Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-*N*′-(4-nitrobenzylidene)-benzohydrazide

Cong-Shan Zhou and Tao Yang*

College of Chemistry and Chemical Engineering, Hunan Institute of Science and Technology, Yueyang, Hunan 414006, People's Republic of China
Correspondence e-mail: zhoucongsh@gmail.com

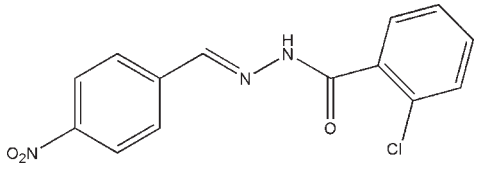
Received 23 December 2009; accepted 24 December 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.113; data-to-parameter ratio = 14.3.

The title Schiff base compound, $C_{14}H_{10}ClN_3O_3$, exists in a *trans* configuration with respect to the C=N bond. The dihedral angle between the two benzene rings is 15.9 (2)°. In the crystal, the molecules are linked into chains along [101] by intermolecular N—H···O hydrogen bonds.

Related literature

For the biological properties of Schiff bases, see: Mohamed *et al.* (2009); Ritter *et al.* (2009); Bagihalli *et al.* (2008). For the crystal structures of Schiff base compounds, see: Fun *et al.* (2008); Shafiq *et al.* (2009); Goh *et al.* (2010). For other related structures, see: Zhou *et al.* (2009); Zhou & Yang (2009).



Experimental

Crystal data

$C_{14}H_{10}ClN_3O_3$
M_r = 303.70
Monoclinic, $P2_1/n$
a = 7.2752 (3) Å
b = 26.4081 (9) Å
c = 7.7284 (3) Å
β = 113.000 (2)°
V = 1366.78 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.936, T_{max} = 0.944
7876 measured reflections
2763 independent reflections
1934 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.113
S = 1.03
2763 reflections
193 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.90 (1)	1.97 (1)	2.855 (2)	169 (2)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Hunan Provincial Natural Science Foundation of China (grant No. 09 J J6022) and the Scientific Research Fund of Hunan Provincial Education Department, China (grant No. 08B031).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5003).

References

Bagihalli, G. B., Avaji, P. G., Patil, S. A. & Badami, P. S. (2008). *Eur. J. Med. Chem.* **43**, 2639–2649.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K., Chantrapromma, S., Jana, S., Hazra, A. & Goswami, S. (2008). *Acta Cryst.* E**64**, o175–o176.
Goh, J. H., Fun, H.-K., Vinayaka, A. C. & Kalluraya, B. (2010). *Acta Cryst.* E**66**, o24.
Mohamed, G. G., Omar, M. M. & Ibrahim, A. A. (2009). *Eur. J. Med. Chem.* **44**, 4801–4812.
Ritter, E., Przybylski, P., Brzezinski, B. & Bartl, F. (2009). *Curr. Org. Chem.* **13**, 241–249.
Shafiq, Z., Yaqub, M., Tahir, M. N., Hussain, A. & Iqbal, M. S. (2009). *Acta Cryst.* E**65**, o2501.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhou, C.-S., Hou, H.-Y. & Yang, T. (2009). *Z. Kristallogr. New Cryst. Struct.* **224**, 37–38.
Zhou, C.-S. & Yang, T. (2009). *Z. Kristallogr. New Cryst. Struct.* **224**, 39–40.

supporting information

Acta Cryst. (2010). E**66**, o290 [https://doi.org/10.1107/S1600536809055330]

2-Chloro-*N*′-(4-nitrobenzylidene)benzohydrazide

Cong-Shan Zhou and Tao Yang

S1. Comment

Schiff bases are a kind of interesting compounds, which possess excellent biological properties, such as antibacterial, antimicrobial, and antitumor (Mohamed *et al.*, 2009; Ritter *et al.*, 2009; Bagihalli *et al.*, 2008). Recently, a large number of Schiff bases derived from the reaction of aldehydes with benzohydrazides have been reported (Fun *et al.*, 2008; Shafiq *et al.*, 2009; Goh *et al.*, 2010). In this paper, the crystal structure of the title new Schiff base compound is reported.

In the title compound (Fig. 1), bond lengths are comparable with those observed in related structures (Zhou *et al.*, 2009; Zhou & Yang, 2009). The molecule exists in a *trans* configuration with respect to the acyclic C═N bond. The molecule is distorted from planarity, with a dihedral angle between the two benzene rings of 15.9 (2)°.

