Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(2-Chlorobenzylidene)-4-nitrobenzohydrazide

Chun-Bao Tang

Department of Chemistry, Jiaying University, Meizhou 514015, People's Republic of China
Correspondence e-mail: chunbao_tang@yahoo.cn

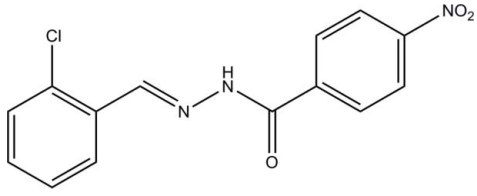
Received 24 December 2011; accepted 25 December 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.146; data-to-parameter ratio = 15.2.

In the title compound, $C_{14}H_{10}ClN_3O_3$, the dihedral angle between the benzene rings is 6.64 (13)°. In the crystal, molecules are linked through N—H···O hydrogen bonds, forming chains running along the c axis direction.

Related literature

For general background to hydrazones, see: Rasras *et al.* (2010); Pyta *et al.* (2010); Angelusiu *et al.* (2010). For related structures, see: Fun *et al.* (2008); Singh & Singh (2010); Ahmad *et al.* (2010); Tang (2010, 2011). For reference bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{10}ClN_3O_3$
M_r = 303.70
Monoclinic, $P2_1/c$
a = 11.2332 (18) Å
b = 13.3778 (18) Å
c = 8.9770 (16) Å
β = 90.408 (2)°
V = 1349.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 298 K
0.18 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.957
10640 measured reflections
2931 independent reflections
1882 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.146
S = 1.03
2931 reflections
193 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.89 (1)	2.06 (1)	2.915 (3)	160 (3)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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*.

Financial support from the Jiaying University research fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2353).

References

Ahmad, T., Zia-ur-Rehman, M., Siddiqui, H. L., Mahmud, S. & Parvez, M. (2010). *Acta Cryst.* E**66**, o976.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Angelusiu, M. V., Barbuceanu, S. F., Draghici, C. & Almajan, G. L. (2010). *Eur. J. Med. Chem.* **45**, 2055–2062.
Bruker (2002). *SMART* and *SAINT* Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K., Sujith, K. V., Patil, P. S., Kalluraya, B. & Chantrapromma, S. (2008). *Acta Cryst.* E**64**, o1961–o1962.
Pyta, K., Przybylski, P., Huczynski, A., Hoser, A., Wozniak, K., Schilf, W., Kamienski, B., Grech, E. & Brzezinski, B. (2010). *J. Mol. Struct.* **970**, 147–154.
Rasras, A. J. M., Al-Tel, T. H., Al-Aboudi, A. F. & Al-Qawasmeh, R. A. (2010). *Eur. J. Med. Chem.* **45**, 2307–2313.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, V. P. & Singh, S. (2010). *Acta Cryst.* E**66**, o1172.
Tang, C.-B. (2010). *Acta Cryst.* E**66**, o2482.
Tang, C.-B. (2011). *Acta Cryst.* E**67**, o271.

supporting information

Acta Cryst. (2012). E**68**, o335 [doi:10.1107/S1600536811055589]

N′-(2-Chlorobenzylidene)-4-nitrobenzohydrazide

Chun-Bao Tang

S1. Comment

Hydrazone compounds have received much attention in biological and structural chemistry in the last few years (Rasras *et al.*, 2010; Pyta *et al.*, 2010; Angelusiu *et al.*, 2010; Fun *et al.*, 2008; Singh & Singh, 2010; Ahmad *et al.*, 2010). As a continuation of our work on the structural study on such compounds (Tang, 2010, 2011), we reports herein on the crystal structure of the title new hydrazone compound.

In the molecule of the title compound (Fig. 1), the dihedral angle between the two benzene rings is 6.64 (13)°. Bond lengths in the compound are normal (Allen *et al.*, 1987) and comparable to those in the similar compounds (Tang, 2010; Tang, 2011).

In the crystal, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains running along the *c* axis direction (Fig. 2).

S2. Experimental

2-Chlorobenzaldehyde (0.1 mmol, 14.1 mg) and 4-nitrobenzohydrazide (0.1 mmol, 18.2 mg) were dissolved in methanol (20 ml). The mixture was stirred at reflux for 10 min to give a clear yellow solution. Yellow needle-shaped crystals of the compound were formed by slow evaporation of the solvent over several days.

