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

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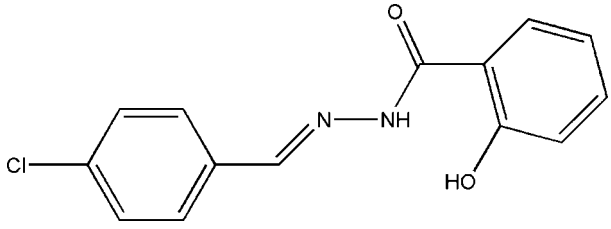
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.067; wR factor = 0.169; data-to-parameter ratio = 17.4.

The title molecule, $C_{14}H_{11}ClN_2O_2$, adopts a *trans* configuration with respect to the C=N double bond. An intramolecular N—H···O hydrogen bond contributes to molecular conformation and the two benzene rings form a dihedral angle of 17.9 (8)°. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into chains running along [10$\bar{1}$].

Related literature

For general background to hydrazones and Schiff bases and their potential pharmacological and antitumor properties, see: Karthikeyan *et al.* (2006); Khattab (2005); Kucukguzel *et al.* (2006); Okabe *et al.* (1993).



Experimental

Crystal data

$C_{14}H_{11}ClN_2O_2$
M_r = 274.70
Monoclinic, $P2_1/n$
a = 4.8557 (6) Å
b = 24.588 (3) Å
c = 11.0903 (13) Å
β = 99.710 (2)°
V = 1305.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 (2) K
0.10 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.977
11227 measured reflections
3126 independent reflections
2402 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.169
S = 1.12
3126 reflections
180 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H2···O1	0.80 (3)	2.01 (3)	2.624 (2)	134 (2)
O1—H1···O2^{i}	0.782 (18)	1.90 (2)	2.647 (2)	159 (3)

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

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*.

This work was supported by the Natural Science Foundation of Anhui Provincial University College (grant No. 2005 KJ137).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2476).

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supplementary materials

Acta Cryst. (2009). E**65**, o84 [**doi:10.1107/S160053680803972X**]

N'-(4-Chlorobenzylidene)-2-hydroxybenzohydrazide

S.-P. Zhang, R. Qiao and S.-C. Shao

Comment

Hydrazones and Schiff bases have attracted much attention for their excellent biological properties, especially for their potential pharmacological and antitumor properties (Kucukguzel *et al.*, 2006; Khattab, 2005; Karthikeyan *et al.*, 2006; Okabe *et al.*, 1993). We are interested in this fields. As a part of ongoing study, we report herein the crystal structure of the title compound, (I).

The molecular structure of (I) (Fig. 1) displays a *trans* configuration about the C=N bond. Intramolecular N—H···O hydrogen bond (Table 1) contributes to molecular conformation - the dihedral angle between the two benzene rings is 17.9 (8)°. In the crystal, the molecules are linked into chains by intermolecular O—H···O hydrongen bonds (Table 1).

Experimental

Equivalent amounts of 2-Hydroxybenzohydrazide and 3-chlorobenzohydrazide were reacted in ethanol (10 mL) for 1 h. After allowing the resulting solution to stand in air for 10 d colourless block-shaped crystals were formed on slow evaporation of the solvent.

Refinement

C-bound H atoms were placed in calculated positions (C—H = 0.93 Å) and constrained to ride on their parent atom, with $U_{iso}(H) = 1.2U_{eq}(C)$. The remaining H atoms were located in a difference map and refined isotropically.

Figures

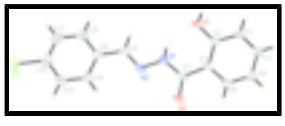

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N'-(4-Chlorobenzylidene)-2-hydroxybenzohydrazide

Crystal data

$C_{14}H_{11}ClN_2O_2$	F_{000} = 568
M_r = 274.70	D_x = 1.398 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 4.8557 (6) Å	Cell parameters from 986 reflections
b = 24.588 (3) Å	θ = 2.1–28.2°