In the crystal structure, intermolecular N—H···O hydrogen bonds link adjacent molecules into chains along the [101] (Table 1 and Fig. 2).

S2. Experimental

4-Nitrobenzaldehyde (1.0 mmol, 151.0 mg) and 2-chlorobenzohydrazide (1.0 mmol, 170.0 mg) were dissolved in methanol (30 ml). The mixture was stirred for 30 min at room temperature. The resulting solution was left in air for a few days, yielding colourless block-shaped crystals.

S3. Refinement

Atom H2A was located in a difference map and refined with a N–H distance restraint of 0.90 (1) Å and U_{iso}(H) = 0.08 Å^2. The remaining H atoms were positioned geometrically (C–H = 0.93 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

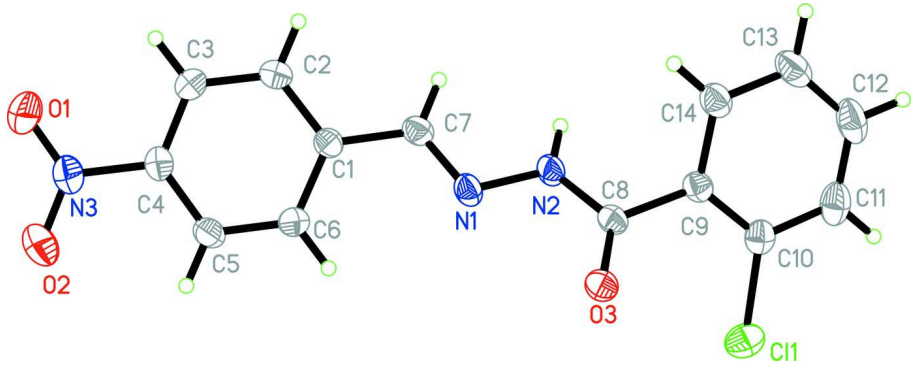


Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

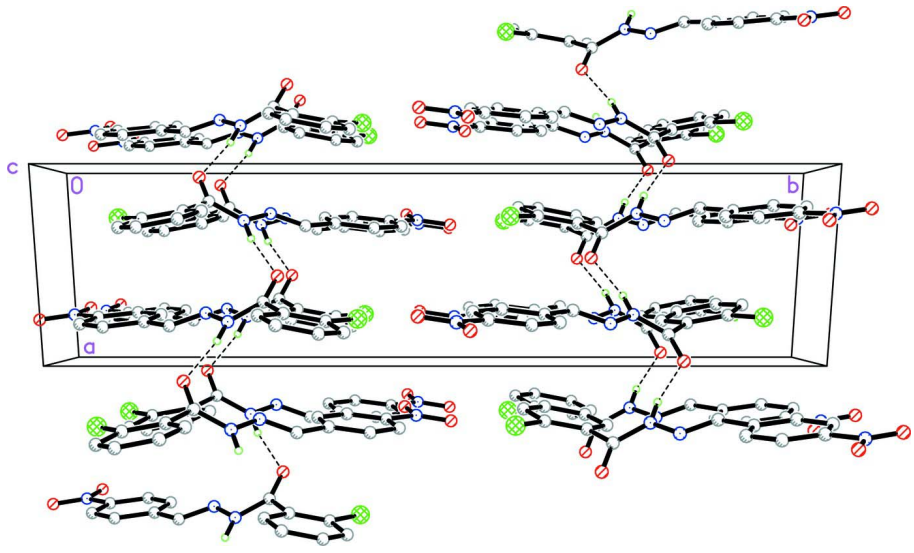


Figure 2

The molecular packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

2-Chloro-*N*′-(4-nitrobenzylidene)benzohydrazide

Crystal data

$C_{14}H_{10}ClN_3O_3$
$M_r = 303.70$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.2752$ (3) Å
$b = 26.4081$ (9) Å
$c = 7.7284$ (3) Å
$\beta = 113.000$ (2)°
$V = 1366.78$ (9) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.476$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1518 reflections
$\theta = 2.4$–24.5°
$\mu = 0.29$ mm^{-1}
$T = 298$ K
Block, colourless
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.936$, $T_{max} = 0.944$
7876 measured reflections
2763 independent reflections
1934 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 26.3°$, $\theta_{min} = 1.5°$
$h = -9\rightarrow9$
$k = -29\rightarrow32$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.113$
$S = 1.03$
2763 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

