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N-(4-Propoxyphenyl)acetamide

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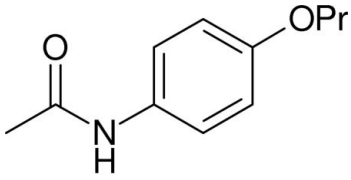
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.115; data-to-parameter ratio = 14.5.

The non-H atoms of the title compound, $C_{11}H_{15}NO_2$, are approximately coplanar. In the crystal structure, an N—H···O hydrogen bond leads to $C(4)$ chains of molecules propagating along [010].

Related literature

For background, see: Haisa *et al.* (1980); Nichols & Frampton (1998); Oswald *et al.* (2002); Hansen *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{15}NO_2$
M_r = 193.24
Orthorhombic, *Pbcn*
a = 11.7776 (11) Å
b = 9.4779 (8) Å
c = 18.8180 (18) Å
V = 2100.6 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 93 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: none
12750 measured reflections
1916 independent reflections
1702 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.06
1916 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 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
N1—H1···O1^{i}	0.884 (17)	1.949 (17)	2.7988 (15)	160.8 (14)

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

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2048).

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supplementary materials

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N-(4-Propoxyphenyl)acetamide

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Comment

The title compound, (I), with *R* = n-Pr, complements the series of molecules with *R* = H [*N*-(4-hydroxyphenyl)acetamide or acetaminophen or paracetamol], *R* = Me [*N*-(4-methoxyphenyl)acetamide; Haisa *et al.* (1980)] and *R* = Et [*N*-(4-ethoxyphenyl)acetamide or phenacetin; Hansen *et al.* (2006)]. Crystallographically, paracetamol is notable for its polymorphism, adopting at least four crystalline forms (Nichols & Frampton, 1998), as well as its participation in a variety of distinctive supramolecular networks (Oswald *et al.*, 2002).

The molecule of (I) is approximately planar, with an r.m.s. deviation from the mean plane of 0.084Å for the non-hydrogen atoms. The short C6—N1 bond length of 1.4145 (17)Å and the bond-angle sum of 360° for N1 suggest some electronic interaction between the π cloud of the benzene ring and the p electrons of N1, C7 and O1. Otherwise, the geometry of (I) may be regarded as normal (Allen *et al.*, 1995).

In the crystal of (I), an N—H···O hydrogen bond (Table 1) links the molecules into C(4) chains propagating in [010] (Fig. 2). The unit-cell packing for (I) results in distinctive zigzag (100) sheets (Fig. 3). There are no aromatic π-π stacking interactions in (I) as the closest benzene ring centroid-centroid separation is greater than 4.51 Å.

Supramolecular C(4) hydrogen bonded chains containing the characteristic ···O=C—N—H··· amide unit are also observed in the crystals of *N*-(4-methoxyphenyl)acetamide (Haisa *et al.*, 1980) and phenacetin (Hansen *et al.*, 2006). However, paracetamol adopts different hydrogen bonding patterns: either –N—H···OH or –O—H···O—H··· hydrogen bonds are seen, depending on the polymorph (Nichols & Frampton, 1998)

Experimental

Paracetamol was treated with K_2CO_3 and 1-iodopropane in acetone to yield the crude pruduct. Recrystallization from acetone yielded colourless prisms of (I).

Refinement

The N-bound hydrogen atom was located in a difference map and its position was freely refined with U_{iso}(H) = 1.2U_{eq}(N). The C-bound hydrogen atoms were geometrically placed (C—H = 0.95–0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate, but not tip, to best fit the electron density.

Figures

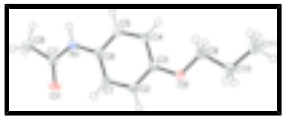

Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

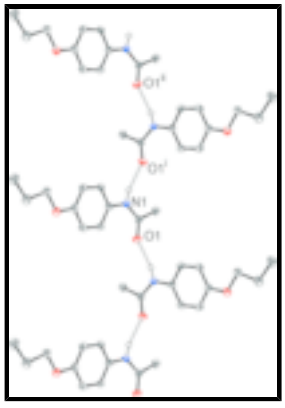

Fig. 2. Fragement of a [010] hydrogen bonded chain of molecules in the crystal of (I) with all H atoms except Hxx omitted for clarity. Symmetry codes: (i) 3/2 − *x*,*y* + 1/2,*z*; (ii) *x*, *y* + 1, *z*.

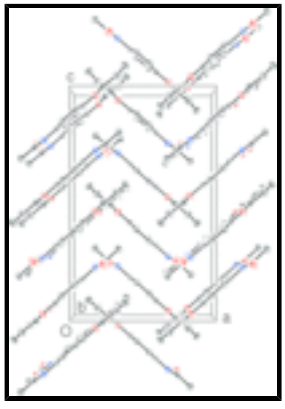

Fig. 3. The unit cell packing for (I), with H atoms omitted for clarity.