S3. Refinement

The amino H atom was located in a difference Fourier map and refined isotropically, with an N—H distance restraint of 0.90 (1) Å. C-bound H atoms were included in calculated positions and refined as riding atoms: C—H = 0.93 Å, with U_{iso}(H) = 1.2U_{eq}(C).

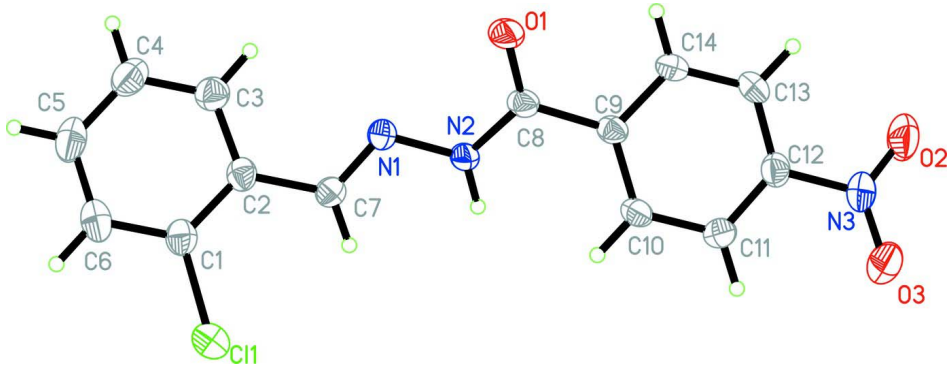


Figure 1

The molecular structure of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

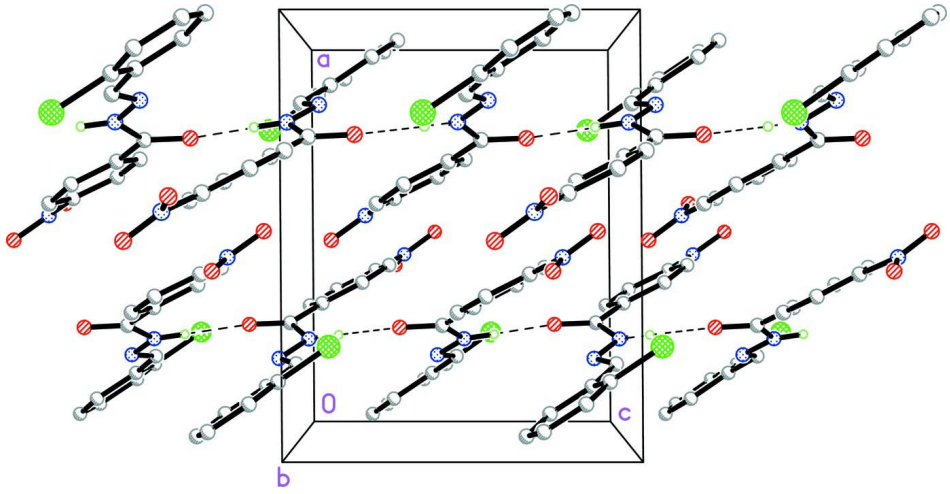


Figure 2

Crystal packing of the title compound, viewed along the b axis, with hydrogen bonds shown as dashed lines.

