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N-(4-Nitrophenyl)propionamide

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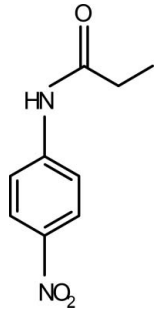
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.147; data-to-parameter ratio = 12.9.

In the title compound, $C_9H_{10}N_2O_3$, the mean planes of the propionamide fragment and the benzene ring make a dihedral angle of 12.86 (2)°. The crystal packing exhibits intermolecular N—H···O hydrogen bonds, which link the molecules into linear chains extended along the *a* axis, and weak C—H···O interactions.

Related literature

For crystal structures of related amides, see: Guo (2004); Gowda *et al.* (2007). For normal ranges of molecular bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_9H_{10}N_2O_3$
M_r = 194.19
Orthorhombic, *Pbca*
a = 9.763 (3) Å
b = 9.278 (3) Å
c = 20.586 (5) Å
V = 1864.7 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
0.20 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.991
8729 measured reflections
1641 independent reflections
1017 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.147
S = 1.04
1641 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.87	2.12	2.960 (3)	163
C5—H5···O2^{ii}	0.93	2.57	3.403 (4)	149

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2289).

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supplementary materials

Acta Cryst. (2007). E**63**, o3903 [**doi:10.1107/S1600536807041372**]

N-(4-Nitrophenyl)propionamide

H.-Y. Zhang, M.-L. Guo, C.-H. Guo and Y.-N. Ye

Comment

The structural studies of amides are of interest (Gowda *et al.*, 2007). As a part of our study of new possible drugs (Guo, 2004), the crystal structure of the title compound (I) is reported herein.

The atom-numbering scheme of the title compound, (I), is illustrated in Fig. 1. The bond distances and angles are normal, within experimental error (Allen *et al.*, 1987).

The intermolecular N1—H1A···O1^{i} hydrogen bond (Table 1) link the molecules into chains (Fig. 2) in the a direction. Further, C5—H5···O2^{ii} controls the packing in the structure.

Experimental

The title compound was prepared by the following procedure. The mixture of concentrated sulfuric acid (1.9 ml) and nitric acid (1.4 ml) was added dropwise into a solution of concentrated sulfuric acid (8 ml) and *N*-phenylpropionamid (3.5 g) with stirring at 0° C temperature. After the acid was added out, intermittently shake the mixture system for 30 min at the room temperature. The mixture was dispersed in ice water (50 ml), after which 4.3 g of the yellow powder product was separated by filtration. The product (0.3 g) was heated and dissolved in ethanol (15 ml). Single crystals were obtained by slow concentration over a period of 3 d at room temperature.

Refinement

The H atom of the NH group was found in a difference Fourier map, but placed in idealized position with N—H = 0.86 Å, and its U_{iso} value was set at 1.2U_{eq}(N). The C-bound H atoms were included in the refinement in the riding model approximation, with C–H = 0.93–0.97 Å and U_{iso} (H) = 1.2 U_{eq} (C) or 1.5U_{eq}(C_{methyl}).

Figures

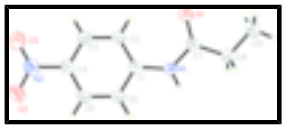

Fig. 1. A view of the structure of (I), showing the atom-numbering scheme. Displacement ellipsoids drawn at the 30% probability level.

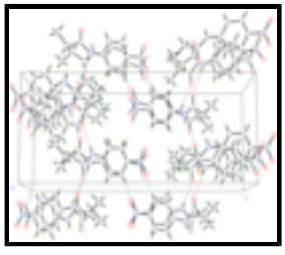

Fig. 2. Packing diagram showing hydrogen bonds interactions drawn as dashed lines, viewed down the *b* axis.

