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(*E*)-4-Bromo-*N*′-(2-chlorobenzylidene)-benzohydrazide

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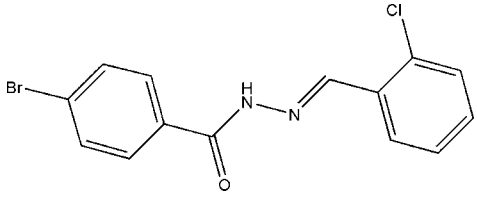
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.094; data-to-parameter ratio = 14.2.

In the title compound, $C_{14}H_{10}BrClN_2O$, the dihedral angle between the two benzene rings is 11.4 (2)°. In the crystal structure, molecules are connected *via* intermolecular N—H···O hydrogen bonds into one-dimensional chains running parallel to the *c* axis.

Related literature

For the biological activity of hydrazones and Schiff bases, see: Bhandari *et al.* (2008); Sinha *et al.* (2008). For a related structure, see: Pan & Yang (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{10}BrClN_2O$ M_r = 337.60
Monoclinic, $P2_1/c$
a = 11.218 (4) Å
b = 13.512 (5) Å
c = 9.200 (3) Å
β = 97.077 (6)°
V = 1383.9 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.16 mm^{-1}
T = 298 K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.491, T_{max} = 0.531
6907 measured reflections
2438 independent reflections
1948 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.03
2438 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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}	0.86	2.12	2.918 (3)	154

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2944).

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supporting information

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(*E*)-4-Bromo-*N*′-(2-chlorobenzylidene)benzohydrazide

Xiao-Hong Shu, Yun-Peng Diao, Mo-Lin Li, Xu Yan and Jia Liu

S1. Comment

Hydrazones and Schiff bases have attracted much attention for their excellent biological properties, especially for their potential pharmacological and antitumor properties (Bhandari *et al.*, 2008; Sinha *et al.*, 2008). In this paper, the crystal structure of the title compound, (I), a new Schiff base compound derived from the condensation reaction of 2-chlorobenzaldehyde with 4-bromobenzohydrazide is reported.

The Schiff base molecule of the compound displays a *trans* configuration with respect to the C=N and C—N bonds (Fig. 1). All the bond lengths are within normal ranges (Allen *et al.*, 1987), and are comparable to those in the related compound *N*′-(2-chlorobenzylidene)-2-hydroxybenzohydrazide (Pan & Yang, 2005). The dihedral angle between the two benzene rings is 11.4 (2)°. In the crystal structure, the $C_{14}H_{10}BrClN_2O$ molecules are connected *via* intermolecular N—H···O hydrogen bonds into one-dimensional chains running parallel to the *c* axis (Table 1 & Fig. 2).

S2. Experimental

2-Chlorobenzaldehyde (0.1 mmol) and 4-bromobenzohydrazide acid hydrazide (0.1 mmol) were dissolved in a 95% ethanol solution (10 ml). The mixture was stirred at room temperature to give a clear colorless solution. Colourless blocks of (I) were formed by gradual evaporation of the solvent over a period of five days at room temperature.

S3. Refinement

All H atoms were placed in geometrically idealized positions, with C—H = 0.93 Å and N—H = 0.86 Å. U_{iso}(H) = 1.2U_{eq}(C,*N*).