N′-(2-Chlorobenzylidene)-4-nitrobenzohydrazide

Crystal data

$C_{14}H_{10}ClN_3O_3$
$M_r = 303.70$
Monoclinic, $P2_1/c$
$a = 11.2332\ (18)$ Å
$b = 13.3778\ (18)$ Å
$c = 8.9770\ (16)$ Å
$\beta = 90.408\ (2)°$
$V = 1349.0\ (4)$ Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.495$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2464 reflections
$\theta = 2.4–24.5°$
$\mu = 0.30$ mm^{-1}
$T = 298$ K
Cut from needle, yellow
0.18 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.949$, $T_{max} = 0.957$
10640 measured reflections
2931 independent reflections
1882 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
$h = -14\rightarrow14$
$k = -14\rightarrow17$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.146$
$S = 1.03$
2931 reflections
193 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.5874P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.23505 (8)	0.62569 (6)	1.10065 (9)	0.0782 (3)
H2	0.246 (3)	0.265 (2)	1.1045 (13)	0.080*
N1	0.18950 (18)	0.33163 (14)	0.9198 (2)	0.0444 (5)
N2	0.23517 (19)	0.25548 (14)	1.0072 (2)	0.0446 (5)
N3	0.4488 (2)	−0.1478 (2)	1.3026 (3)	0.0667 (7)
O1	0.26845 (19)	0.15983 (13)	0.80373 (18)	0.0620 (5)
O2	0.4173 (3)	−0.23176 (19)	1.2688 (3)	0.1126 (10)
O3	0.5111 (2)	−0.12928 (18)	1.4092 (3)	0.0902 (8)
C1	0.1488 (2)	0.59971 (19)	0.9450 (3)	0.0513 (6)
C2	0.1308 (2)	0.50090 (18)	0.8991 (3)	0.0452 (6)
C3	0.0625 (2)	0.4872 (2)	0.7698 (3)	0.0553 (7)
H3	0.0493	0.4227	0.7348	0.066*
C4	0.0149 (3)	0.5657 (3)	0.6941 (3)	0.0679 (8)
H4	−0.0312	0.5541	0.6094	0.082*
C5	0.0344 (3)	0.6622 (2)	0.7416 (4)	0.0709 (9)
H5	0.0020	0.7154	0.6885	0.085*
C6	0.1015 (3)	0.6800 (2)	0.8673 (4)	0.0644 (8)
H6	0.1149	0.7450	0.8998	0.077*
C7	0.1807 (2)	0.41629 (18)	0.9816 (3)	0.0463 (6)
H7	0.2061	0.4247	1.0796	0.056*
C8	0.2731 (2)	0.17126 (17)	0.9389 (3)	0.0434 (6)
C9	0.3213 (2)	0.09038 (17)	1.0373 (2)	0.0392 (5)
C10	0.3769 (2)	0.10957 (18)	1.1718 (3)	0.0443 (6)
H10	0.3845	0.1751	1.2052	0.053*
C11	0.4216 (2)	0.03155 (19)	1.2576 (3)	0.0495 (6)
H11	0.4605	0.0441	1.3474	0.059*
C12	0.4069 (2)	−0.06443 (19)	1.2070 (3)	0.0479 (6)
C13	0.3536 (2)	−0.08568 (19)	1.0728 (3)	0.0558 (7)
H13	0.3456	−0.1514	1.0404	0.067*
C14	0.3122 (2)	−0.00768 (19)	0.9871 (3)	0.0539 (7)
H14	0.2777	−0.0207	0.8947	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1009 (6)	0.0532 (5)	0.0802 (6)	−0.0085 (4)	−0.0221 (5)	−0.0047 (4)

N1	0.0560 (12)	0.0374 (11)	0.0397 (11)	−0.0027 (9)	−0.0030 (9)	0.0046 (9)
N2	0.0662 (13)	0.0345 (11)	0.0329 (11)	−0.0010 (9)	−0.0045 (9)	−0.0007 (9)
N3	0.0637 (15)	0.0569 (16)	0.0792 (18)	0.0213 (12)	−0.0113 (13)	0.0006 (14)
O1	0.1089 (16)	0.0463 (10)	0.0308 (10)	−0.0018 (10)	−0.0020 (9)	−0.0018 (8)
O2	0.134 (2)	0.0514 (15)	0.152 (3)	0.0189 (14)	−0.0636 (19)	0.0076 (15)
O3	0.1053 (18)	0.0902 (18)	0.0747 (16)	0.0349 (14)	−0.0268 (14)	−0.0009 (13)
C1	0.0545 (14)	0.0475 (15)	0.0518 (15)	−0.0003 (12)	0.0045 (12)	0.0070 (12)
C2	0.0504 (13)	0.0428 (14)	0.0425 (14)	0.0001 (11)	0.0078 (11)	0.0052 (11)
C3	0.0590 (16)	0.0573 (17)	0.0496 (16)	0.0051 (13)	−0.0006 (12)	−0.0021 (13)
C4	0.0709 (19)	0.078 (2)	0.0548 (17)	0.0151 (16)	−0.0082 (14)	0.0057 (16)
C5	0.081 (2)	0.063 (2)	0.068 (2)	0.0191 (16)	0.0024 (17)	0.0202 (16)
C6	0.0742 (19)	0.0443 (16)	0.075 (2)	0.0044 (14)	0.0094 (16)	0.0094 (14)
C7	0.0579 (14)	0.0440 (14)	0.0369 (13)	−0.0017 (11)	−0.0019 (11)	0.0026 (11)
C8	0.0579 (14)	0.0369 (13)	0.0353 (13)	−0.0113 (11)	−0.0005 (10)	0.0003 (10)
C9	0.0476 (12)	0.0365 (12)	0.0337 (12)	−0.0051 (10)	0.0043 (10)	−0.0016 (10)
C10	0.0510 (13)	0.0369 (13)	0.0450 (14)	−0.0038 (10)	−0.0014 (11)	−0.0087 (11)
C11	0.0507 (14)	0.0530 (16)	0.0446 (14)	0.0034 (12)	−0.0080 (11)	−0.0057 (12)
C12	0.0468 (13)	0.0443 (14)	0.0526 (15)	0.0089 (11)	0.0004 (11)	0.0007 (12)
C13	0.0694 (17)	0.0355 (13)	0.0625 (18)	0.0044 (12)	−0.0095 (14)	−0.0119 (12)
C14	0.0749 (18)	0.0416 (14)	0.0450 (14)	−0.0001 (13)	−0.0130 (13)	−0.0117 (12)