N-(4-Propoxyphenyl)acetamide

Crystal data

$C_{11}H_{15}NO_2$	F_{000} = 832
M_r = 193.24	D_x = 1.222 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 6098 reflections
a = 11.7776 (11) Å	θ = 2.4–28.7º
b = 9.4779 (8) Å	μ = 0.08 mm^{-1}
c = 18.8180 (18) Å	*T* = 93 (2) K
V = 2100.6 (3) Å^3	Prism, colourless
Z = 8	0.20 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer	1702 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.027
Monochromator: graphite	θ_{max} = 25.3º
T = 93(2) K	θ_{min} = 2.8º
ω and φ scans	*h* = −14→14
Absorption correction: none	*k* = −10→11

12750 measured reflections
1916 independent reflections

$l = -22 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.115$
$S = 1.06$
1916 reflections
132 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difmap and geom
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.5326P]$ 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}
Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.54255 (11)	0.29534 (13)	0.34000 (7)	0.0215 (3)
H1A	0.5712	0.2107	0.3197	0.026*
C2	0.45492 (11)	0.29033 (14)	0.38907 (7)	0.0226 (3)
H2	0.4242	0.2015	0.4023	0.027*
C3	0.41105 (11)	0.41241 (14)	0.41933 (7)	0.0207 (3)
C4	0.45639 (11)	0.54225 (14)	0.39988 (7)	0.0219 (3)
H4	0.4274	0.6268	0.4200	0.026*
C5	0.54437 (11)	0.54724 (13)	0.35089 (7)	0.0210 (3)
H5	0.5752	0.6361	0.3378	0.025*
C6	0.58849 (10)	0.42529 (13)	0.32056 (7)	0.0182 (3)
C7	0.74534 (11)	0.34160 (14)	0.24285 (7)	0.0211 (3)
C8	0.83580 (12)	0.39449 (15)	0.19276 (8)	0.0281 (4)
H8A	0.8423	0.4972	0.1971	0.042*
H8B	0.8152	0.3700	0.1438	0.042*
H8C	0.9087	0.3506	0.2048	0.042*
C9	0.27433 (12)	0.51676 (14)	0.49810 (7)	0.0245 (3)

H9A	0.2452	0.5813	0.4610	0.029*
H9B	0.3321	0.5676	0.5265	0.029*
C10	0.17881 (12)	0.46751 (16)	0.54514 (8)	0.0316 (4)
H10A	0.2092	0.4020	0.5814	0.038*
H10B	0.1227	0.4153	0.5161	0.038*
C11	0.12012 (14)	0.59032 (16)	0.58193 (8)	0.0351 (4)
H11A	0.0586	0.5544	0.6120	0.053*
H11B	0.0887	0.6545	0.5461	0.053*
H11C	0.1752	0.6412	0.6114	0.053*
N1	0.67758 (9)	0.44174 (12)	0.27083 (6)	0.0193 (3)
H1	0.6928 (14)	0.5298 (18)	0.2586 (7)	0.023*
O1	0.73594 (9)	0.21529 (10)	0.25639 (5)	0.0298 (3)
O2	0.32328 (8)	0.39351 (10)	0.46613 (5)	0.0257 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0241 (7)	0.0167 (7)	0.0237 (7)	0.0015 (5)	−0.0002 (5)	−0.0011 (5)
C2	0.0252 (7)	0.0182 (7)	0.0246 (7)	−0.0031 (5)	0.0005 (5)	0.0019 (5)
C3	0.0199 (7)	0.0236 (7)	0.0187 (6)	0.0002 (5)	−0.0009 (5)	0.0020 (5)
C4	0.0247 (7)	0.0183 (7)	0.0228 (7)	0.0025 (5)	0.0002 (5)	−0.0023 (5)
C5	0.0222 (7)	0.0173 (7)	0.0235 (7)	−0.0014 (5)	−0.0007 (5)	0.0015 (5)
C6	0.0183 (6)	0.0191 (7)	0.0174 (6)	0.0009 (5)	−0.0039 (5)	0.0009 (5)
C7	0.0201 (7)	0.0211 (8)	0.0220 (7)	0.0022 (5)	−0.0027 (5)	−0.0005 (5)
C8	0.0259 (7)	0.0272 (8)	0.0313 (8)	0.0028 (6)	0.0045 (6)	−0.0004 (6)
C9	0.0247 (7)	0.0245 (7)	0.0243 (7)	0.0029 (6)	0.0012 (6)	0.0001 (6)
C10	0.0279 (8)	0.0344 (9)	0.0326 (8)	0.0007 (6)	0.0083 (6)	−0.0021 (6)
C11	0.0326 (8)	0.0397 (9)	0.0329 (8)	0.0064 (7)	0.0087 (7)	0.0012 (7)
N1	0.0209 (6)	0.0151 (6)	0.0218 (6)	−0.0007 (4)	0.0015 (4)	0.0008 (4)
O1	0.0313 (6)	0.0180 (6)	0.0401 (6)	0.0052 (4)	0.0057 (4)	0.0021 (4)
O2	0.0262 (5)	0.0238 (5)	0.0270 (5)	0.0000 (4)	0.0080 (4)	0.0000 (4)

