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N′-(2,4-Dichlorobenzylidene)-4-hydroxybenzohydrazide

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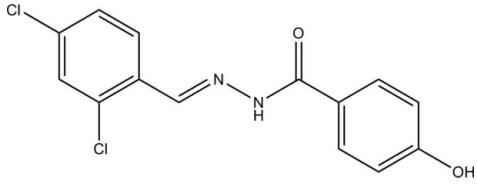
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.114; data-to-parameter ratio = 15.3.

The title hydrazone compound, $C_{14}H_{10}Cl_2N_2O_2$, was synthesized by the reaction of 2,4-dichlorobenzaldehyde and 4-hydroxybenzohydrazide. The molecule adopts an *E* geometry with respect to the azomethine group and the dihedral angle between the aromatic rings is 7.0 (2)°. In the crystal, molecules are linked through intermolecular N—H···Cl and O—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For the structures and properties of hydrazones, see: Carvalho *et al.* (2010); Liu (2010); Fun *et al.* (2008); Wang *et al.* (2010); Singh *et al.* (2009); Zhu *et al.* (2009); Vijayakumar *et al.* (2009); Tameem *et al.* (2010).



Experimental

Crystal data

$C_{14}H_{10}Cl_2N_2O_2$
M_r = 309.14
Monoclinic, $P2_1/c$
a = 7.6687 (11) Å
b = 11.9591 (17) Å
c = 15.043 (2) Å
β = 103.200 (2)°
V = 1343.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 298 K
0.17 × 0.13 × 0.13 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.922, T_{max} = 0.940
6784 measured reflections
2838 independent reflections
2385 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.05
2838 reflections
185 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Cl2^{i}	0.89 (1)	2.85 (1)	3.7228 (16)	167 (2)
O2—H2A···O1^{ii}	0.82	1.97	2.7624 (19)	162

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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 Yichun University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5726).

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supplementary materials

Acta Cryst. (2010). E**66**, o3143 [**doi:10.1107/S1600536810045502**]

N'-(2,4-Dichlorobenzylidene)-4-hydroxybenzohydrazide

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Comment

The hydrazone compounds bearing –CH=N—NH—C(O)- groups have been received much attention for their structures (Carvalho *et al.*, 2010; Liu, 2010; Fun *et al.*, 2008; Wang *et al.*, 2010) and properties (Singh *et al.*, 2009; Zhu *et al.*, 2009; Vijayakumar *et al.*, 2009; Tameem *et al.*, 2010). In this paper, the title new hydrazone compound is reported.

The molecular structure of the title compound is shown in Fig. 1. The molecule adopts an *E* geometry with respect to the azomethine group. The dihedral angle between the two aromatic rings C1—C6 and C9—C14 is 7.0 (2)°. In the crystal structure, molecules are linked through intermolecular N–H···Cl and O–H···O hydrogen bonds to form a three-dimensional network (Table 1, Fig. 2).

Experimental

Equimolar quantities (0.1 mmol each) of 2,4-dichlorobenzaldehyde and 4-hydroxybenzohydrazide were mixed and stirred in methanol for 30 min at reflux. After keeping the filtrate in air for a few days, colorless blocks of the title compound were formed.

Refinement

H2 attached to N2 was located from a difference Fourier map, and refined with N–H distance restrained to 0.90 (1) Å, and with U_{iso} restrained to 0.08 Å^2. The remaining H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å, O—H distance of 0.85 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Figures

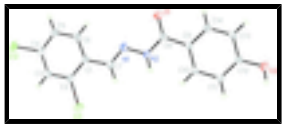

Fig. 1. Molecular structure of the title compound, with 30% ellipsoids.

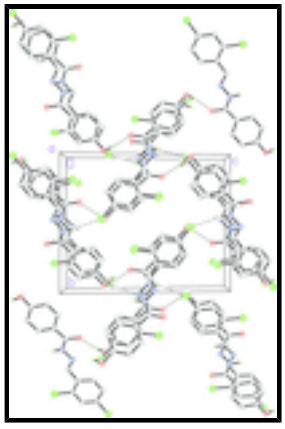

Fig. 2. The molecular packing of the title compound, viewed along the *a* axis. Hydrogen bonds are drawn as thin dashed lines.

N'-(2,4-Dichlorobenzylidene)-4-hydroxybenzohydrazide

Crystal data

$C_{14}H_{10}Cl_2N_2O_2$	$F(000) = 632$
$M_r = 309.14$	$D_x = 1.529$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3439 reflections
$a = 7.6687$ (11) Å	$\theta = 2.2$–$28.1°$
$b = 11.9591$ (17) Å	$\mu = 0.49$ mm^{-1}
$c = 15.043$ (2) Å	$T = 298$ K
$\beta = 103.200$ (2)°	Block, colorless
$V = 1343.2$ (3) Å^3	0.17 × 0.13 × 0.13 mm
$Z = 4$	

