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N′-(2-Nitrobenzoyl)benzohydrazide

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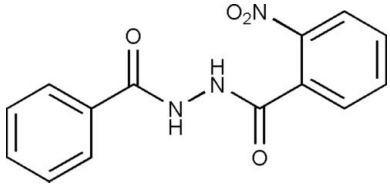
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.124; data-to-parameter ratio = 16.6.

In the title compound, $C_{14}H_{11}N_3O_4$, the dihedral angle between the two benzene rings is 8.1 (2)°. The molecules are linked into chains through N—H···O hydrogen bonds.

Related literature

This structure report is an extension of our work on the characterization of hydrazide derivatives (Qiu, Fang *et al.*, 2006; Qiu, Luo *et al.*, 2006).



Experimental

Crystal data

$C_{14}H_{11}N_3O_4$
M_r = 285.26
Monoclinic, $P2_1/n$
a = 8.2363 (16) Å
b = 12.834 (3) Å
c = 12.955 (3) Å
β = 92.78 (3)°
V = 1367.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.16 × 0.08 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.988, T_{max} = 0.991
10170 measured reflections
3313 independent reflections
1747 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.124
S = 0.95
3313 reflections
199 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H8···O1^{i}	0.90 (2)	1.99 (2)	2.8825 (18)	178.0 (15)
N1—H7···O2^{ii}	0.91 (2)	1.93 (2)	2.8216 (19)	165.8 (17)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: BI2195).

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supplementary materials

Acta Cryst. (2007). E**63**, o3208 [**doi:10.1107/S1600536807028024**]

N'-(2-Nitrobenzoyl)benzohydrazide

S.-L. Yang and Z.-G. Luo

Comment

This structure report is an extension of our work on the characterization of hydrazide derivatives (Qiu, Fang *et al.*, 2006; Qiu, Luo *et al.*, 2006).

In the title compound (Fig. 1), the dihedral angle between the two benzene rings is 8.1 (2) °. The molecules are linked through intermolecular N—H···O hydrogen bonds into chains running along the *a*-axis (Fig. 2).

Experimental

The title compound was synthesized by reaction of equivalent amounts of benzohydrazide (0.14 g, 1 mmol) and 2-nitrobenzoyl chloride (0.19 g, 1 mmol) in ethyl acetate (25 ml) for 3 h at 373–393 K. Single crystals for X-ray diffraction analysis were obtained by evaporation of an ethyl acetate solution.

Refinement

Atoms H7 and H8 were located in a difference Fourier map and refined isotropically without restraint. The refined N—H distances are 0.91 (2) and 0.90 (2) Å. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

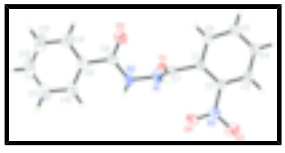

Fig. 1. The molecular structure of the title compound showing displacement ellipsoids at 30% probability for non-H atoms.

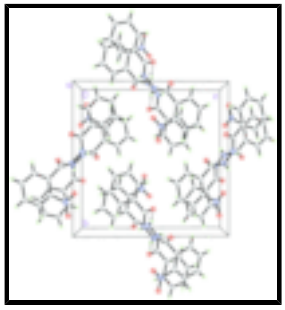

Fig. 2. View along the direction of propagation of the hydrogen-bonded chains (the *a*-axis).

N'-(2-Nitrobenzoyl)benzohydrazide

Crystal data

$C_{14}H_{11}N_3O_4$

$M_r = 285.26$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.2363\ (16)$ Å

$b = 12.834\ (3)$ Å

$c = 12.955\ (3)$ Å

$\beta = 92.78\ (3)^o$

$V = 1367.8\ (5)$ Å^3

$Z = 4$

$F_{000} = 592$

$D_x = 1.385$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 2796 reflections

$\theta = 4.2–25^o$

$\mu = 0.10$ mm^{-1}

$T = 298\ (2)$ K

Block, colourless

0.16 × 0.08 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.988$, $T_{max} = 0.991$

10170 measured reflections

3313 independent reflections

1747 reflections with $I > 2\sigma(I)$

$R_{int} = 0.032$

$\theta_{max} = 28.3^o$

$\theta_{min} = 2.2^o$

$h = -10\rightarrow10$

$k = -17\rightarrow17$

$l = -17\rightarrow17$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.124$

$S = 0.95$

3313 reflections

199 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

$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0064 (15)