c = 11.0903 (13) Å	μ = 0.29 mm^{-1}
β = 99.710 (2)º	T = 298 (2) K
V = 1305.1 (3) Å^3	Block, colourless
Z = 4	0.10 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3126 independent reflections
Radiation source: fine-focus sealed tube	2402 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 298(2) K	θ_{max} = 28.2º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→6
T_{min} = 0.972, T_{max} = 0.977	k = −32→31
11227 measured reflections	l = −14→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.067	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.169	$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.4971P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max}$ = 0.072
3126 reflections	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
180 parameters	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Cl1	−0.39445 (17)	1.00945 (3)	0.73436 (9)	0.0851 (3)
O1	0.9734 (4)	0.73796 (8)	0.50406 (15)	0.0610 (5)
N1	0.6996 (4)	0.76768 (8)	0.67797 (18)	0.0476 (5)
O2	0.8154 (4)	0.72610 (8)	0.85960 (14)	0.0618 (5)
N2	0.5245 (4)	0.80391 (8)	0.72149 (16)	0.0465 (5)
C7	0.8405 (4)	0.73021 (9)	0.75183 (18)	0.0442 (5)
C1	1.0293 (4)	0.69349 (9)	0.69718 (18)	0.0411 (5)
C8	0.3878 (5)	0.83421 (10)	0.6399 (2)	0.0507 (6)
H8	0.4112	0.8294	0.5591	0.061*
C3	1.2815 (5)	0.66229 (11)	0.5401 (2)	0.0531 (6)
H3	1.3252	0.6657	0.4619	0.064*
C2	1.0942 (4)	0.69832 (9)	0.57896 (18)	0.0423 (5)
C4	1.4019 (5)	0.62186 (11)	0.6157 (2)	0.0588 (6)
H4	1.5299	0.5984	0.5892	0.071*
C9	0.1965 (5)	0.87608 (10)	0.6674 (2)	0.0485 (5)
C6	1.1533 (5)	0.65119 (11)	0.7705 (2)	0.0562 (6)
H6	1.1112	0.6471	0.8487	0.067*
C13	−0.0225 (6)	0.93008 (11)	0.8045 (3)	0.0648 (7)
H13	−0.0453	0.9389	0.8838	0.078*
C14	0.1588 (6)	0.88896 (11)	0.7845 (2)	0.0571 (6)
H14	0.2561	0.8698	0.8506	0.069*
C12	−0.1684 (5)	0.95778 (10)	0.7069 (3)	0.0579 (6)
C5	1.3350 (6)	0.61556 (12)	0.7309 (2)	0.0623 (7)
H5	1.4127	0.5873	0.7812	0.075*
C10	0.0436 (6)	0.90483 (13)	0.5712 (3)	0.0713 (8)
H10	0.0643	0.8963	0.4915	0.086*
C11	−0.1375 (6)	0.94547 (13)	0.5903 (3)	0.0763 (9)
H11	−0.2377	0.9644	0.5245	0.092*
H1	1.053 (6)	0.7435 (12)	0.449 (2)	0.081 (10)*
H2	0.708 (5)	0.7692 (10)	0.607 (2)	0.051 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0716 (5)	0.0602 (5)	0.1249 (8)	0.0104 (3)	0.0203 (5)	0.0032 (4)
O1	0.0751 (11)	0.0777 (13)	0.0384 (9)	0.0191 (9)	0.0334 (8)	0.0132 (8)
N1	0.0595 (11)	0.0569 (12)	0.0316 (9)	0.0026 (9)	0.0223 (8)	−0.0021 (8)
O2	0.0829 (12)	0.0735 (12)	0.0359 (8)	0.0106 (9)	0.0301 (8)	0.0019 (8)
N2	0.0528 (10)	0.0519 (11)	0.0384 (10)	−0.0043 (8)	0.0186 (8)	−0.0053 (8)
C7	0.0513 (12)	0.0507 (13)	0.0346 (10)	−0.0096 (10)	0.0191 (9)	−0.0043 (9)
C1	0.0452 (11)	0.0483 (12)	0.0321 (10)	−0.0081 (9)	0.0136 (8)	−0.0037 (9)
C8	0.0585 (13)	0.0622 (15)	0.0342 (11)	−0.0036 (11)	0.0154 (10)	−0.0046 (10)
C3	0.0599 (13)	0.0668 (16)	0.0365 (11)	0.0045 (11)	0.0192 (10)	−0.0054 (11)
C2	0.0459 (11)	0.0513 (13)	0.0320 (10)	−0.0042 (9)	0.0133 (8)	−0.0009 (9)

C4	0.0632 (15)	0.0669 (16)	0.0471 (13)	0.0129 (12)	0.0117 (11)	−0.0114 (12)
C9	0.0514 (12)	0.0545 (14)	0.0401 (11)	−0.0073 (10)	0.0094 (9)	−0.0007 (10)
C6	0.0744 (16)	0.0621 (15)	0.0352 (11)	0.0040 (12)	0.0182 (11)	0.0028 (11)
C13	0.0829 (18)	0.0613 (16)	0.0554 (15)	0.0062 (14)	0.0266 (13)	0.0019 (13)
C14	0.0732 (16)	0.0579 (15)	0.0432 (13)	0.0118 (12)	0.0182 (11)	0.0090 (11)
C12	0.0519 (13)	0.0492 (14)	0.0732 (17)	−0.0039 (11)	0.0120 (12)	0.0066 (12)
C5	0.0808 (18)	0.0614 (16)	0.0441 (13)	0.0150 (13)	0.0084 (12)	0.0032 (12)
C10	0.0768 (18)	0.090 (2)	0.0453 (14)	0.0106 (16)	0.0059 (12)	0.0040 (14)
C11	0.0708 (18)	0.090 (2)	0.0633 (18)	0.0143 (16)	−0.0019 (14)	0.0168 (16)