Data collection

Bruker SMART CCD diffractometer	2838 independent reflections
Radiation source: fine-focus sealed tube	2385 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.019$
ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.922$, $T_{max} = 0.940$	$k = -7 \rightarrow 15$
6784 measured reflections	$l = -19 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.114$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.4165P]$ where $P = (F_o^2 + 2F_c^2)/3$
2838 reflections	$(\Delta/\sigma)_{max} < 0.001$
185 parameters	$\Delta\rho_{max} = 0.37$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.58$ 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}
Cl1	1.05089 (9)	0.19236 (5)	0.07396 (3)	0.0590 (2)
Cl2	0.99147 (8)	0.02938 (5)	−0.26115 (4)	0.05604 (19)
N1	0.7367 (2)	0.47578 (12)	−0.05039 (10)	0.0350 (3)
N2	0.7130 (2)	0.55434 (12)	0.01223 (10)	0.0363 (3)
O1	0.5166 (2)	0.65200 (12)	−0.09421 (8)	0.0476 (4)
O2	0.5103 (2)	0.96168 (11)	0.24525 (9)	0.0472 (4)
H2A	0.5329	0.9360	0.2971	0.071*
C1	0.8721 (2)	0.30387 (14)	−0.07778 (12)	0.0322 (4)
C2	0.9708 (2)	0.20915 (15)	−0.04294 (12)	0.0360 (4)
C3	1.0075 (2)	0.12484 (15)	−0.09862 (12)	0.0388 (4)
H3	1.0745	0.0628	−0.0741	0.047*
C4	0.9423 (2)	0.13500 (15)	−0.19144 (12)	0.0372 (4)
C5	0.8419 (2)	0.22625 (15)	−0.22950 (12)	0.0385 (4)
H5	0.7984	0.2313	−0.2924	0.046*
C6	0.8074 (2)	0.30948 (15)	−0.17268 (12)	0.0351 (4)
H6	0.7395	0.3709	−0.1979	0.042*
C7	0.8350 (2)	0.39312 (15)	−0.01809 (12)	0.0365 (4)
H7	0.8840	0.3892	0.0444	0.044*
C8	0.5992 (2)	0.64163 (14)	−0.01442 (11)	0.0325 (4)
C9	0.5824 (2)	0.72236 (13)	0.05731 (11)	0.0307 (4)
C10	0.6378 (2)	0.70117 (15)	0.15075 (12)	0.0358 (4)
H10	0.6907	0.6329	0.1704	0.043*
C11	0.6154 (2)	0.77948 (15)	0.21432 (11)	0.0375 (4)
H11	0.6530	0.7637	0.2763	0.045*
C12	0.5367 (2)	0.88225 (14)	0.18611 (11)	0.0338 (4)

C13	0.4802 (3)	0.90445 (15)	0.09322 (12)	0.0391 (4)
H13	0.4276	0.9729	0.0736	0.047*
C14	0.5020 (3)	0.82533 (14)	0.03025 (11)	0.0370 (4)
H14	0.4623	0.8408	−0.0317	0.044*
H2	0.767 (3)	0.542 (2)	0.0707 (8)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0820 (4)	0.0559 (3)	0.0333 (3)	0.0123 (3)	0.0010 (2)	−0.0002 (2)
Cl2	0.0620 (3)	0.0532 (3)	0.0521 (3)	0.0072 (2)	0.0113 (2)	−0.0228 (2)
N1	0.0433 (8)	0.0303 (7)	0.0336 (7)	−0.0054 (6)	0.0135 (6)	−0.0062 (6)
N2	0.0461 (8)	0.0315 (7)	0.0307 (7)	0.0008 (6)	0.0074 (6)	−0.0064 (6)
O1	0.0696 (10)	0.0455 (8)	0.0266 (6)	0.0091 (7)	0.0087 (6)	−0.0004 (5)
O2	0.0715 (9)	0.0374 (7)	0.0341 (7)	0.0030 (6)	0.0149 (7)	−0.0066 (5)
C1	0.0344 (9)	0.0301 (8)	0.0339 (8)	−0.0059 (6)	0.0117 (7)	−0.0039 (7)
C2	0.0391 (9)	0.0356 (9)	0.0327 (8)	−0.0034 (7)	0.0071 (7)	−0.0019 (7)
C3	0.0398 (10)	0.0332 (9)	0.0426 (10)	0.0007 (7)	0.0077 (8)	−0.0033 (7)
C4	0.0367 (9)	0.0364 (9)	0.0406 (9)	−0.0051 (7)	0.0132 (7)	−0.0114 (7)
C5	0.0429 (10)	0.0425 (10)	0.0308 (8)	−0.0025 (8)	0.0098 (7)	−0.0034 (7)
C6	0.0377 (9)	0.0326 (9)	0.0360 (9)	−0.0027 (7)	0.0106 (7)	0.0006 (7)
C7	0.0433 (10)	0.0348 (9)	0.0321 (8)	−0.0041 (7)	0.0097 (7)	−0.0045 (7)
C8	0.0410 (9)	0.0302 (8)	0.0279 (8)	−0.0062 (7)	0.0111 (7)	0.0000 (6)
C9	0.0356 (9)	0.0285 (8)	0.0291 (8)	−0.0048 (6)	0.0098 (6)	−0.0003 (6)
C10	0.0418 (10)	0.0357 (9)	0.0299 (8)	0.0070 (7)	0.0082 (7)	0.0037 (7)
C11	0.0443 (10)	0.0422 (10)	0.0251 (8)	0.0050 (8)	0.0060 (7)	0.0015 (7)
C12	0.0416 (9)	0.0304 (8)	0.0314 (8)	−0.0062 (7)	0.0124 (7)	−0.0032 (7)
C13	0.0576 (11)	0.0261 (8)	0.0342 (9)	0.0001 (8)	0.0117 (8)	0.0045 (7)
C14	0.0528 (11)	0.0319 (9)	0.0259 (8)	−0.0026 (7)	0.0082 (7)	0.0037 (6)

