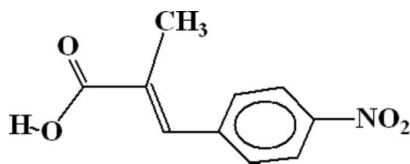
Received 10 July 2008; accepted 3 August 2008

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.134; data-to-parameter ratio = 18.0.

The title compound, $\text{C}_{10}\text{H}_9\text{NO}_4$, forms $R_2^2(8)$ dimers due to intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding in the crystal structure. Two dimers are further linked to each other through two intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming an $R_3^3(7)$ ring motif. The nitro groups form an intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond mimicking a five-membered ring. As a result of these hydrogen bonds, polymeric sheets are formed. The aromatic ring makes a dihedral angle of 42.84 (8°) with the carboxylate group and an angle of 8.01 (14°) with the nitro group. There is a π -interaction ($\text{N}-\text{O}\cdots\pi$) between the nitro group and the aromatic ring, with a distance of 3.7572 (14) Å between the N atom and the centroid of the aromatic ring.

Related literature

For related literature, see: Bernstein *et al.* (1995); Fujii *et al.* (2002); Ma & Hayes (2004); Muhammad *et al.* (2007, 2008a,b); Muhammad, Ali, Tahir & Zia-ur-Rehman (2008); Muhammad, Tahir, Ali, Zia-ur-Rehman & Kashmiri (2008); Muhammad, Tahir, Zia-ur-Rehman & Ali (2008); Muhammad, Tahir, Zia-ur-Rehman, Ali & Shaheen, (2008); Niaz *et al.* (2008).



Experimental

Crystal data

$\text{C}_{10}\text{H}_9\text{NO}_4$	$\gamma = 87.686$ (2°)
$M_r = 207.18$	$V = 479.21$ (4) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.3878$ (3) Å	Mo $K\alpha$ radiation
$b = 8.1050$ (5) Å	$\mu = 0.11$ mm ⁻¹
$c = 8.3402$ (4) Å	$T = 296$ (2) K
$\alpha = 75.793$ (2°)	$0.25 \times 0.20 \times 0.18$ mm
$\beta = 81.835$ (3°)	

Data collection

Bruker Kappa APEXII CCD diffractometer	9039 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	2518 independent reflections
$T_{\min} = 0.970$, $T_{\max} = 0.981$	1926 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.134$	$\Delta\rho_{\text{max}} = 0.24$ e Å ⁻³
$S = 1.02$	$\Delta\rho_{\text{min}} = -0.21$ e Å ⁻³
2518 reflections	
140 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{O2}^{\text{i}}$	0.93 (2)	1.71 (2)	2.6333 (15)	177 (2)
$\text{C3}-\text{H3}\cdots\text{O1}$	0.93	2.31	2.7080 (17)	105
$\text{C8}-\text{H8}\cdots\text{O1}^{\text{ii}}$	0.93	2.55	3.3471 (17)	144
$\text{C9}-\text{H9}\cdots\text{O2}^{\text{iii}}$	0.93	2.60	3.4912 (17)	161

Symmetry codes: (i) $-x, -y, -z + 1$; (ii) $x, y + 1, z$; (iii) $-x, -y + 1, -z + 1$.

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2; data reduction: SAINT (Bruker, 2007); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

The authors acknowledge the Higher Education Commission, Islamabad, Pakistan, for funding the purchase of the diffractometer at GCU, Lahore and for financial support to Niaz Muhammad for PhD studies under the Indigenous Scholarship Scheme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2087).