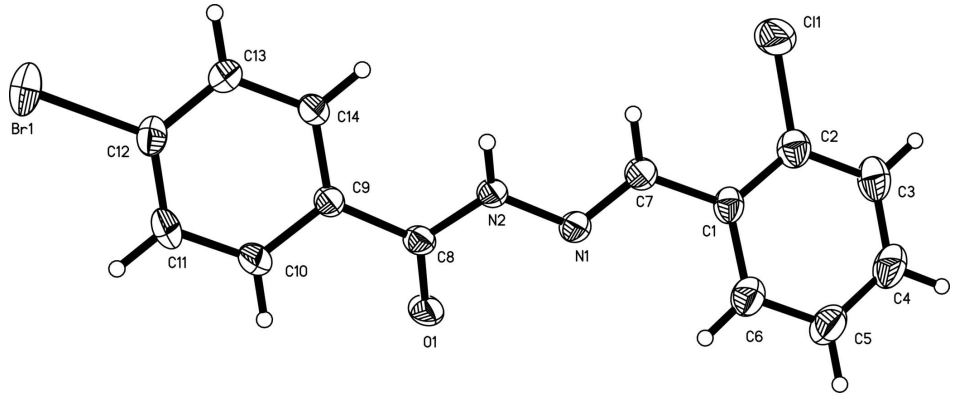

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

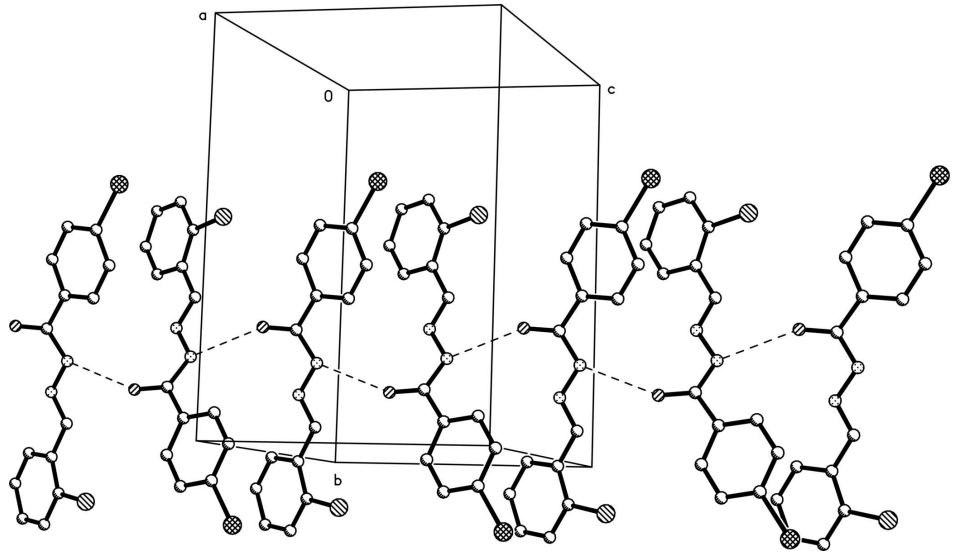

Figure 2

The one-dimensional chains structure along *c* axis. The donor···acceptor for the intermolecular hydrogen bonds are shown as dashed lines.