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}
O1	0.07092 (13)	−0.01088 (8)	0.37340 (8)	0.0562 (3)
C7	0.19938 (19)	−0.05391 (11)	0.39718 (12)	0.0458 (4)
O2	0.43196 (14)	0.15833 (9)	0.48726 (9)	0.0617 (3)
C2	0.28541 (18)	−0.23966 (11)	0.34355 (11)	0.0467 (4)
N2	0.24453 (17)	0.04930 (10)	0.54726 (10)	0.0557 (4)
C8	0.31783 (18)	0.14319 (12)	0.54234 (11)	0.0480 (4)
C1	0.27361 (17)	−0.13295 (11)	0.32778 (11)	0.0441 (4)
N3	0.21728 (19)	−0.28640 (11)	0.43411 (11)	0.0644 (4)
O4	0.13109 (17)	−0.23342 (11)	0.48638 (10)	0.0794 (4)
N1	0.29262 (18)	−0.02943 (11)	0.48098 (11)	0.0567 (4)
C5	0.4118 (2)	−0.15825 (13)	0.16931 (13)	0.0609 (5)
H5	0.4553	−0.1303	0.1105	0.073*
C6	0.3380 (2)	−0.09398 (12)	0.23843 (12)	0.0566 (4)
H6	0.3311	−0.0229	0.2249	0.068*
C3	0.3582 (2)	−0.30420 (12)	0.27425 (13)	0.0548 (4)
H3	0.3643	−0.3755	0.2867	0.066*
C9	0.25532 (18)	0.22508 (12)	0.61152 (12)	0.0516 (4)
C4	0.4212 (2)	−0.26365 (13)	0.18751 (13)	0.0577 (4)
H4	0.4703	−0.3072	0.1408	0.069*
C10	0.1773 (2)	0.20236 (14)	0.70013 (14)	0.0636 (5)
H10	0.1600	0.1333	0.7185	0.076*
O3	0.2459 (3)	−0.37735 (12)	0.45241 (13)	0.1253 (7)
C14	0.2827 (2)	0.32818 (14)	0.58496 (16)	0.0727 (5)
H14	0.3383	0.3442	0.5262	0.087*
C11	0.1241 (2)	0.2825 (2)	0.76252 (16)	0.0848 (7)
H11	0.0716	0.2673	0.8226	0.102*
C12	0.1499 (3)	0.3842 (2)	0.7347 (2)	0.1023 (9)
H12	0.1147	0.4380	0.7762	0.123*
C13	0.2263 (3)	0.40685 (16)	0.6470 (2)	0.0994 (8)
H13	0.2409	0.4761	0.6283	0.119*
H8	0.146 (2)	0.0389 (12)	0.5726 (12)	0.060 (5)*
H7	0.382 (2)	−0.0660 (15)	0.5020 (14)	0.078 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0534 (7)	0.0529 (7)	0.0630 (7)	0.0075 (5)	0.0112 (6)	0.0014 (5)
C7	0.0465 (9)	0.0409 (8)	0.0512 (9)	−0.0023 (7)	0.0150 (8)	−0.0010 (7)
O2	0.0573 (7)	0.0653 (8)	0.0640 (7)	0.0040 (5)	0.0176 (6)	−0.0002 (6)
C2	0.0517 (9)	0.0440 (8)	0.0453 (8)	−0.0049 (7)	0.0115 (7)	−0.0024 (7)
N2	0.0523 (8)	0.0541 (8)	0.0623 (9)	0.0022 (7)	0.0200 (7)	−0.0199 (6)
C8	0.0463 (9)	0.0522 (10)	0.0456 (9)	0.0055 (7)	0.0034 (8)	−0.0038 (7)
C1	0.0447 (9)	0.0427 (8)	0.0456 (8)	−0.0022 (6)	0.0100 (7)	−0.0042 (6)
N3	0.0843 (11)	0.0494 (9)	0.0616 (9)	−0.0037 (7)	0.0239 (8)	0.0058 (7)
O4	0.0975 (10)	0.0758 (9)	0.0687 (8)	−0.0047 (7)	0.0438 (8)	0.0031 (6)
N1	0.0536 (9)	0.0549 (8)	0.0621 (9)	0.0107 (7)	0.0090 (8)	−0.0197 (7)
C5	0.0698 (12)	0.0679 (11)	0.0465 (9)	−0.0038 (9)	0.0190 (9)	−0.0021 (8)
C6	0.0681 (11)	0.0478 (9)	0.0554 (10)	−0.0008 (7)	0.0188 (9)	0.0010 (7)
C3	0.0613 (11)	0.0427 (8)	0.0610 (10)	−0.0036 (7)	0.0087 (9)	−0.0114 (7)
C9	0.0488 (10)	0.0524 (10)	0.0529 (10)	0.0066 (7)	−0.0046 (8)	−0.0112 (7)
C4	0.0624 (11)	0.0601 (10)	0.0519 (10)	−0.0005 (8)	0.0151 (8)	−0.0169 (8)
C10	0.0613 (11)	0.0712 (11)	0.0587 (11)	0.0040 (9)	0.0060 (9)	−0.0213 (9)
O3	0.1998 (19)	0.0605 (9)	0.1222 (13)	0.0202 (10)	0.0747 (13)	0.0333 (9)
C14	0.0831 (14)	0.0571 (11)	0.0767 (13)	0.0068 (9)	−0.0091 (11)	−0.0064 (9)
C11	0.0757 (14)	0.1096 (19)	0.0690 (13)	0.0188 (12)	0.0030 (11)	−0.0430 (12)
C12	0.1058 (19)	0.0932 (19)	0.105 (2)	0.0409 (14)	−0.0203 (16)	−0.0565 (16)
C13	0.123 (2)	0.0572 (12)	0.114 (2)	0.0236 (13)	−0.0272 (17)	−0.0266 (13)