References

- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2005). *SADABS*. Bruker AXS Inc. Madison, Wisconsin, USA.
- Bruker (2007). *APEX2* and *SAINTE*. Bruker AXS Inc. Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Fujii, T., Shimaya, C., Yano, A., Terado, K., Sugino, H. & Fukuda, H. (2002). *Biotechnol. Lett.* **24**, 151–154.
- Ma, G. & Hayes, S. E. J. (2004). *Labelled Compd. Radiopharm.* **47**, 895–901.
- Muhammad, N., Ali, S., Tahir, M. N. & Zia-ur-Rehman (2008). *Acta Cryst.* **E64**, o1373.
- Muhammad, N., Tahir, M. N., Ali, S. & Zia-ur-Rehman (2008a). *Acta Cryst.* **E64**, m946–m947.
- Muhammad, N., Tahir, M. N., Ali, S. & Zia-ur-Rehman (2008b). *Acta Cryst.* **E64**, m978.
- Muhammad, N., Tahir, M. N., Ali, S., Zia-ur-Rehman & Kashmiri, M. A. (2008). *Acta Cryst.* **E64**, o1456.
- Muhammad, N., Tahir, M. N., Zia-ur-Rehman & Ali, S. (2008). *Acta Cryst.* **E64**, o1458.
- Muhammad, N., Tahir, M. N., Zia-ur-Rehman, Ali, S. & Shaheen, F. (2008). *Acta Cryst.* **E64**, o1542.

Muhammad, N., Zia-ur-Rehman, Ali, S. & Meetsma, A. (2007). *Acta Cryst.* **E63**, o2174–o2175.
Niaz, M., Tahir, M. N., Zia-ur-Rehman, Ali, S. & Khan, I. U. (2008). *Acta Cryst.* **E64**, o733.

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2008). E64, o1717-o1718 [doi:10.1107/S1600536808024999]

2-Methyl-3-(4-nitrophenyl)acrylic acid

N. Muhammad, M. N. Tahir, Zia-ur-Rehman and S. Ali

Comment

Cinnamic acid derivatives are widely used chemicals in a variety of fields (Ma *et al.*, 2004). They have been applied as antibacterial agents for suppression of bacterial growth (Fujii *et al.*, 2002). In wine, cinnamic acid and its derivatives join benzoic acid derivatives and flavonoids in creating pigments and tannin agents that give each vintage its characteristic bouquet and color. The title compound has been prepared in continuation of synthesizing various derivatives of cinnamic acids (Niaz *et al.*, 2008; Muhammad, Ali, Tahir & Zia-ur-Rehman, 2008; Muhammad, Tahir, Ali, Zia-ur-Rehman & Kashmiri, 2008) and their tin complexes (Muhammad *et al.*, 2008*a,b*).

The crystal structures of 3-(4-isopropylphenyl)-2-methylacrylic acid (Muhammad, Tahir, Ali, Zia-ur-Rehman & Kashmiri, 2008), of 3-(4-chlorophenyl)-2-methylacrylic acid (Muhammad, Tahir, Zia-ur-Rehman, Ali & Shaheen, 2008) and of 3-(4-bromophenyl)-2-methylacrylic acid (Muhammad *et al.*, 2007) have been reported. The title compound differs from these compounds due to the nitro group at *para* position. In the crystal structure of the title compound, the exocyclic C_{sp2}—C_{sp2} bonds are of 1.4770 (18) and 1.4880 (18) Å, the C=C is of 1.3376 (18) Å. The C—O bond length 1.2996 (16) Å is normal, much like the C=O bond length of 1.2300 (15) Å. The resonant N—O bond lengths are equal (1.2185 (16) and 1.2204 (17) Å). There is an intermolecular H-bond of C—H \cdots O type (Table 1, Fig 1). Centrosymmetric R₂²(8) dimers (Bernstein *et al.* 1995) are formed due to the intermolecular O1—H1 \cdots O2ⁱ [symmetry code: *i* = -*x*, -*y*, -*z* + 1] hydrogen bonding. Two adjacent dimers are linked to each other through two intermolecular H-bonds of C—H \cdots O type forming an R₃³(7) motif (Bernstein *et al.* 1995). The group of two dimers are linked to each other by intermolecular H-bonding (Table 1, Fig 2). There exist an N1—O4 \cdots Cgⁱⁱ [symmetry code: *ii* = -*x* + 1, -*y* + 2, -*z*] interaction with a distance of 3.7572 (14) Å between the N-atom and the centroid of the (C4—C9) aromatic ring. The aromatic ring makes a dihedral angle of 42.84 (8)° with the carboxylate (O1/C1/O2) moiety and 8.01 (14)° with the (N1/O3/O4) nitro group. Due to the intermolecular H-bonding polymeric sheets are formed.