(*E*)-4-Bromo-*N*′-(2-chlorobenzylidene)benzohydrazide

Crystal data

$C_{14}H_{10}BrClN_2O$
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Hall symbol: -P 2ybc
a = 11.218 (4) Å
b = 13.512 (5) Å
c = 9.200 (3) Å
β = 97.077 (6)°
V = 1383.9 (8) Å^3
Z = 4
$F(000)$ = 672
D_x = 1.620 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2695 reflections
θ = 2.4–26.2°
μ = 3.16 mm^{-1}
T = 298 K
Block, colorless
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.491, T_{max} = 0.531
6907 measured reflections
2438 independent reflections
1948 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.1°, θ_{min} = 1.8°
h = −13→13
k = −10→16
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.03
2438 reflections
172 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.9326P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ 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}
Br1	0.45713 (4)	1.17921 (3)	0.84354 (5)	0.07653 (18)
Cl1	0.23484 (10)	0.37589 (7)	0.63350 (10)	0.0790 (3)
N1	0.1872 (2)	0.66418 (16)	0.4378 (2)	0.0423 (5)
N2	0.2302 (2)	0.74288 (16)	0.5254 (2)	0.0419 (5)
H2	0.2331	0.7398	0.6191	0.050*
O1	0.2623 (2)	0.83236 (15)	0.3250 (2)	0.0555 (6)
C1	0.1301 (3)	0.4950 (2)	0.4158 (3)	0.0439 (7)
C2	0.1495 (3)	0.3987 (2)	0.4655 (3)	0.0521 (7)
C3	0.1046 (3)	0.3167 (2)	0.3829 (4)	0.0634 (9)
H3	0.1184	0.2529	0.4190	0.076*
C4	0.0401 (3)	0.3319 (3)	0.2483 (4)	0.0674 (10)
H4	0.0100	0.2781	0.1924	0.081*
C5	0.0197 (3)	0.4264 (3)	0.1954 (4)	0.0670 (10)
H5	−0.0245	0.4358	0.1041	0.080*
C6	0.0637 (3)	0.5072 (3)	0.2759 (4)	0.0558 (8)
H6	0.0497	0.5705	0.2378	0.067*
C7	0.1768 (3)	0.5816 (2)	0.5014 (3)	0.0448 (7)
H7	0.1987	0.5760	0.6019	0.054*
C8	0.2680 (3)	0.82507 (19)	0.4591 (3)	0.0402 (6)
C9	0.3160 (2)	0.90782 (19)	0.5568 (3)	0.0387 (6)
C10	0.3159 (3)	1.0028 (2)	0.4976 (4)	0.0639 (10)
H10	0.2873	1.0121	0.3993	0.077*
C11	0.3572 (4)	1.0832 (2)	0.5811 (4)	0.0687 (10)
H11	0.3549	1.1463	0.5404	0.082*
C12	0.4020 (3)	1.0687 (2)	0.7257 (3)	0.0485 (7)
C13	0.4055 (3)	0.9757 (2)	0.7869 (3)	0.0502 (7)
H13	0.4371	0.9667	0.8844	0.060*
C14	0.3620 (3)	0.8957 (2)	0.7029 (3)	0.0432 (6)
H14	0.3635	0.8330	0.7447	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0834 (3)	0.0523 (2)	0.0923 (3)	−0.02495 (18)	0.0047 (2)	−0.02263 (19)
Cl1	0.1214 (8)	0.0504 (5)	0.0598 (6)	0.0029 (5)	−0.0099 (5)	0.0011 (4)
N1	0.0549 (14)	0.0366 (13)	0.0344 (12)	0.0020 (10)	0.0014 (10)	−0.0050 (10)
N2	0.0650 (15)	0.0336 (12)	0.0262 (11)	−0.0013 (10)	0.0018 (10)	−0.0021 (9)
O1	0.0959 (17)	0.0437 (12)	0.0263 (11)	0.0018 (11)	0.0054 (10)	0.0010 (8)
C1	0.0496 (16)	0.0391 (15)	0.0445 (16)	−0.0057 (12)	0.0120 (13)	−0.0079 (13)
C2	0.0590 (19)	0.0442 (17)	0.0542 (18)	−0.0014 (14)	0.0108 (15)	−0.0081 (14)
C3	0.076 (2)	0.0392 (17)	0.077 (3)	−0.0050 (15)	0.017 (2)	−0.0117 (16)
C4	0.076 (2)	0.058 (2)	0.066 (2)	−0.0167 (18)	0.0048 (19)	−0.0232 (18)
C5	0.069 (2)	0.071 (2)	0.058 (2)	−0.0143 (18)	−0.0046 (17)	−0.0136 (18)
C6	0.0590 (19)	0.0543 (19)	0.0540 (19)	−0.0083 (15)	0.0061 (15)	−0.0098 (15)
C7	0.0588 (18)	0.0397 (16)	0.0360 (15)	−0.0021 (13)	0.0058 (13)	−0.0027 (12)
C8	0.0519 (17)	0.0352 (14)	0.0332 (15)	0.0075 (12)	0.0038 (12)	0.0004 (11)
C9	0.0510 (16)	0.0333 (14)	0.0322 (14)	0.0015 (12)	0.0067 (12)	−0.0004 (11)
C10	0.105 (3)	0.0416 (17)	0.0414 (18)	−0.0093 (17)	−0.0061 (17)	0.0104 (14)
C11	0.103 (3)	0.0325 (17)	0.068 (2)	−0.0132 (17)	0.001 (2)	0.0098 (16)
C12	0.0519 (17)	0.0397 (16)	0.0542 (19)	−0.0110 (13)	0.0078 (14)	−0.0071 (14)
C13	0.0638 (19)	0.0464 (17)	0.0384 (16)	−0.0065 (14)	−0.0024 (14)	−0.0024 (13)
C14	0.0570 (17)	0.0341 (14)	0.0381 (15)	−0.0007 (12)	0.0042 (12)	0.0041 (12)

Geometric parameters (Å, º)