Geometric parameters (Å, °)

C1—C2	1.3856 (19)	C8—H8A	0.9800
C1—C6	1.3941 (18)	C8—H8B	0.9800
C1—H1A	0.9500	C8—H8C	0.9800
C2—C3	1.3894 (18)	C9—O2	1.4349 (16)
C2—H2	0.9500	C9—C10	1.506 (2)
C3—O2	1.3697 (16)	C9—H9A	0.9900
C3—C4	1.3905 (18)	C9—H9B	0.9900
C4—C5	1.3877 (19)	C10—C11	1.521 (2)
C4—H4	0.9500	C10—H10A	0.9900
C5—C6	1.3899 (17)	C10—H10B	0.9900
C5—H5	0.9500	C11—H11A	0.9800
C6—N1	1.4145 (17)	C11—H11B	0.9800
C7—O1	1.2289 (17)	C11—H11C	0.9800
C7—N1	1.3471 (17)	N1—H1	0.884 (17)
C7—C8	1.5083 (19)		

C2—C1—C6	119.62 (12)	H8A—C8—H8C	109.5
C2—C1—H1A	120.2	H8B—C8—H8C	109.5
C6—C1—H1A	120.2	O2—C9—C10	107.12 (11)
C1—C2—C3	121.44 (12)	O2—C9—H9A	110.3
C1—C2—H2	119.3	C10—C9—H9A	110.3
C3—C2—H2	119.3	O2—C9—H9B	110.3
O2—C3—C2	115.80 (11)	C10—C9—H9B	110.3
O2—C3—C4	125.09 (12)	H9A—C9—H9B	108.5
C2—C3—C4	119.10 (12)	C9—C10—C11	111.72 (12)
C5—C4—C3	119.46 (11)	C9—C10—H10A	109.3
C5—C4—H4	120.3	C11—C10—H10A	109.3
C3—C4—H4	120.3	C9—C10—H10B	109.3
C4—C5—C6	121.58 (11)	C11—C10—H10B	109.3
C4—C5—H5	119.2	H10A—C10—H10B	107.9
C6—C5—H5	119.2	C10—C11—H11A	109.5
C5—C6—C1	118.80 (12)	C10—C11—H11B	109.5
C5—C6—N1	117.21 (11)	H11A—C11—H11B	109.5
C1—C6—N1	123.98 (11)	C10—C11—H11C	109.5
O1—C7—N1	123.50 (12)	H11A—C11—H11C	109.5
O1—C7—C8	121.12 (12)	H11B—C11—H11C	109.5
N1—C7—C8	115.38 (12)	C7—N1—C6	128.33 (11)
C7—C8—H8A	109.5	C7—N1—H1	116.3 (10)
C7—C8—H8B	109.5	C6—N1—H1	115.3 (10)
H8A—C8—H8B	109.5	C3—O2—C9	117.79 (10)
C7—C8—H8C	109.5		

C6—C1—C2—C3	0.3 (2)	C2—C1—C6—N1	−179.72 (11)
C1—C2—C3—O2	178.89 (11)	O2—C9—C10—C11	−179.87 (12)
C1—C2—C3—C4	−0.1 (2)	O1—C7—N1—C6	2.0 (2)
O2—C3—C4—C5	−178.96 (12)	C8—C7—N1—C6	−177.89 (12)
C2—C3—C4—C5	−0.1 (2)	C5—C6—N1—C7	168.77 (12)
C3—C4—C5—C6	0.1 (2)	C1—C6—N1—C7	−11.8 (2)
C4—C5—C6—C1	0.17 (19)	C2—C3—O2—C9	−179.29 (11)
C4—C5—C6—N1	179.59 (11)	C4—C3—O2—C9	−0.40 (18)
C2—C1—C6—C5	−0.34 (19)	C10—C9—O2—C3	178.51 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.884 (17)	1.949 (17)	2.7988 (15)	160.8 (14)

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*.