Experimental

The title compound was prepared according to a reported procedure (Muhammad *et al.*, 2007). A mixture of 4-nitrobenzaldehyde (1.51 g, 10 mmol), methylmalonic acid (2.36 g, 20 mmol) and piperidine (1.98 ml, 20 mmol) in a pyridine (12.5 ml) solution was heated on a steam-bath for 24 h. The reaction mixture was cooled and added to a mixture of 25 ml of concentrated HCl and 50 g of ice. The precipitate formed in the acidified mixture was filtered off and washed with ice-cold water. The product was recrystallized from ethanol. The yield was 79%.

Refinement

The coordinates of H-atom attached with O1 were refined. The H-atoms attached with C-atoms were positioned geometrically, C—H = 0.93, and 0.96 Å for aromatic and methyl H, and constrained to ride on their parent atoms. The H-atoms were treated as isotropic with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{O})$, where $x = 1.5$ for methyl H, and $x = 1.2$ for all other H atoms.

Figures

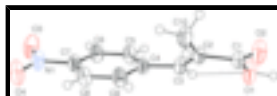


Fig. 1. ORTEP drawing of the title compound, $\text{C}_{11}\text{H}_{12}\text{O}_2$ with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii. The intramolecular H-bonds are shown by dotted lines.

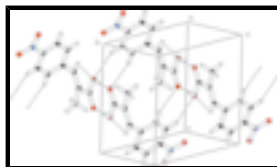


Fig. 2. The packing figure (PLATON: Spek, 2003) which shows the dimeric nature of the compound and the interlinkages of the dimers.

2-Methyl-3-(4-nitrophenyl)acrylic acid

Crystal data

$\text{C}_{10}\text{H}_9\text{NO}_4$	$Z = 2$
$M_r = 207.18$	$F_{000} = 216$
Triclinic, $P\bar{1}$	$D_x = 1.436 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 7.3878 (3) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 8.1050 (5) \text{ \AA}$	Cell parameters from 2518 reflections
$c = 8.3402 (4) \text{ \AA}$	$\theta = 2.5\text{--}29.1^\circ$
$\alpha = 75.793 (2)^\circ$	$\mu = 0.11 \text{ mm}^{-1}$
$\beta = 81.835 (3)^\circ$	$T = 296 (2) \text{ K}$
$\gamma = 87.686 (2)^\circ$	Prismatic, colourless
$V = 479.21 (4) \text{ \AA}^3$	$0.25 \times 0.20 \times 0.18 \text{ mm}$

Data collection

Bruker Kappa APEXII CCD diffractometer	2518 independent reflections
Radiation source: fine-focus sealed tube	1926 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.023$
Detector resolution: 7.4 pixels mm^{-1}	$\theta_{\text{max}} = 29.1^\circ$
$T = 296(2) \text{ K}$	$\theta_{\text{min}} = 2.5^\circ$
ω scans	$h = -10 \rightarrow 9$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -11 \rightarrow 9$
$T_{\text{min}} = 0.970$, $T_{\text{max}} = 0.981$	$l = -11 \rightarrow 11$

9039 measured reflections

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.134$

$S = 1.02$

2518 reflections

140 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.0915P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$

Extinction coefficient: ?