$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.233P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.25382 (9)	0.09582 (2)	0.73742 (9)	0.0617 (2)
N1	0.2283 (2)	0.28721 (7)	0.5887 (2)	0.0434 (4)
N2	0.2675 (2)	0.25629 (7)	0.7434 (2)	0.0437 (4)
N3	0.2493 (3)	0.47567 (8)	0.0679 (3)	0.0637 (6)
O1	0.2747 (4)	0.52006 (8)	0.1124 (3)	0.1069 (8)
O2	0.2156 (4)	0.46052 (8)	−0.0899 (3)	0.0983 (7)
O3	0.0453 (2)	0.19654 (5)	0.57474 (19)	0.0498 (4)
C1	0.2747 (3)	0.36895 (8)	0.4821 (3)	0.0388 (5)
C2	0.3001 (3)	0.42028 (8)	0.5248 (3)	0.0505 (6)
H2	0.3247	0.4311	0.6464	0.061*
C3	0.2892 (3)	0.45526 (8)	0.3895 (3)	0.0525 (6)
H3	0.3032	0.4896	0.4176	0.063*
C4	0.2573 (3)	0.43846 (8)	0.2119 (3)	0.0447 (5)
C5	0.2344 (3)	0.38808 (8)	0.1647 (3)	0.0469 (5)
H5	0.2143	0.3776	0.0438	0.056*
C6	0.2420 (3)	0.35350 (8)	0.3006 (3)	0.0443 (5)
H6	0.2249	0.3193	0.2704	0.053*
C7	0.2910 (3)	0.33266 (8)	0.6288 (3)	0.0435 (5)
H7	0.3480	0.3427	0.7541	0.052*
C8	0.1706 (3)	0.21195 (8)	0.7239 (3)	0.0396 (5)
C9	0.2232 (3)	0.18436 (8)	0.9059 (3)	0.0392 (5)
C10	0.2608 (3)	0.13269 (8)	0.9245 (3)	0.0452 (5)
C11	0.3086 (3)	0.10918 (10)	1.0973 (4)	0.0612 (7)
H11	0.3399	0.0749	1.1108	0.073*
C12	0.3095 (4)	0.13687 (12)	1.2487 (4)	0.0680 (8)
H12	0.3372	0.1207	1.3631	0.082*
C13	0.2705 (4)	0.18759 (11)	1.2333 (3)	0.0623 (7)
H13	0.2722	0.2058	1.3369	0.075*
C14	0.2289 (3)	0.21163 (9)	1.0648 (3)	0.0496 (6)
H14	0.2042	0.2463	1.0553	0.060*
H2A	0.359 (3)	0.2671 (9)	0.853 (2)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0603 (4)	0.0542 (4)	0.0718 (4)	0.0013 (3)	0.0270 (3)	−0.0108 (3)
N1	0.0437 (10)	0.0494 (11)	0.0319 (9)	−0.0017 (8)	0.0091 (7)	0.0068 (8)
N2	0.0462 (10)	0.0469 (10)	0.0281 (9)	−0.0076 (8)	0.0039 (7)	0.0049 (8)
N3	0.0825 (15)	0.0591 (14)	0.0531 (13)	0.0030 (11)	0.0302 (11)	0.0129 (11)
O1	0.197 (3)	0.0488 (12)	0.0902 (16)	−0.0089 (14)	0.0720 (17)	0.0117 (11)
O2	0.160 (2)	0.0860 (15)	0.0546 (12)	−0.0099 (14)	0.0489 (13)	0.0119 (11)
O3	0.0535 (9)	0.0502 (9)	0.0318 (8)	−0.0070 (7)	0.0017 (7)	0.0008 (7)
C1	0.0362 (10)	0.0422 (12)	0.0357 (11)	0.0003 (9)	0.0117 (9)	0.0005 (9)
C2	0.0632 (14)	0.0485 (13)	0.0383 (12)	−0.0032 (11)	0.0182 (10)	−0.0059 (10)
C3	0.0667 (15)	0.0382 (12)	0.0521 (14)	−0.0037 (10)	0.0228 (11)	−0.0026 (10)
C4	0.0457 (12)	0.0454 (12)	0.0444 (12)	0.0019 (10)	0.0190 (10)	0.0082 (10)
C5	0.0524 (13)	0.0518 (13)	0.0360 (11)	0.0026 (11)	0.0167 (10)	−0.0014 (10)
C6	0.0502 (12)	0.0402 (11)	0.0407 (12)	0.0004 (9)	0.0156 (10)	−0.0030 (10)
C7	0.0436 (12)	0.0493 (13)	0.0337 (11)	−0.0019 (10)	0.0108 (9)	−0.0021 (9)
C8	0.0395 (11)	0.0454 (12)	0.0303 (10)	0.0019 (9)	0.0096 (9)	0.0013 (9)
C9	0.0333 (10)	0.0472 (13)	0.0329 (10)	−0.0032 (9)	0.0084 (8)	0.0005 (9)
C10	0.0351 (11)	0.0488 (13)	0.0479 (13)	−0.0033 (9)	0.0120 (9)	0.0057 (10)
C11	0.0505 (14)	0.0609 (16)	0.0635 (16)	−0.0018 (11)	0.0129 (12)	0.0220 (13)
C12	0.0601 (15)	0.090 (2)	0.0450 (15)	−0.0131 (14)	0.0106 (12)	0.0225 (15)
C13	0.0604 (15)	0.089 (2)	0.0369 (13)	−0.0178 (14)	0.0182 (11)	−0.0050 (13)
C14	0.0478 (12)	0.0586 (14)	0.0399 (12)	−0.0076 (11)	0.0145 (10)	0.0018 (11)

