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Ethyl 2-(4-nitrophenoxy)acetate

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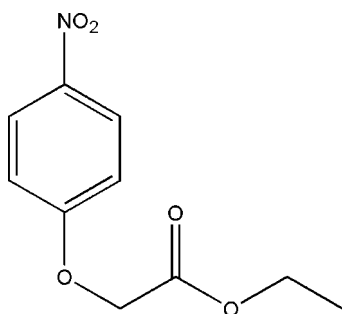
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.068; wR factor = 0.156; data-to-parameter ratio = 14.9.

In the title molecule, $\text{C}_{10}\text{H}_{11}\text{NO}_5$, the methyl C atom deviates by 0.830 (6) Å from the mean plane of the remaining non-H atoms. In the crystal, weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into layers parallel to the bc plane.

Related literature

For the structure of *tert*-butyl 2-(4-nitrophenoxy)acetate, see: Ali *et al.* (2011). For general background to ferroelectric organics, see: Fu *et al.* (2009); Ye *et al.* (2006).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{11}\text{NO}_5$
 $M_r = 225.20$
 Monoclinic, $P2_1/c$

$a = 5.3848$ (11) Å
 $b = 8.4482$ (17) Å
 $c = 24.238$ (5) Å

$\beta = 92.59$ (3)°
 $V = 1101.5$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.11$ mm⁻¹
 $T = 293$ K
 $0.3 \times 0.3 \times 0.2$ mm

Data collection

Rigaku Mercury CCD diffractometer
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
 $T_{\min} = 0.968$, $T_{\max} = 0.978$

9279 measured reflections
 2169 independent reflections
 1157 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.089$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.156$
 $S = 1.01$
 2169 reflections

146 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H2A}\cdots\text{O4}^{\text{i}}$	0.93	2.53	3.177 (4)	127
$\text{C10}-\text{H10B}\cdots\text{O1}^{\text{ii}}$	0.96	2.58	3.513 (6)	164

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The author is grateful to the starter fund of Southeast University for financial support to buy the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5259).

References

- Ali, Q., Anis, I., Raza Shah, M. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o532.
 Fu, D.-W., Ge, J.-Z., Dai, J., Ye, H.-Y. & Qu, Z.-R. (2009). *Inorg. Chem. Commun.* **12**, 994–997.
 Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Ye, Q., Song, Y.-M., Wang, G.-X., Chen, K. & Fu, D.-W. (2006). *J. Am. Chem. Soc.* **128**, 6554–6555.

supporting information

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Ethyl 2-(4-nitrophenoxy)acetate

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S1. Comment

The title compound, (I), has been obtained during the search for new organic compounds which demonstrate ferroelectric phase changes (Fu *et al.*, 2009; Ye *et al.*, 2006). Though the measured dielectric constant of (I) showed no dielectric disuniformity in the range 120–385 K (mp. 393–402 K), herewith we present its crystal structure.

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in *tert*-butyl 2-(4-nitrophenoxy)acetate (Ali *et al.*, 2011). Atom C10 deviates at 0.830 (6) Å from the mean plane of the rest non-H atoms. Weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into layers parallel to *bc* plane.

S2. Experimental

4-Nitro-phenol (7 g) and 1-Bromo-butan-2-one (8.5 g) were dissolved in acetone, kalium carbonicum (7.5 g) was added to the mixture. Then the mixture was heated and refluxed by mechanical stirring at 70°C. Yellow solid was filtered off. This solid was dissolved in ethanol and single crystals suitable for X-ray structure analysis were obtained by the slow evaporation of the above solution after 3 days in air.

S3. Refinement

All H atoms were placed in calculated positions (N—H = 0.89 Å; C—H = 0.93 Å for *Csp*² atoms and C—H = 0.96 Å and 0.97 Å for *Csp*³ atoms), assigned fixed *U*_{iso} values [*U*_{iso} = 1.2 *U*_{eq}(*Csp*²) and 1.5 *U*_{eq}(*Csp*³, *N*)] and allowed to ride.