Geometric parameters (Å, °)

Cl1—C2	1.7369 (18)	C5—C6	1.377 (2)
Cl2—C4	1.7372 (18)	C5—H5	0.9300
N1—C7	1.270 (2)	C6—H6	0.9300
N1—N2	1.372 (2)	C7—H7	0.9300
N2—C8	1.361 (2)	C8—C9	1.475 (2)
N2—H2	0.894 (10)	C9—C10	1.396 (2)
O1—C8	1.229 (2)	C9—C14	1.396 (2)
O2—C12	1.348 (2)	C10—C11	1.377 (2)
O2—H2A	0.8200	C10—H10	0.9300
C1—C2	1.396 (2)	C11—C12	1.392 (2)
C1—C6	1.402 (2)	C11—H11	0.9300
C1—C7	1.464 (2)	C12—C13	1.391 (2)
C2—C3	1.380 (2)	C13—C14	1.376 (2)
C3—C4	1.377 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.382 (3)		

C7—N1—N2	115.49 (14)	N1—C7—H7	119.5
C8—N2—N1	119.98 (14)	C1—C7—H7	119.5
C8—N2—H2	122.6 (18)	O1—C8—N2	121.20 (16)
N1—N2—H2	117.1 (18)	O1—C8—C9	122.47 (16)
C12—O2—H2A	109.5	N2—C8—C9	116.33 (14)
C2—C1—C6	117.17 (16)	C10—C9—C14	117.80 (15)
C2—C1—C7	121.73 (15)	C10—C9—C8	124.10 (15)
C6—C1—C7	121.09 (16)	C14—C9—C8	118.08 (14)
C3—C2—C1	122.21 (16)	C11—C10—C9	121.24 (16)
C3—C2—Cl1	117.13 (14)	C11—C10—H10	119.4
C1—C2—Cl1	120.66 (14)	C9—C10—H10	119.4
C4—C3—C2	118.28 (17)	C10—C11—C12	120.19 (15)
C4—C3—H3	120.9	C10—C11—H11	119.9
C2—C3—H3	120.9	C12—C11—H11	119.9
C3—C4—C5	121.92 (16)	O2—C12—C13	117.99 (16)
C3—C4—Cl2	117.99 (14)	O2—C12—C11	122.74 (15)
C5—C4—Cl2	120.08 (14)	C13—C12—C11	119.26 (16)
C6—C5—C4	118.79 (16)	C14—C13—C12	120.10 (16)
C6—C5—H5	120.6	C14—C13—H13	120.0
C4—C5—H5	120.6	C12—C13—H13	120.0
C5—C6—C1	121.61 (17)	C13—C14—C9	121.41 (15)
C5—C6—H6	119.2	C13—C14—H14	119.3
C1—C6—H6	119.2	C9—C14—H14	119.3
N1—C7—C1	120.95 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cl2^{i}	0.89 (1)	2.85 (1)	3.7228 (16)	167 (2)
O2—H2A···O1^{ii}	0.82	1.97	2.7624 (19)	162

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

Fig. 1

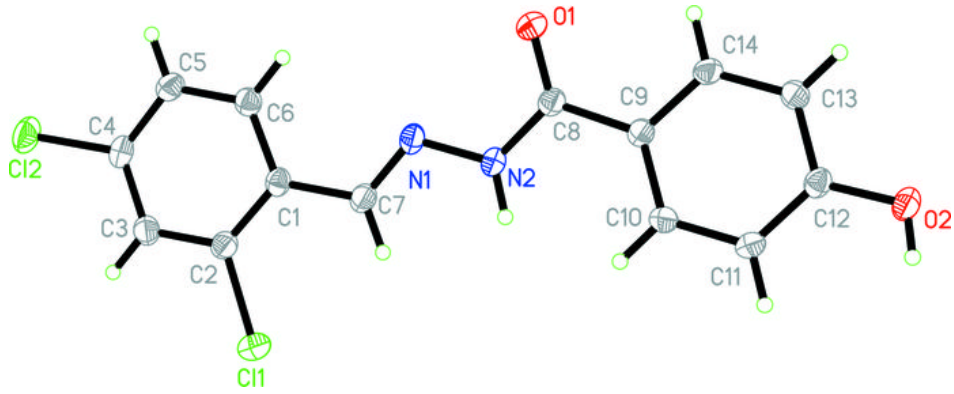

Fig. 2