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.04661 (16)	0.13519 (13)	0.29456 (12)	0.0547 (4)
O2	0.09796 (15)	0.16087 (12)	0.54300 (12)	0.0526 (3)
O3	0.52309 (18)	1.11600 (15)	-0.36244 (14)	0.0661 (4)
O4	0.35761 (19)	1.23296 (13)	-0.18699 (15)	0.0648 (4)
N1	0.41247 (18)	1.10856 (14)	-0.23745 (14)	0.0466 (4)
C1	0.10453 (16)	0.21896 (15)	0.39150 (15)	0.0357 (3)
C2	0.17797 (17)	0.39231 (15)	0.31101 (16)	0.0362 (3)
C3	0.17195 (18)	0.45348 (15)	0.14759 (16)	0.0378 (3)
C4	0.22936 (17)	0.62471 (15)	0.04743 (15)	0.0361 (3)
C5	0.3308 (2)	0.64219 (16)	-0.11015 (16)	0.0424 (4)
C6	0.39099 (19)	0.80039 (17)	-0.20464 (16)	0.0425 (4)
C7	0.34487 (18)	0.94026 (15)	-0.14089 (15)	0.0375 (4)
C8	0.2375 (2)	0.92912 (16)	0.01030 (17)	0.0432 (4)
C9	0.1804 (2)	0.76957 (16)	0.10462 (16)	0.0430 (4)
C10	0.2580 (2)	0.47901 (17)	0.42356 (17)	0.0480 (4)
H1	-0.005 (3)	0.032 (3)	0.355 (2)	0.0656*
H3	0.12727	0.38114	0.09157	0.0454*
H5	0.35821	0.54652	-0.15208	0.0508*
H6	0.46089	0.81202	-0.30868	0.0510*
H8	0.20402	1.02624	0.04821	0.0518*
H9	0.10844	0.75935	0.20750	0.0516*
H10A	0.33667	0.40104	0.48836	0.0719*
H10B	0.16126	0.51574	0.49695	0.0719*
H10C	0.32723	0.57588	0.35757	0.0719*

Atomic displacement parameters (\AA^2)

U^{11} U^{22} U^{33} U^{12} U^{13} U^{23}

supplementary materials

O1	0.0855 (8)	0.0371 (5)	0.0397 (5)	-0.0259 (5)	-0.0071 (5)	-0.0026 (4)
O2	0.0801 (7)	0.0381 (5)	0.0357 (5)	-0.0229 (5)	-0.0058 (5)	0.0008 (4)
O3	0.0862 (8)	0.0524 (7)	0.0487 (6)	-0.0249 (6)	0.0068 (6)	0.0033 (5)
O4	0.1010 (9)	0.0290 (5)	0.0614 (7)	-0.0085 (5)	-0.0120 (6)	-0.0036 (5)
N1	0.0638 (7)	0.0340 (6)	0.0385 (6)	-0.0119 (5)	-0.0133 (5)	0.0030 (5)
C1	0.0399 (6)	0.0288 (6)	0.0353 (6)	-0.0057 (5)	-0.0021 (5)	-0.0028 (4)
C2	0.0379 (6)	0.0278 (5)	0.0392 (6)	-0.0052 (5)	-0.0024 (5)	-0.0019 (5)
C3	0.0443 (6)	0.0284 (6)	0.0380 (6)	-0.0068 (5)	-0.0037 (5)	-0.0029 (5)
C4	0.0416 (6)	0.0294 (6)	0.0342 (6)	-0.0041 (5)	-0.0064 (5)	-0.0004 (4)
C5	0.0569 (8)	0.0300 (6)	0.0375 (6)	-0.0005 (5)	-0.0009 (5)	-0.0062 (5)
C6	0.0521 (7)	0.0360 (6)	0.0338 (6)	-0.0020 (5)	0.0023 (5)	-0.0023 (5)
C7	0.0468 (7)	0.0281 (6)	0.0343 (6)	-0.0062 (5)	-0.0093 (5)	0.0017 (5)
C8	0.0607 (8)	0.0292 (6)	0.0380 (6)	0.0016 (5)	-0.0052 (6)	-0.0062 (5)
C9	0.0554 (8)	0.0348 (6)	0.0334 (6)	-0.0009 (5)	0.0030 (5)	-0.0029 (5)
C10	0.0626 (8)	0.0353 (7)	0.0437 (7)	-0.0160 (6)	-0.0124 (6)	0.0001 (5)

Geometric parameters (Å, °)