Geometric parameters (Å, °)

O1—C7	1.2197 (18)	C5—H5	0.930
C7—N1	1.336 (2)	C6—H6	0.930
C7—C1	1.5050 (19)	C3—C4	1.364 (2)
O2—C8	1.2230 (18)	C3—H3	0.930
C2—C3	1.380 (2)	C9—C10	1.374 (2)
C2—C1	1.387 (2)	C9—C14	1.388 (2)
C2—N3	1.454 (2)	C4—H4	0.930
N2—C8	1.351 (2)	C10—C11	1.392 (2)
N2—N1	1.3958 (17)	C10—H10	0.930
N2—H8	0.90 (2)	C14—C13	1.385 (3)
C8—C9	1.489 (2)	C14—H14	0.930
C1—C6	1.389 (2)	C11—C12	1.374 (4)
N3—O3	1.2119 (19)	C11—H11	0.930
N3—O4	1.2131 (18)	C12—C13	1.356 (4)
N1—H7	0.91 (2)	C12—H12	0.930
C5—C4	1.375 (2)	C13—H13	0.930
C5—C6	1.380 (2)		
O1—C7—N1	123.78 (14)	C1—C6—H6	119.2
O1—C7—C1	121.80 (15)	C4—C3—C2	120.12 (15)
N1—C7—C1	114.19 (13)	C4—C3—H3	119.9

