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Methyl *N*-(4-nitrophenyl)carbamate

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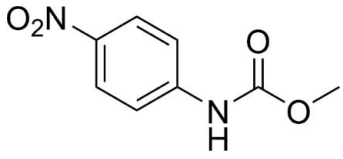
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.074; wR factor = 0.162; data-to-parameter ratio = 12.8.

In the title molecule, $C_8H_8N_2O_4$, the nitro and methoxycarbonyl groups are twisted from the plane of aromatic ring by 5.1 (1) and 6.2 (1)°, respectively. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules related by translation along the *b* axis into chains. Weak intermolecular C—H···O interactions link further these chains into sheets parallel to the *bc* plane.

Related literature

For the preparation of the title compound, see: Wilshire (1990). For a related structure, see: Yakimanski *et al.* (1997).



Experimental

Crystal data

$C_8H_8N_2O_4$
M_r = 196.16
Triclinic, $P\overline{1}$
a = 7.4269 (11) Å
b = 8.1003 (12) Å
c = 8.5376 (12) Å
α = 101.634 (2)°
β = 97.914 (2)°
γ = 116.660 (2)°
V = 434.04 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 K
0.40 × 0.30 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
4507 measured reflections
1686 independent reflections
1539 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.162
S = 1.26
1686 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2^{i}	0.93	2.57	3.471 (3)	163
C1—H1B···O4^{ii}	0.96	2.53	3.324 (4)	140
N1—H1···O3^{iii}	0.82 (3)	2.20 (4)	3.016 (3)	170 (3)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5074).

References

Bruker (1997). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wilshire, J. F. K. (1990). *Aust. J. Chem.* **43**, 1817–1826.
Yakimanski, A. V., Kolb, U., Matveeva, G. N., Voigt-Martin, I. G. & Tenkovtsev, A. V. (1997). *Acta Cryst.* A**53**, 603–614.

supporting information

Acta Cryst. (2011). E**67**, o1494 [doi:10.1107/S1600536811018757]

Methyl *N*-(4-nitrophenyl)carbamate

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S1. Comment

4-Nitrophenylhexyl derivatives are studied in the crystal engineering and design of nonlinear optical (NLO) materials (Yakimanski et al., 1997). Herewith we report the crystal structure of the title compound (I).

In (I) (Fig. 1), all bond lengths and angles are normal and comparable with those observed in 4-nitrophenyl-hexyl-urethane (Yakimanski et al., 1997). The nitro and methoxycarbonyl groups are twisted from the plane of aromatic ring at 5.1 (1) and 6.2 (1)°, respectively. In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules related by translation along axis b<*i*> into chains. Weak intermolecular C—H···O interactions (Table 1) link further these chains into sheets parallel to bc<*i*> plane.

S2. Experimental

The title compound was synthesized according to Wilshire (1990). Crystals of (I) suitable for X-ray diffraction were grown by slow evaporation of a chloroform-methanol (2:1) solution of the title compound under 293 K.

S3. Refinement

C-bound H atoms were positioned in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C). Atom H1 was located on difference map and isotropically refined.