N-(4-Nitrophenyl)propionamide

Crystal data

$C_9H_{10}N_2O_3$	F_{000} = 816
M_r = 194.19	D_x = 1.383 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2057 reflections
a = 9.763 (3) Å	θ = 2.9–24.5º
b = 9.278 (3) Å	μ = 0.11 mm^{-1}
c = 20.586 (5) Å	*T* = 294 (2) K
V = 1864.7 (9) Å^3	Prism, yellow
Z = 8	0.20 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1641 independent reflections
Radiation source: fine-focus sealed tube	1017 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.081
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −11→11
T_{min} = 0.982, T_{max} = 0.991	*k* = −10→11
8729 measured reflections	*l* = −17→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.147	$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.9116P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
1641 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
127 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}
N1	0.18357 (19)	0.9563 (2)	0.29421 (10)	0.0490 (6)
H1A	0.1012	0.9815	0.2834	0.059*
N2	0.2399 (3)	0.5853 (3)	0.50795 (12)	0.0682 (7)
O1	0.39868 (18)	0.9788 (2)	0.25400 (9)	0.0669 (6)
O2	0.1359 (2)	0.5464 (3)	0.53559 (11)	0.0961 (9)
O3	0.3528 (3)	0.5507 (3)	0.52575 (13)	0.1157 (11)
C1	0.2042 (2)	0.8624 (3)	0.34674 (12)	0.0454 (6)
C2	0.3325 (3)	0.8307 (3)	0.37243 (13)	0.0571 (8)
H2	0.4107	0.8714	0.3544	0.069*
C3	0.3431 (3)	0.7388 (3)	0.42472 (13)	0.0610 (8)
H3	0.4286	0.7164	0.4418	0.073*
C4	0.2270 (3)	0.6805 (3)	0.45151 (12)	0.0517 (7)
C5	0.0993 (3)	0.7117 (3)	0.42755 (14)	0.0628 (8)
H5	0.0213	0.6728	0.4467	0.075*
C6	0.0888 (3)	0.8013 (3)	0.37478 (13)	0.0571 (8)
H6	0.0028	0.8214	0.3575	0.069*
C7	0.2767 (2)	1.0102 (3)	0.25161 (13)	0.0482 (7)
C8	0.2166 (3)	1.1091 (3)	0.20158 (13)	0.0621 (8)
H8A	0.1601	1.1802	0.2234	0.074*
H8B	0.1576	1.0534	0.1732	0.074*
C9	0.3215 (4)	1.1863 (4)	0.16084 (15)	0.0781 (10)
H9A	0.3810	1.2412	0.1885	0.117*
H9B	0.2760	1.2498	0.1310	0.117*
H9C	0.3745	1.1170	0.1370	0.117*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0357 (11)	0.0592 (14)	0.0521 (13)	0.0042 (10)	0.0024 (10)	0.0042 (11)
N2	0.0761 (18)	0.0759 (18)	0.0526 (15)	−0.0125 (15)	−0.0074 (15)	0.0018 (13)
O1	0.0400 (11)	0.0934 (16)	0.0671 (12)	0.0023 (10)	0.0083 (9)	0.0103 (11)
O2	0.0899 (17)	0.125 (2)	0.0737 (16)	−0.0340 (16)	−0.0031 (13)	0.0328 (14)
O3	0.0864 (18)	0.156 (3)	0.105 (2)	0.0068 (18)	−0.0091 (15)	0.0637 (19)
C1	0.0402 (14)	0.0492 (15)	0.0470 (14)	−0.0025 (12)	0.0020 (11)	−0.0107 (12)
C2	0.0388 (15)	0.077 (2)	0.0559 (16)	−0.0029 (14)	0.0029 (12)	0.0080 (15)
C3	0.0468 (16)	0.082 (2)	0.0541 (17)	0.0034 (15)	−0.0014 (13)	−0.0003 (16)
C4	0.0583 (17)	0.0542 (17)	0.0426 (14)	−0.0076 (14)	−0.0006 (12)	−0.0047 (13)

C5	0.0494 (16)	0.079 (2)	0.0599 (18)	−0.0151 (15)	0.0022 (14)	0.0044 (16)
C6	0.0384 (14)	0.075 (2)	0.0584 (17)	−0.0057 (13)	0.0009 (13)	0.0062 (15)
C7	0.0415 (15)	0.0529 (16)	0.0504 (14)	−0.0009 (12)	0.0038 (12)	−0.0063 (13)
C8	0.0606 (18)	0.0648 (19)	0.0608 (17)	−0.0031 (15)	0.0014 (14)	0.0095 (15)
C9	0.093 (2)	0.073 (2)	0.068 (2)	−0.0058 (19)	0.0159 (18)	0.0125 (17)

Geometric parameters (Å, °)