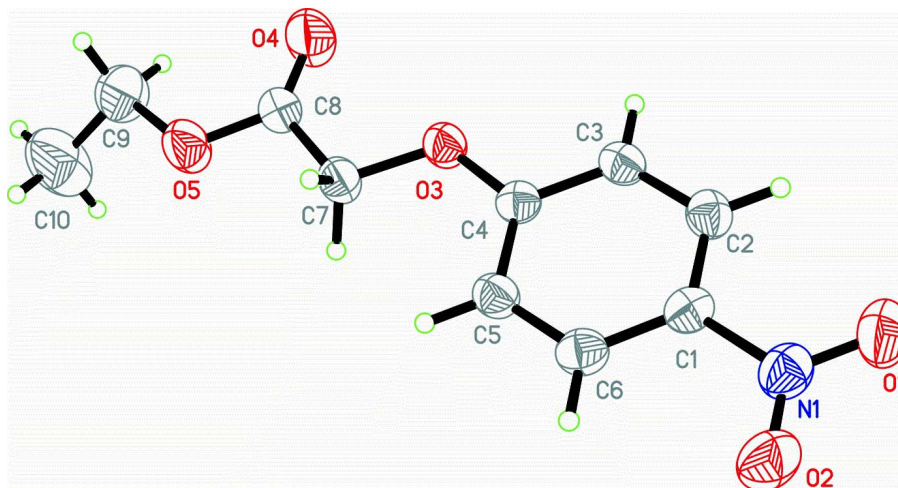


Figure 1

The molecular structure of (I) showing the atomic numbering and 40% probability displacement ellipsoids.

Ethyl 2-(4-nitrophenoxy)acetate

Crystal data

 $C_{10}H_{11}NO_5$ $M_r = 225.20$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 5.3848$ (11) Å $b = 8.4482$ (17) Å $c = 24.238$ (5) Å $\beta = 92.59$ (3)° $V = 1101.5$ (4) Å³ $Z = 4$ $F(000) = 472$ $D_x = 1.358$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3450 reflections

 $\theta = 3.4$ – 26.0° $\mu = 0.11$ mm⁻¹ $T = 293$ K

Block, colourless

 $0.3 \times 0.3 \times 0.2$ mm

Data collection

Rigaku Mercury CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω scans

Absorption correction: multi-scan

(CrystalClear; Rigaku, 2005)

 $T_{\min} = 0.968$, $T_{\max} = 0.978$

9279 measured reflections

2169 independent reflections

1157 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.089$ $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.4^\circ$ $h = -6 \rightarrow 6$ $k = -10 \rightarrow 10$ $l = -29 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.068$ $wR(F^2) = 0.156$ $S = 1.01$

2169 reflections

146 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from

neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.35P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.20$ e Å⁻³ $\Delta\rho_{\min} = -0.21$ e Å⁻³Extinction correction: *SHELXL97* (Sheldrick,2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.011 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O3	0.2402 (3)	0.9062 (2)	0.43476 (7)	0.0593 (5)
C4	0.3764 (4)	0.8226 (3)	0.47348 (10)	0.0502 (6)
C3	0.2863 (5)	0.8248 (3)	0.52630 (10)	0.0559 (7)

H3A	0.1438	0.8824	0.5331	0.067*
C1	0.6184 (5)	0.6596 (3)	0.55727 (11)	0.0540 (7)
C7	0.3224 (5)	0.9043 (3)	0.38008 (10)	0.0598 (7)
H7A	0.3228	0.7968	0.3661	0.072*
H7B	0.4902	0.9458	0.3794	0.072*
C6	0.7118 (5)	0.6582 (3)	0.50557 (11)	0.0600 (7)
H6A	0.8565	0.6024	0.4992	0.072*
O5	0.2362 (4)	1.0156 (3)	0.29508 (8)	0.0930 (8)
C5	0.5909 (4)	0.7396 (3)	0.46316 (11)	0.0568 (7)
H5A	0.6527	0.7389	0.4279	0.068*
N1	0.7460 (5)	0.5687 (3)	0.60109 (11)	0.0713 (7)
C2	0.4062 (5)	0.7424 (3)	0.56848 (11)	0.0588 (7)
H2A	0.3454	0.7424	0.6038	0.071*
O1	0.6650 (5)	0.5737 (3)	0.64727 (10)	0.1141 (10)
O2	0.9260 (4)	0.4885 (3)	0.59049 (9)	0.0938 (8)
C8	0.1488 (5)	1.0048 (4)	0.34495 (11)	0.0640 (8)
O4	−0.0361 (4)	1.0635 (3)	0.35870 (9)	0.1103 (10)
C9	0.0983 (7)	1.1139 (6)	0.25442 (15)	0.1140 (14)
H9A	−0.0259	1.0504	0.2344	0.137*
H9B	0.0140	1.1987	0.2730	0.137*
C10	0.2659 (8)	1.1779 (7)	0.21723 (18)	0.157 (2)
H10A	0.1762	1.2415	0.1902	0.235*
H10B	0.3491	1.0935	0.1991	0.235*
H10C	0.3863	1.2424	0.2371	0.235*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0581 (11)	0.0663 (12)	0.0541 (11)	0.0116 (9)	0.0075 (8)	0.0024 (9)
C4	0.0496 (15)	0.0462 (15)	0.0547 (15)	−0.0030 (12)	0.0012 (12)	−0.0033 (13)
C3	0.0522 (15)	0.0567 (17)	0.0594 (16)	−0.0004 (13)	0.0083 (12)	−0.0025 (14)
C1	0.0535 (16)	0.0467 (15)	0.0612 (17)	−0.0028 (13)	−0.0046 (13)	0.0025 (14)
C7	0.0612 (16)	0.0655 (18)	0.0534 (16)	0.0049 (14)	0.0104 (13)	0.0001 (14)
C6	0.0551 (16)	0.0554 (17)	0.0694 (18)	0.0060 (13)	0.0020 (14)	−0.0043 (16)
O5	0.0837 (14)	0.130 (2)	0.0668 (13)	0.0279 (14)	0.0152 (11)	0.0294 (14)
C5	0.0539 (16)	0.0596 (17)	0.0574 (15)	0.0025 (13)	0.0079 (12)	−0.0056 (14)
N1	0.0725 (17)	0.0681 (17)	0.0725 (18)	−0.0037 (14)	−0.0054 (14)	0.0084 (15)
C2	0.0636 (17)	0.0562 (17)	0.0568 (16)	−0.0076 (14)	0.0050 (13)	0.0006 (14)
O1	0.1161 (19)	0.153 (3)	0.0734 (16)	0.0334 (17)	0.0087 (14)	0.0313 (17)
O2	0.0892 (16)	0.0956 (17)	0.0954 (17)	0.0293 (14)	−0.0086 (13)	0.0132 (14)
C8	0.0609 (17)	0.076 (2)	0.0554 (16)	0.0006 (16)	0.0055 (14)	0.0000 (15)
O4	0.0937 (17)	0.161 (3)	0.0771 (15)	0.0615 (17)	0.0125 (13)	0.0127 (15)
C9	0.101 (3)	0.160 (4)	0.080 (2)	0.023 (3)	−0.002 (2)	0.043 (3)
C10	0.149 (4)	0.196 (5)	0.129 (4)	0.053 (4)	0.043 (3)	0.081 (4)