Geometric parameters (Å, º)

Cl1—C10	1.727 (2)	C4—C5	1.372 (3)
N1—C7	1.278 (3)	C5—C6	1.377 (3)
N1—N2	1.382 (2)	C5—H5	0.93
N2—C8	1.344 (3)	C6—H6	0.93
N2—H2A	0.895 (10)	C7—H7	0.93
N3—O2	1.214 (3)	C8—C9	1.495 (3)
N3—O1	1.215 (3)	C9—C10	1.388 (3)
N3—C4	1.468 (3)	C9—C14	1.410 (3)
O3—C8	1.226 (2)	C10—C11	1.388 (3)
C1—C6	1.389 (3)	C11—C12	1.378 (4)
C1—C2	1.390 (3)	C11—H11	0.93
C1—C7	1.454 (3)	C12—C13	1.365 (4)
C2—C3	1.374 (3)	C12—H12	0.93
C2—H2	0.93	C13—C14	1.372 (3)
C3—C4	1.373 (3)	C13—H13	0.93
C3—H3	0.93	C14—H14	0.93
C7—N1—N2	114.29 (16)	N1—C7—C1	121.13 (18)
C8—N2—N1	119.69 (15)	N1—C7—H7	119.4
C8—N2—H2A	123.1 (17)	C1—C7—H7	119.4
N1—N2—H2A	117.2 (17)	O3—C8—N2	124.00 (18)

O2—N3—O1	123.4 (2)	O3—C8—C9	123.06 (18)
O2—N3—C4	118.2 (2)	N2—C8—C9	112.86 (16)
O1—N3—C4	118.3 (2)	C10—C9—C14	118.30 (18)
C6—C1—C2	118.74 (19)	C10—C9—C8	122.97 (18)
C6—C1—C7	121.58 (19)	C14—C9—C8	118.69 (18)
C2—C1—C7	119.64 (19)	C11—C10—C9	120.3 (2)
C3—C2—C1	120.8 (2)	C11—C10—Cl1	117.86 (19)
C3—C2—H2	119.6	C9—C10—Cl1	121.83 (16)
C1—C2—H2	119.6	C12—C11—C10	119.7 (2)
C4—C3—C2	118.7 (2)	C12—C11—H11	120.1
C4—C3—H3	120.6	C10—C11—H11	120.1
C2—C3—H3	120.6	C13—C12—C11	121.0 (2)
C5—C4—C3	122.3 (2)	C13—C12—H12	119.5
C5—C4—N3	118.8 (2)	C11—C12—H12	119.5
C3—C4—N3	118.8 (2)	C12—C13—C14	119.9 (2)
C4—C5—C6	118.4 (2)	C12—C13—H13	120.1
C4—C5—H5	120.8	C14—C13—H13	120.1
C6—C5—H5	120.8	C13—C14—C9	120.7 (2)
C5—C6—C1	121.0 (2)	C13—C14—H14	119.6
C5—C6—H6	119.5	C9—C14—H14	119.6
C1—C6—H6	119.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O3^{i}	0.90 (1)	1.97 (1)	2.855 (2)	169 (2)

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