Br1—C12	1.903 (3)	C5—C6	1.377 (4)
Cl1—C2	1.742 (3)	C5—H5	0.9300
N1—C7	1.272 (4)	C6—H6	0.9300
N1—N2	1.385 (3)	C7—H7	0.9300
N2—C8	1.359 (3)	C8—C9	1.493 (4)
N2—H2	0.8600	C9—C14	1.388 (4)
O1—C8	1.232 (3)	C9—C10	1.394 (4)
C1—C2	1.388 (4)	C10—C11	1.378 (5)
C1—C6	1.415 (4)	C10—H10	0.9300
C1—C7	1.470 (4)	C11—C12	1.377 (5)
C2—C3	1.401 (4)	C11—H11	0.9300
C3—C4	1.371 (5)	C12—C13	1.376 (4)
C3—H3	0.9300	C13—C14	1.383 (4)
C4—C5	1.375 (5)	C13—H13	0.9300
C4—H4	0.9300	C14—H14	0.9300
C7—N1—N2	116.8 (2)	N1—C7—H7	120.1
C8—N2—N1	118.2 (2)	C1—C7—H7	120.1
C8—N2—H2	120.9	O1—C8—N2	122.3 (3)
N1—N2—H2	120.9	O1—C8—C9	120.9 (2)
C2—C1—C6	116.9 (3)	N2—C8—C9	116.8 (2)
C2—C1—C7	122.6 (3)	C14—C9—C10	117.9 (3)
C6—C1—C7	120.5 (3)	C14—C9—C8	123.9 (2)

C1—C2—C3	122.1 (3)	C10—C9—C8	118.1 (2)
C1—C2—Cl1	120.3 (2)	C11—C10—C9	121.6 (3)
C3—C2—Cl1	117.5 (3)	C11—C10—H10	119.2
C4—C3—C2	119.1 (3)	C9—C10—H10	119.2
C4—C3—H3	120.5	C12—C11—C10	118.9 (3)
C2—C3—H3	120.5	C12—C11—H11	120.5
C3—C4—C5	120.3 (3)	C10—C11—H11	120.5
C3—C4—H4	119.8	C13—C12—C11	121.0 (3)
C5—C4—H4	119.8	C13—C12—Br1	119.5 (2)
C4—C5—C6	120.9 (3)	C11—C12—Br1	119.5 (2)
C4—C5—H5	119.5	C12—C13—C14	119.6 (3)
C6—C5—H5	119.5	C12—C13—H13	120.2
C5—C6—C1	120.7 (3)	C14—C13—H13	120.2
C5—C6—H6	119.7	C13—C14—C9	120.9 (3)
C1—C6—H6	119.7	C13—C14—H14	119.6
N1—C7—C1	119.9 (3)	C9—C14—H14	119.6

C7—N1—N2—C8	165.4 (3)	N1—N2—C8—C9	−178.9 (2)
C6—C1—C2—C3	−0.9 (5)	O1—C8—C9—C14	−157.9 (3)
C7—C1—C2—C3	180.0 (3)	N2—C8—C9—C14	22.8 (4)
C6—C1—C2—Cl1	177.7 (2)	O1—C8—C9—C10	21.4 (4)
C7—C1—C2—Cl1	−1.4 (4)	N2—C8—C9—C10	−158.0 (3)
C1—C2—C3—C4	0.5 (5)	C14—C9—C10—C11	−1.6 (5)
Cl1—C2—C3—C4	−178.1 (3)	C8—C9—C10—C11	179.1 (3)
C2—C3—C4—C5	−0.2 (6)	C9—C10—C11—C12	1.4 (6)
C3—C4—C5—C6	0.3 (6)	C10—C11—C12—C13	−0.1 (6)
C4—C5—C6—C1	−0.7 (6)	C10—C11—C12—Br1	−179.0 (3)
C2—C1—C6—C5	1.0 (5)	C11—C12—C13—C14	−1.0 (5)
C7—C1—C6—C5	−179.9 (3)	Br1—C12—C13—C14	177.9 (2)
N2—N1—C7—C1	179.2 (2)	C12—C13—C14—C9	0.8 (5)
C2—C1—C7—N1	160.0 (3)	C10—C9—C14—C13	0.5 (5)
C6—C1—C7—N1	−19.1 (4)	C8—C9—C14—C13	179.7 (3)
N1—N2—C8—O1	1.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.12	2.918 (3)	154

Symmetry code: (i) *x*, −*y*+3/2, *z*+1/2.