N1—C7	1.359 (3)	C3—H3	0.9300
N1—C1	1.403 (3)	C4—C5	1.372 (4)
N1—H1A	0.8670	C5—C6	1.372 (4)
N2—O3	1.206 (3)	C5—H5	0.9300
N2—O2	1.218 (3)	C6—H6	0.9300
N2—C4	1.465 (4)	C7—C8	1.499 (4)
O1—C7	1.227 (3)	C8—C9	1.505 (4)
C1—C6	1.387 (3)	C8—H8A	0.9700
C1—C2	1.391 (3)	C8—H8B	0.9700
C2—C3	1.377 (4)	C9—H9A	0.9600
C2—H2	0.9300	C9—H9B	0.9600
C3—C4	1.371 (4)	C9—H9C	0.9600
C7—N1—C1	129.1 (2)	C6—C5—H5	120.6
C7—N1—H1A	110.8	C5—C6—C1	121.1 (3)
C1—N1—H1A	119.9	C5—C6—H6	119.5
O3—N2—O2	122.8 (3)	C1—C6—H6	119.5
O3—N2—C4	118.7 (3)	O1—C7—N1	122.4 (2)
O2—N2—C4	118.5 (3)	O1—C7—C8	123.6 (2)
C6—C1—C2	119.1 (2)	N1—C7—C8	114.0 (2)
C6—C1—N1	117.3 (2)	C7—C8—C9	114.0 (2)
C2—C1—N1	123.6 (2)	C7—C8—H8A	108.7
C3—C2—C1	119.7 (3)	C9—C8—H8A	108.7
C3—C2—H2	120.1	C7—C8—H8B	108.7
C1—C2—H2	120.1	C9—C8—H8B	108.7
C4—C3—C2	119.8 (3)	H8A—C8—H8B	107.6
C4—C3—H3	120.1	C8—C9—H9A	109.5
C2—C3—H3	120.1	C8—C9—H9B	109.5
C3—C4—C5	121.5 (3)	H9A—C9—H9B	109.5
C3—C4—N2	119.1 (3)	C8—C9—H9C	109.5
C5—C4—N2	119.3 (2)	H9A—C9—H9C	109.5
C4—C5—C6	118.7 (3)	H9B—C9—H9C	109.5
C4—C5—H5	120.6		
C7—N1—C1—C6	−167.6 (2)	O2—N2—C4—C5	−6.3 (4)
C7—N1—C1—C2	13.8 (4)	C3—C4—C5—C6	1.2 (4)
C6—C1—C2—C3	0.5 (4)	N2—C4—C5—C6	179.8 (3)
N1—C1—C2—C3	179.0 (2)	C4—C5—C6—C1	−1.4 (4)
C1—C2—C3—C4	−0.7 (4)	C2—C1—C6—C5	0.6 (4)
C2—C3—C4—C5	−0.2 (4)	N1—C1—C6—C5	−178.1 (2)
C2—C3—C4—N2	−178.8 (3)	C1—N1—C7—O1	1.1 (4)
O3—N2—C4—C3	−6.5 (4)	C1—N1—C7—C8	−179.6 (2)
O2—N2—C4—C3	172.3 (3)	O1—C7—C8—C9	−9.5 (4)

O3—N2—C4—C5	174.9 (3)	N1—C7—C8—C9	171.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.87	2.12	2.960 (3)	163
C5—H5···O2^{ii}	0.93	2.57	3.403 (4)	149

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

Fig. 1

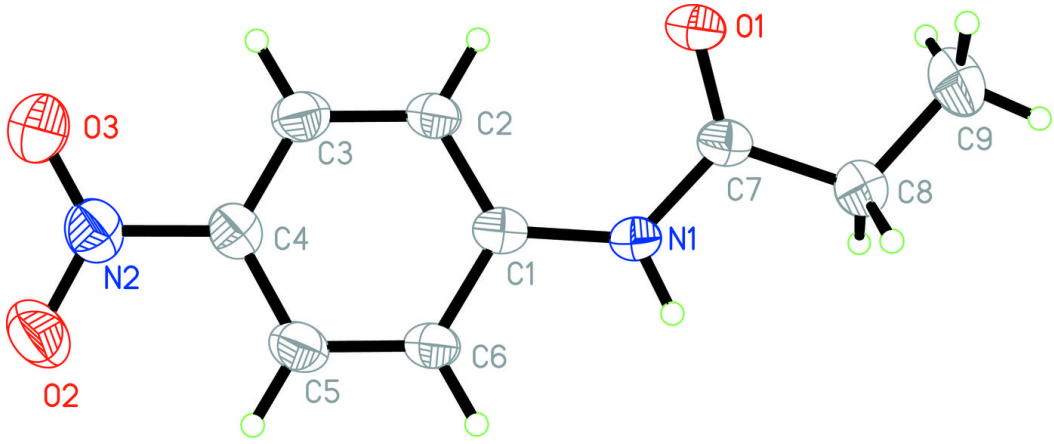

Fig. 2