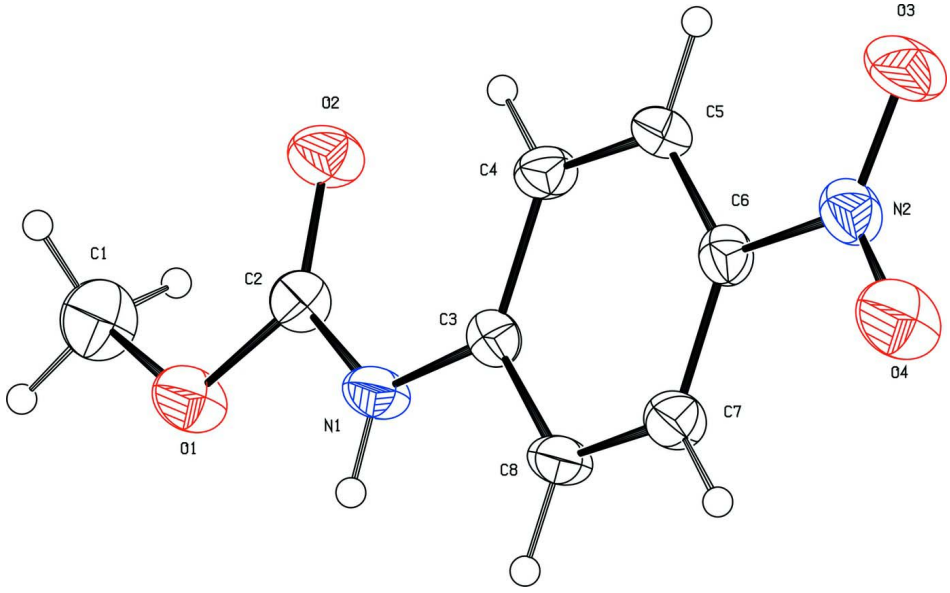

Figure 1

A view of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

Methyl *N*-(4-nitrophenyl)carbamate

Crystal data

$C_8H_8N_2O_4$
$M_r = 196.16$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.4269$ (11) Å
$b = 8.1003$ (12) Å
$c = 8.5376$ (12) Å
$\alpha = 101.634$ (2)°
$\beta = 97.914$ (2)°
$\gamma = 116.660$ (2)°
$V = 434.04$ (11) Å^3
$Z = 2$
$F(000) = 204$
$D_x = 1.501$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2193 reflections
$\theta = 2.5$–28.2°
$\mu = 0.12$ mm^{-1}
$T = 298$ K
Block, yellow
0.40 × 0.30 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4507 measured reflections
1686 independent reflections
1539 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.5°$
$h = -9\rightarrow9$
$k = -9\rightarrow9$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.162$
$S = 1.26$
1686 reflections
132 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.2842P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2798 (6)	0.1171 (5)	0.4095 (4)	0.0645 (10)
H1A	0.4024	0.2283	0.4846	0.097*
H1B	0.2871	0.0023	0.4122	0.097*
H1C	0.1582	0.1095	0.4419	0.097*
C2	0.2591 (4)	0.2904 (4)	0.2229 (3)	0.0400 (6)
C3	0.2433 (4)	0.4234 (4)	−0.0116 (3)	0.0351 (6)
C4	0.2670 (4)	0.5997 (4)	0.0750 (3)	0.0391 (6)
H4	0.2853	0.6318	0.1891	0.047*
C5	0.2633 (4)	0.7260 (4)	−0.0091 (3)	0.0399 (6)
H5	0.2796	0.8445	0.0481	0.048*
C6	0.2355 (4)	0.6774 (4)	−0.1782 (3)	0.0377 (6)
C7	0.2141 (5)	0.5042 (4)	−0.2666 (3)	0.0427 (7)
H7	0.1979	0.4739	−0.3804	0.051*
C8	0.2173 (4)	0.3786 (4)	−0.1826 (3)	0.0415 (7)
H8	0.2018	0.2607	−0.2405	0.050*
N2	0.2288 (4)	0.8111 (4)	−0.2670 (3)	0.0479 (6)
N1	0.2450 (4)	0.2846 (4)	0.0624 (3)	0.0436 (6)
O1	0.2673 (4)	0.1340 (3)	0.2437 (2)	0.0538 (6)
O2	0.2635 (4)	0.4136 (3)	0.3310 (2)	0.0545 (6)
O3	0.2327 (4)	0.9584 (3)	−0.1911 (3)	0.0695 (7)
O4	0.2176 (4)	0.7718 (4)	−0.4139 (3)	0.0733 (8)
H1	0.235 (5)	0.187 (5)	0.001 (4)	0.059 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.089 (3)	0.073 (2)	0.0476 (18)	0.045 (2)	0.0229 (17)	0.0351 (17)
C2	0.0426 (16)	0.0416 (16)	0.0391 (14)	0.0211 (13)	0.0138 (12)	0.0152 (13)
C3	0.0356 (14)	0.0342 (14)	0.0388 (14)	0.0188 (12)	0.0108 (11)	0.0128 (11)
C4	0.0481 (16)	0.0400 (15)	0.0286 (12)	0.0224 (13)	0.0106 (11)	0.0064 (11)
C5	0.0458 (16)	0.0310 (14)	0.0441 (15)	0.0224 (13)	0.0101 (12)	0.0061 (11)