Fig. 1

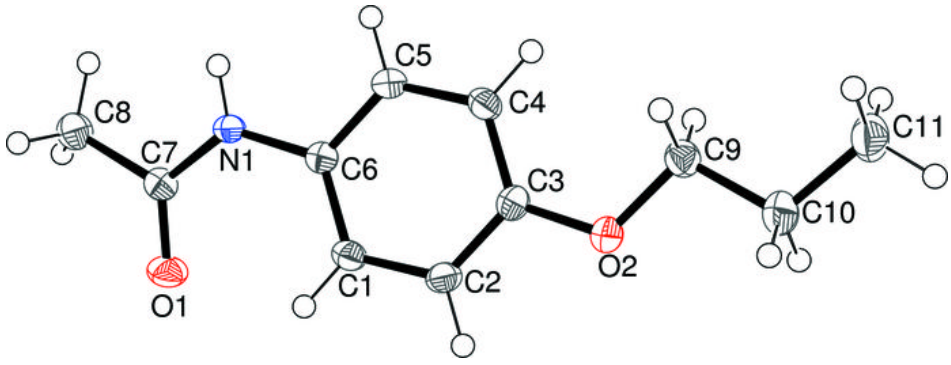

Fig. 2

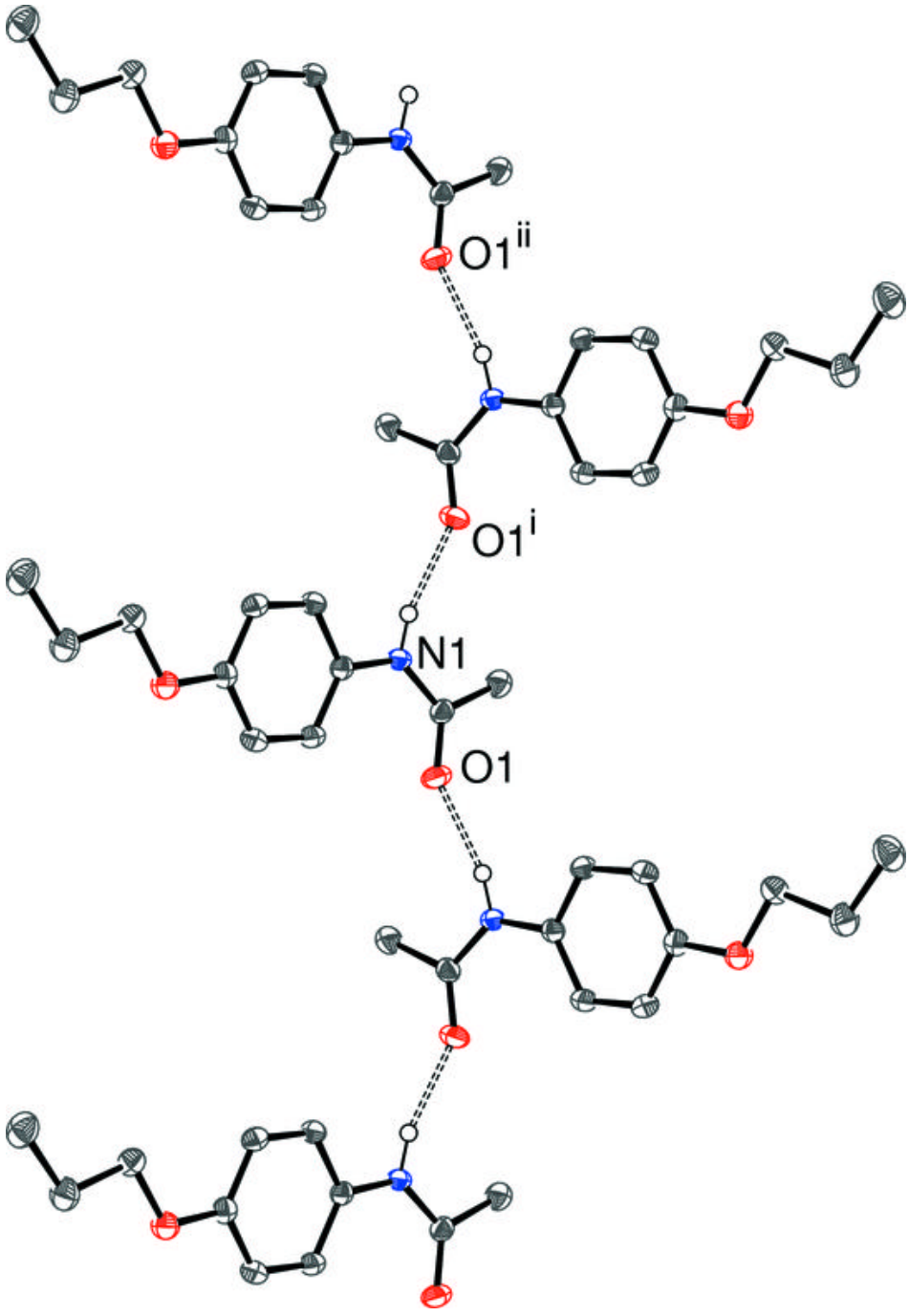

Fig. 3