O1—C1	1.2996 (16)	C5—C6	1.3832 (19)
O2—C1	1.2300 (15)	C6—C7	1.3774 (19)
O3—N1	1.2204 (17)	C7—C8	1.3759 (19)
O4—N1	1.2185 (16)	C8—C9	1.3855 (19)
O1—H1	0.93 (2)	C3—H3	0.9300
N1—C7	1.4698 (17)	C5—H5	0.9300
C1—C2	1.4880 (18)	C6—H6	0.9300
C2—C3	1.3376 (18)	C8—H8	0.9300
C2—C10	1.4965 (19)	C9—H9	0.9300
C3—C4	1.4770 (18)	C10—H10A	0.9600
C4—C9	1.3887 (18)	C10—H10B	0.9600
C4—C5	1.3951 (18)	C10—H10C	0.9600
O1...C8 ⁱ	3.3471 (17)	C4...H10C	2.7200
O1...C6 ⁱⁱ	3.4128 (19)	C4...H3 ⁱⁱ	3.0300
O1...O2 ⁱⁱⁱ	2.6333 (15)	C9...H10C	2.6400
O2...O1 ⁱⁱⁱ	2.6333 (15)	C10...H9	2.8300
O2...C1 ⁱⁱⁱ	3.3657 (16)	C10...H10B ^v	3.0700
O2...N1 ^{iv}	3.1112 (17)	H1...O1 ⁱⁱⁱ	2.882 (17)
O1...H1 ⁱⁱⁱ	2.882 (17)	H1...O2 ⁱⁱⁱ	1.71 (2)
O1...H3	2.3100	H1...C1 ⁱⁱⁱ	2.59 (2)
O1...H8 ⁱ	2.5500	H1...H1 ⁱⁱⁱ	2.36 (2)
O2...H10B	2.8600	H3...O1	2.3100
O2...H10A	2.5900	H3...H5	2.5900
O2...H1 ⁱⁱⁱ	1.71 (2)	H3...C4 ⁱⁱ	3.0300
O2...H9 ^v	2.6000	H5...O4 ⁱ	2.6300
O3...H6	2.4400	H5...H3	2.5900
O3...H10A ^{vi}	2.7600	H6...O3	2.4400
O3...H6 ^{vii}	2.6500	H6...O3 ^{vii}	2.6500

O3...H10C ^{viii}	2.7800	H6...C2 ^x	3.0800
O4...H5 ^{ix}	2.6300	H8...O1 ^{ix}	2.5500
O4...H8	2.4200	H8...O4	2.4200
O4...H10A ^{vi}	2.7400	H9...C2	2.9300
O4...H10C ^{viii}	2.8500	H9...C10	2.8300
N1...O2 ^{vi}	3.1112 (17)	H9...H10C	2.4200
N1...C8 ^{viii}	3.378 (2)	H9...O2 ^v	2.6000
C1...O2 ⁱⁱⁱ	3.3657 (16)	H10A...O2	2.5900
C2...C6 ^x	3.5837 (19)	H10A...O3 ^{iv}	2.7600
C6...O1 ⁱⁱ	3.4128 (19)	H10A...O4 ^{iv}	2.7400
C6...C2 ^x	3.5837 (19)	H10B...O2	2.8600
C8...N1 ^{viii}	3.378 (2)	H10B...C1 ^v	3.0800
C8...O1 ^{ix}	3.3471 (17)	H10B...C2 ^v	2.9500
C9...C10	3.1937 (19)	H10B...C10 ^v	3.0700
C10...C9	3.1937 (19)	H10B...H10B ^v	2.4000
C1...H10B ^v	3.0800	H10C...C4	2.7200
C1...H1 ⁱⁱⁱ	2.59 (2)	H10C...C9	2.6400
C2...H9	2.9300	H10C...H9	2.4200
C2...H10B ^v	2.9500	H10C...O3 ^{viii}	2.7800
C2...H6 ^x	3.0800	H10C...O4 ^{viii}	2.8500
C1—O1—H1	111.6 (12)	C7—C8—C9	118.33 (12)
O3—N1—O4	123.45 (13)	C4—C9—C8	120.81 (12)
O3—N1—C7	118.21 (12)	C2—C3—H3	117.00
O4—N1—C7	118.33 (12)	C4—C3—H3	117.00
O1—C1—O2	122.55 (12)	C4—C5—H5	120.00
O1—C1—C2	116.77 (11)	C6—C5—H5	120.00
O2—C1—C2	120.68 (11)	C5—C6—H6	121.00
C1—C2—C10	115.28 (11)	C7—C6—H6	121.00
C3—C2—C10	126.40 (12)	C7—C8—H8	121.00
C1—C2—C3	118.29 (11)	C9—C8—H8	121.00
C2—C3—C4	126.35 (12)	C4—C9—H9	120.00
C3—C4—C9	121.47 (11)	C8—C9—H9	120.00
C5—C4—C9	119.09 (12)	C2—C10—H10A	109.00
C3—C4—C5	119.41 (11)	C2—C10—H10B	109.00
C4—C5—C6	120.66 (12)	C2—C10—H10C	109.00
C5—C6—C7	118.38 (12)	H10A—C10—H10B	109.00
N1—C7—C6	119.04 (11)	H10A—C10—H10C	110.00
N1—C7—C8	118.35 (11)	H10B—C10—H10C	109.00
C6—C7—C8	122.61 (12)		
O3—N1—C7—C6	-7.7 (2)	C2—C3—C4—C9	-44.9 (2)
O3—N1—C7—C8	172.34 (13)	C3—C4—C5—C6	-178.09 (13)
O4—N1—C7—C6	173.58 (14)	C9—C4—C5—C6	3.7 (2)
O4—N1—C7—C8	-6.4 (2)	C3—C4—C9—C8	179.06 (13)
O1—C1—C2—C3	3.07 (18)	C5—C4—C9—C8	-2.7 (2)
O1—C1—C2—C10	-174.99 (12)	C4—C5—C6—C7	-1.4 (2)