Geometric parameters (Å, º)

Cl1—C1	1.729 (3)	C4—H4	0.9300
N1—C7	1.265 (3)	C5—C6	1.373 (4)
N1—N2	1.382 (3)	C5—H5	0.9300
N2—C8	1.353 (3)	C6—H6	0.9300
N2—H2	0.891 (10)	C7—H7	0.9300
N3—O3	1.207 (3)	C8—C9	1.495 (3)
N3—O2	1.216 (3)	C9—C10	1.380 (3)
N3—C12	1.482 (3)	C9—C14	1.390 (3)
O1—C8	1.224 (3)	C10—C11	1.389 (3)
C1—C6	1.385 (4)	C10—H10	0.9300
C1—C2	1.399 (3)	C11—C12	1.372 (3)
C2—C3	1.399 (3)	C11—H11	0.9300
C2—C7	1.462 (3)	C12—C13	1.371 (3)
C3—C4	1.358 (4)	C13—C14	1.375 (4)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.377 (5)	C14—H14	0.9300
C7—N1—N2	116.14 (19)	N1—C7—C2	120.1 (2)
C8—N2—N1	118.26 (19)	N1—C7—H7	119.9
C8—N2—H2	122 (2)	C2—C7—H7	119.9
N1—N2—H2	120 (2)	O1—C8—N2	122.8 (2)
O3—N3—O2	123.6 (3)	O1—C8—C9	120.5 (2)
O3—N3—C12	119.0 (3)	N2—C8—C9	116.7 (2)
O2—N3—C12	117.4 (3)	C10—C9—C14	119.4 (2)
C6—C1—C2	122.0 (3)	C10—C9—C8	122.8 (2)

C6—C1—Cl1	117.5 (2)	C14—C9—C8	117.8 (2)
C2—C1—Cl1	120.5 (2)	C9—C10—C11	120.3 (2)
C1—C2—C3	116.5 (2)	C9—C10—H10	119.8
C1—C2—C7	121.9 (2)	C11—C10—H10	119.8
C3—C2—C7	121.6 (2)	C12—C11—C10	118.5 (2)
C4—C3—C2	121.7 (3)	C12—C11—H11	120.7
C4—C3—H3	119.2	C10—C11—H11	120.7
C2—C3—H3	119.2	C13—C12—C11	122.4 (2)
C3—C4—C5	120.6 (3)	C13—C12—N3	119.2 (2)
C3—C4—H4	119.7	C11—C12—N3	118.4 (2)
C5—C4—H4	119.7	C12—C13—C14	118.5 (2)
C6—C5—C4	120.1 (3)	C12—C13—H13	120.7
C6—C5—H5	119.9	C14—C13—H13	120.7
C4—C5—H5	119.9	C13—C14—C9	120.7 (2)
C5—C6—C1	119.1 (3)	C13—C14—H14	119.6
C5—C6—H6	120.4	C9—C14—H14	119.6
C1—C6—H6	120.4		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.89 (1)	2.06 (1)	2.915 (3)	160 (3)

Symmetry code: (i) x, $-y+1/2$, $z+1/2$.