C6	0.0362 (14)	0.0361 (15)	0.0429 (14)	0.0185 (12)	0.0089 (11)	0.0150 (12)
C7	0.0567 (18)	0.0455 (17)	0.0338 (14)	0.0307 (15)	0.0129 (12)	0.0129 (12)
C8	0.0562 (18)	0.0350 (15)	0.0365 (14)	0.0271 (14)	0.0122 (12)	0.0051 (11)
N2	0.0539 (15)	0.0430 (15)	0.0545 (15)	0.0282 (13)	0.0137 (12)	0.0194 (12)
N1	0.0675 (17)	0.0398 (14)	0.0324 (12)	0.0334 (13)	0.0155 (11)	0.0101 (10)
O1	0.0864 (16)	0.0512 (13)	0.0429 (11)	0.0426 (12)	0.0242 (11)	0.0254 (10)
O2	0.0838 (16)	0.0558 (13)	0.0366 (11)	0.0421 (12)	0.0224 (10)	0.0157 (10)
O3	0.106 (2)	0.0434 (13)	0.0709 (16)	0.0476 (14)	0.0179 (14)	0.0174 (11)
O4	0.120 (2)	0.0758 (17)	0.0552 (15)	0.0635 (17)	0.0334 (14)	0.0378 (13)

Geometric parameters (Å, º)

C1—O1	1.444 (3)	C4—H4	0.9300
C1—H1A	0.9600	C5—C6	1.378 (4)
C1—H1B	0.9600	C5—H5	0.9300
C1—H1C	0.9600	C6—C7	1.379 (4)
C2—O2	1.200 (3)	C6—N2	1.456 (3)
C2—O1	1.340 (3)	C7—C8	1.364 (4)
C2—N1	1.350 (3)	C7—H7	0.9300
C3—C4	1.390 (4)	C8—H8	0.9300
C3—C8	1.394 (4)	N2—O4	1.211 (3)
C3—N1	1.400 (3)	N2—O3	1.223 (3)
C4—C5	1.370 (4)	N1—H1	0.82 (3)
O1—C1—H1A	109.5	C6—C5—H5	120.0
O1—C1—H1B	109.5	C5—C6—C7	121.6 (2)
H1A—C1—H1B	109.5	C5—C6—N2	119.7 (2)
O1—C1—H1C	109.5	C7—C6—N2	118.7 (2)
H1A—C1—H1C	109.5	C8—C7—C6	118.3 (2)
H1B—C1—H1C	109.5	C8—C7—H7	120.9
O2—C2—O1	124.7 (3)	C6—C7—H7	120.9
O2—C2—N1	126.5 (3)	C7—C8—C3	121.3 (2)
O1—C2—N1	108.8 (2)	C7—C8—H8	119.3
C4—C3—C8	119.3 (2)	C3—C8—H8	119.3
C4—C3—N1	124.0 (2)	O4—N2—O3	122.3 (3)
C8—C3—N1	116.7 (2)	O4—N2—C6	118.9 (2)
C5—C4—C3	119.5 (2)	O3—N2—C6	118.9 (2)
C5—C4—H4	120.3	C2—N1—C3	127.9 (2)
C3—C4—H4	120.3	C2—N1—H1	116 (2)
C4—C5—C6	120.0 (2)	C3—N1—H1	116 (2)
C4—C5—H5	120.0	C2—O1—C1	115.7 (2)
C8—C3—C4—C5	0.4 (4)	C5—C6—N2—O4	175.4 (3)
N1—C3—C4—C5	179.9 (3)	C7—C6—N2—O4	−4.5 (4)
C3—C4—C5—C6	0.2 (4)	C5—C6—N2—O3	−5.3 (4)
C4—C5—C6—C7	−1.0 (4)	C7—C6—N2—O3	174.8 (3)
C4—C5—C6—N2	179.2 (2)	O2—C2—N1—C3	3.5 (5)
C5—C6—C7—C8	1.2 (4)	O1—C2—N1—C3	−176.5 (3)

N2—C6—C7—C8	−179.0 (2)	C4—C3—N1—C2	3.4 (5)
C6—C7—C8—C3	−0.6 (4)	C8—C3—N1—C2	−177.0 (3)
C4—C3—C8—C7	−0.2 (4)	O2—C2—O1—C1	0.8 (4)
N1—C3—C8—C7	−179.8 (3)	N1—C2—O1—C1	−179.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O2^{i}	0.93	2.57	3.471 (3)	163
C4—H4···O2	0.93	2.30	2.892 (3)	121
C1—H1*B*···O4^{ii}	0.96	2.53	3.324 (4)	140
N1—H1···O3^{iii}	0.82 (3)	2.20 (4)	3.016 (3)	170 (3)

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