supplementary materials

O2—C1—C2—C3	-176.04 (13)	C5—C6—C7—N1	178.15 (13)
O2—C1—C2—C10	5.90 (18)	C5—C6—C7—C8	-1.9 (2)
C1—C2—C3—C4	176.84 (12)	N1—C7—C8—C9	-177.24 (13)
C10—C2—C3—C4	-5.3 (2)	C6—C7—C8—C9	2.8 (2)
C2—C3—C4—C5	136.88 (15)	C7—C8—C9—C4	-0.4 (2)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -y+1, -z$; (iii) $-x, -y, -z+1$; (iv) $x, y-1, z+1$; (v) $-x, -y+1, -z+1$; (vi) $x, y+1, z-1$; (vii) $-x+1, -y+2, -z-1$; (viii) $-x+1, -y+2, -z$; (ix) $x, y+1, z$; (x) $-x+1, -y+1, -z$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱⁱⁱ	0.93 (2)	1.71 (2)	2.6333 (15)	177 (2)
C3—H3 \cdots O1	0.93	2.31	2.7080 (17)	105
C8—H8 \cdots O1 ^{ix}	0.93	2.55	3.3471 (17)	144
C9—H9 \cdots O2 ^v	0.93	2.60	3.4912 (17)	161

Symmetry codes: (iii) $-x, -y, -z+1$; (ix) $x, y+1, z$; (v) $-x, -y+1, -z+1$.

Fig. 1

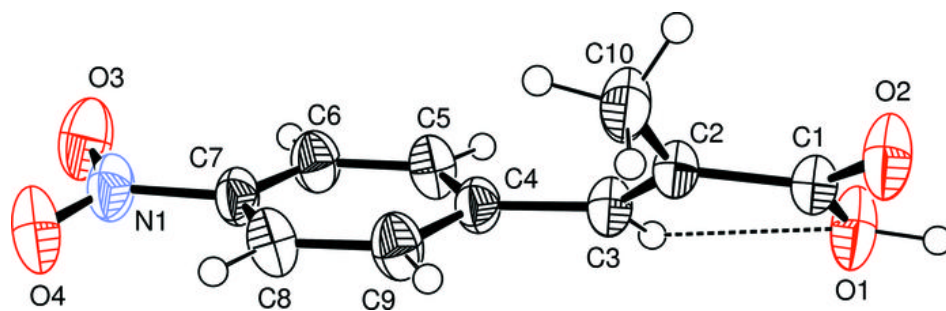


Fig. 2