C3—C2—C1	121.76 (14)	C2—C3—H3	119.9
C3—C2—N3	118.30 (14)	C10—C9—C14	119.84 (15)
C1—C2—N3	119.93 (13)	C10—C9—C8	122.86 (15)
C8—N2—N1	118.42 (13)	C14—C9—C8	117.27 (15)
C8—N2—H8	124.3 (10)	C3—C4—C5	119.76 (14)
N1—N2—H8	113.9 (11)	C3—C4—H4	120.1
O2—C8—N2	121.83 (14)	C5—C4—H4	120.1
O2—C8—C9	122.48 (15)	C9—C10—C11	120.12 (19)
N2—C8—C9	115.64 (13)	C9—C10—H10	119.9
C2—C1—C6	116.82 (13)	C11—C10—H10	119.9
C2—C1—C7	127.23 (13)	C13—C14—C9	119.2 (2)
C6—C1—C7	115.95 (13)	C13—C14—H14	120.4
O3—N3—O4	122.98 (15)	C9—C14—H14	120.4
O3—N3—C2	118.43 (15)	C12—C11—C10	119.5 (2)
O4—N3—C2	118.57 (14)	C12—C11—H11	120.2
C7—N1—N2	120.06 (14)	C10—C11—H11	120.2
C7—N1—H7	123.4 (12)	C13—C12—C11	120.48 (19)
N2—N1—H7	116.2 (12)	C13—C12—H12	119.8
C4—C5—C6	119.98 (15)	C11—C12—H12	119.8
C4—C5—H5	120.0	C12—C13—C14	120.8 (2)
C6—C5—H5	120.0	C12—C13—H13	119.6
C5—C6—C1	121.55 (15)	C14—C13—H13	119.6
C5—C6—H6	119.2		
N1—N2—C8—O2	−5.4 (2)	C2—C1—C6—C5	−0.8 (2)
N1—N2—C8—C9	177.18 (13)	C7—C1—C6—C5	178.91 (15)
C3—C2—C1—C6	0.3 (2)	C1—C2—C3—C4	0.1 (3)
N3—C2—C1—C6	−178.52 (15)	N3—C2—C3—C4	178.94 (15)
C3—C2—C1—C7	−179.32 (15)	O2—C8—C9—C10	−153.43 (17)
N3—C2—C1—C7	1.9 (2)	N2—C8—C9—C10	24.0 (2)
O1—C7—C1—C2	−108.89 (18)	O2—C8—C9—C14	24.7 (2)
N1—C7—C1—C2	76.56 (19)	N2—C8—C9—C14	−157.83 (15)
O1—C7—C1—C6	71.49 (19)	C2—C3—C4—C5	−0.1 (3)
N1—C7—C1—C6	−103.06 (16)	C6—C5—C4—C3	−0.4 (3)
C3—C2—N3—O3	9.7 (3)	C14—C9—C10—C11	0.8 (3)
C1—C2—N3—O3	−171.39 (17)	C8—C9—C10—C11	178.90 (15)
C3—C2—N3—O4	−168.42 (15)	C10—C9—C14—C13	−1.9 (3)
C1—C2—N3—O4	10.5 (2)	C8—C9—C14—C13	179.82 (16)
O1—C7—N1—N2	0.1 (2)	C9—C10—C11—C12	0.2 (3)
C1—C7—N1—N2	174.57 (13)	C10—C11—C12—C13	0.1 (3)
C8—N2—N1—C7	−103.18 (17)	C11—C12—C13—C14	−1.3 (4)
C4—C5—C6—C1	0.8 (3)	C9—C14—C13—C12	2.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H8···O1^{i}	0.90 (2)	1.99 (2)	2.8825 (18)	178.0 (15)
N1—H7···O2^{ii}	0.91 (2)	1.93 (2)	2.8216 (19)	165.8 (17)

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

Fig. 1

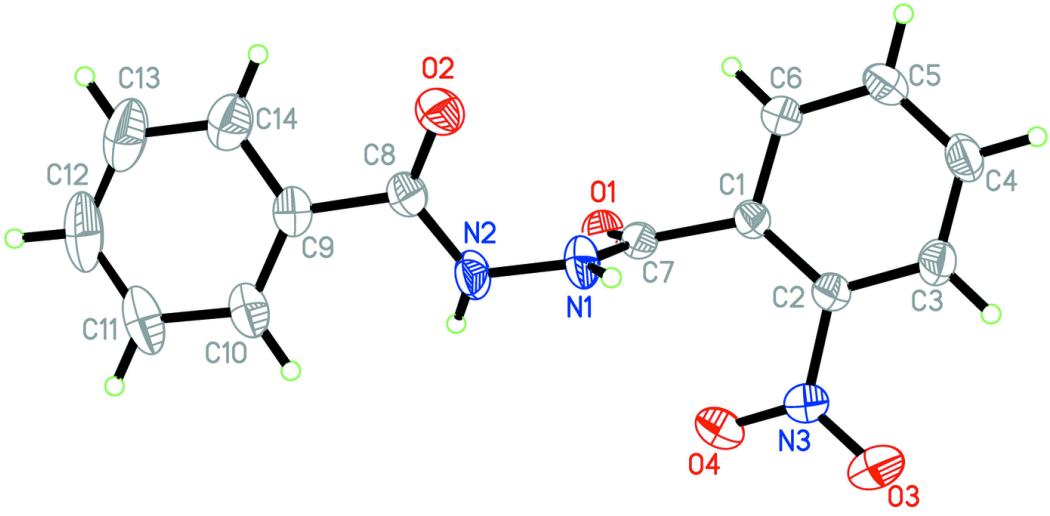

Fig. 2