Geometric parameters (Å, °)

Cl1—C12	1.739 (3)	C4—C5	1.379 (3)
O1—C2	1.349 (3)	C4—H4	0.9300
O1—H1	0.782 (18)	C9—C14	1.379 (3)
N1—C7	1.341 (3)	C9—C10	1.386 (4)
N1—N2	1.374 (3)	C6—C5	1.367 (3)
N1—H2	0.80 (3)	C6—H6	0.9300
O2—C7	1.226 (2)	C13—C12	1.371 (4)
N2—C8	1.269 (3)	C13—C14	1.383 (4)
C7—C1	1.487 (3)	C13—H13	0.9300
C1—C6	1.393 (3)	C14—H14	0.9300
C1—C2	1.404 (3)	C12—C11	1.360 (4)
C8—C9	1.453 (3)	C5—H5	0.9300
C8—H8	0.9300	C10—C11	1.371 (4)
C3—C4	1.367 (3)	C10—H10	0.9300
C3—C2	1.389 (3)	C11—H11	0.9300
C3—H3	0.9300		
C2—O1—H1	112 (2)	C14—C9—C8	123.4 (2)
C7—N1—N2	120.86 (18)	C10—C9—C8	118.6 (2)
C7—N1—H2	122.0 (18)	C5—C6—C1	122.0 (2)
N2—N1—H2	117.1 (18)	C5—C6—H6	119.0
C8—N2—N1	114.23 (18)	C1—C6—H6	119.0
O2—C7—N1	121.9 (2)	C12—C13—C14	119.7 (2)
O2—C7—C1	121.1 (2)	C12—C13—H13	120.2
N1—C7—C1	117.02 (17)	C14—C13—H13	120.2
C6—C1—C2	117.7 (2)	C9—C14—C13	120.5 (2)
C6—C1—C7	116.82 (18)	C9—C14—H14	119.7
C2—C1—C7	125.5 (2)	C13—C14—H14	119.7
N2—C8—C9	122.9 (2)	C11—C12—C13	121.0 (3)
N2—C8—H8	118.6	C11—C12—Cl1	120.2 (2)
C9—C8—H8	118.6	C13—C12—Cl1	118.8 (2)
C4—C3—C2	120.5 (2)	C6—C5—C4	119.4 (2)
C4—C3—H3	119.7	C6—C5—H5	120.3
C2—C3—H3	119.7	C4—C5—H5	120.3
O1—C2—C3	120.60 (18)	C11—C10—C9	121.8 (3)
O1—C2—C1	119.55 (19)	C11—C10—H10	119.1
C3—C2—C1	119.9 (2)	C9—C10—H10	119.1
C3—C4—C5	120.4 (2)	C12—C11—C10	119.1 (3)

C3—C4—H4	119.8	C12—C11—H11	120.5
C5—C4—H4	119.8	C10—C11—H11	120.5
C14—C9—C10	117.9 (2)		
C7—N1—N2—C8	−174.7 (2)	N2—C8—C9—C10	−176.0 (2)
N2—N1—C7—O2	1.3 (3)	C2—C1—C6—C5	0.7 (4)
N2—N1—C7—C1	−178.79 (18)	C7—C1—C6—C5	−178.7 (2)
O2—C7—C1—C6	6.2 (3)	C10—C9—C14—C13	−1.2 (4)
N1—C7—C1—C6	−173.7 (2)	C8—C9—C14—C13	178.6 (2)
O2—C7—C1—C2	−173.2 (2)	C12—C13—C14—C9	0.8 (4)
N1—C7—C1—C2	6.9 (3)	C14—C13—C12—C11	−0.1 (4)
N1—N2—C8—C9	−178.5 (2)	C14—C13—C12—Cl1	−179.8 (2)
C4—C3—C2—O1	−179.4 (2)	C1—C6—C5—C4	1.0 (4)
C4—C3—C2—C1	0.5 (4)	C3—C4—C5—C6	−2.0 (4)
C6—C1—C2—O1	178.4 (2)	C14—C9—C10—C11	0.9 (4)
C7—C1—C2—O1	−2.2 (3)	C8—C9—C10—C11	−178.9 (3)
C6—C1—C2—C3	−1.5 (3)	C13—C12—C11—C10	−0.2 (4)
C7—C1—C2—C3	177.9 (2)	Cl1—C12—C11—C10	179.5 (2)
C2—C3—C4—C5	1.3 (4)	C9—C10—C11—C12	−0.2 (5)
N2—C8—C9—C14	4.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2···O1	0.80 (3)	2.01 (3)	2.624 (2)	134 (2)
O1—H1···O2^{i}	0.782 (18)	1.90 (2)	2.647 (2)	159 (3)

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

Fig. 1