Geometric parameters (Å, °)

O3—C4	1.362 (3)	O5—C8	1.320 (3)
O3—C7	1.416 (3)	O5—C9	1.465 (4)
C4—C5	1.384 (3)	C5—H5A	0.9300
C4—C3	1.390 (3)	N1—O2	1.220 (3)
C3—C2	1.374 (3)	N1—O1	1.220 (3)
C3—H3A	0.9300	C2—H2A	0.9300
C1—C6	1.371 (3)	C8—O4	1.174 (3)
C1—C2	1.377 (3)	C9—C10	1.412 (5)
C1—N1	1.458 (3)	C9—H9A	0.9700
C7—C8	1.499 (4)	C9—H9B	0.9700
C7—H7A	0.9700	C10—H10A	0.9600
C7—H7B	0.9700	C10—H10B	0.9600
C6—C5	1.376 (3)	C10—H10C	0.9600
C6—H6A	0.9300		
C4—O3—C7	117.25 (19)	C4—C5—H5A	120.4
O3—C4—C5	124.5 (2)	O2—N1—O1	122.2 (3)
O3—C4—C3	115.4 (2)	O2—N1—C1	119.5 (3)
C5—C4—C3	120.1 (2)	O1—N1—C1	118.3 (3)
C2—C3—C4	120.5 (2)	C3—C2—C1	118.5 (2)
C2—C3—H3A	119.8	C3—C2—H2A	120.8
C4—C3—H3A	119.8	C1—C2—H2A	120.8
C6—C1—C2	121.8 (2)	O4—C8—O5	125.0 (3)
C6—C1—N1	118.8 (2)	O4—C8—C7	126.4 (3)
C2—C1—N1	119.5 (2)	O5—C8—C7	108.7 (2)
O3—C7—C8	108.2 (2)	C10—C9—O5	109.1 (3)
O3—C7—H7A	110.1	C10—C9—H9A	109.9
C8—C7—H7A	110.1	O5—C9—H9A	109.9
O3—C7—H7B	110.1	C10—C9—H9B	109.9
C8—C7—H7B	110.1	O5—C9—H9B	109.9
H7A—C7—H7B	108.4	H9A—C9—H9B	108.3
C1—C6—C5	119.8 (2)	C9—C10—H10A	109.5
C1—C6—H6A	120.1	C9—C10—H10B	109.5
C5—C6—H6A	120.1	H10A—C10—H10B	109.5
C8—O5—C9	117.7 (3)	C9—C10—H10C	109.5
C6—C5—C4	119.3 (2)	H10A—C10—H10C	109.5
C6—C5—H5A	120.4	H10B—C10—H10C	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C2—H2A $\cdots$ O4 ⁱ	0.93	2.53	3.177 (4)	127
C10—H10B $\cdots$ O1 ⁱⁱ	0.96	2.58	3.513 (6)	164

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x, -y+3/2, z-1/2$.