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N′-(2,4-Dichlorobenzylidene)-2-hydroxy-3-methylbenzohydrazide

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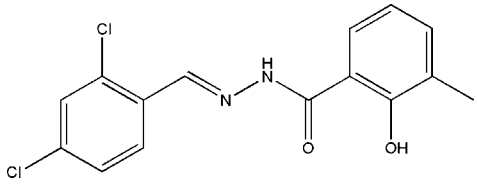
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.130; data-to-parameter ratio = 16.5.

In the title compound, $C_{15}H_{12}Cl_2N_2O_2$, the dihedral angle between the two benzene rings is 6.3 (2)°. The molecule adopts an *E* configuration with respect to the C=N bond. An intramolecular O—H···O hydrogen bond is observed. In the crystal structure, the molecules are linked through intermolecular N—H···O and C—H···O hydrogen bonds to form chains running along [101].

Related literature

For the biological properties of hydrazone compounds, see: Patil *et al.* (2010); Cukurovali *et al.* (2006). For related structures, see: Mohd Lair *et al.* (2009); Lin & Sang (2009); Suleiman Gwaram *et al.* (2010); Li & Ban (2009); Lo & Ng (2009); Ning & Xu (2009); Zhu *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{12}Cl_2N_2O_2$
M_r = 323.17
Monoclinic, $P2_1/n$
a = 7.137 (1) Å
b = 28.146 (2) Å
c = 8.130 (1) Å
β = 115.098 (1)°
V = 1478.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.917, T_{max} = 0.928
8543 measured reflections
3211 independent reflections
2439 reflections with $I > 2\sigma(I)$
R_{int} = 0.080

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 1.08
3211 reflections
195 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.96	2.6689 (19)	144
N2—H2···O2^{i}	0.90 (1)	2.13 (1)	2.9905 (19)	161 (2)
C7—H7···O2^{i}	0.93	2.45	3.264 (2)	146

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5073).

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supplementary materials

Acta Cryst. (2010). E**66**, o1048 [**doi:10.1107/S1600536810012419**]

N'-(2,4-Dichlorobenzylidene)-2-hydroxy-3-methylbenzohydrazide

Y.-Y. Han and Q.-R. Zhao

Comment

Hydrazone compounds have been widely investigated for their biological properties (Patil *et al.*, 2010; Cukurovali *et al.*, 2006). Furthermore, the crystal structures of the hydrazone compounds have also attracted much attention in recent years (Mohd Lair *et al.*, 2009; Lin & Sang, 2009; Suleiman Gwaram *et al.*, 2010). In the present work, the title new hydrazone compound is reported.

In the title molecule (Fig. 1), the dihedral angle between the two benzene rings is 6.3 (2)°. The molecule adopts an *E* configuration with respect to the C═N bond. There is an intramolecular O—H···O hydrogen bond (Table 1) in the molecule. All the bond lengths are within normal ranges (Allen *et al.*, 1987), and are comparable to those observed in related structures (Li & Ban, 2009; Lo & Ng, 2009; Ning & Xu, 2009; Zhu *et al.*, 2009).

In the crystal structure, molecules are linked through intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) to form chains running along the [101] (Fig. 2).

Experimental

A mixture of 2,4-dichlorobenzaldehyde (0.174 g, 1 mmol) and 2-hydroxy-3-methylbenzohydrazide (0.166 g, 1 mmol) in methanol (50 ml) was stirred at room temperature for 1 h. The mixture was filtered to remove impurities, and then left at room temperature. After a few days, single crystals of the title compound, suitable for X-ray diffraction, were formed.

Refinement

Atom H2 was located in a difference Fourier map and refined isotropically, with the N–H distance restrained to 0.90 (1) Å. Other H atoms were positioned geometrically and refined using the riding-model approximation, with C–H = 0.93 or 0.96 Å, O–H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C and O).

Figures

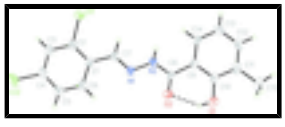

Fig. 1. The molecular structure of the title compound with atom labels and 30% probability displacement ellipsoids for non-H atoms. An intramolecular hydrogen bond is shown as a dashed line.

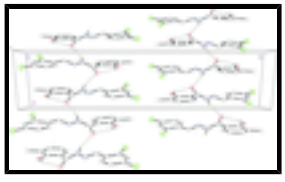

Fig. 2. The molecular packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

N'-(2,4-Dichlorobenzylidene)-2-hydroxy-3-methylbenzohydrazide

Crystal data

$C_{15}H_{12}Cl_2N_2O_2$	$F(000) = 664$
$M_r = 323.17$	$D_x = 1.451$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 3312 reflections
$a = 7.137$ (1) Å	$\theta = 2.7$–$26.7°$
$b = 28.146$ (2) Å	$\mu = 0.44$ mm^{-1}
$c = 8.130$ (1) Å	$T = 298$ K
$\beta = 115.098$ (1)°	Block, colourless
$V = 1478.9$ (3) Å^3	0.20 × 0.20 × 0.17 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3211 independent reflections
Radiation source: fine-focus sealed tube	2439 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.080$
ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -7 \rightarrow 9$
$T_{min} = 0.917$, $T_{max} = 0.928$	$k = -35 \rightarrow 29$
8543 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.130$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.0199P]$ where $P = (F_o^2 + 2F_c^2)/3$
3211 reflections	$(\Delta/\sigma)_{max} = 0.001$
195 parameters	$\Delta\rho_{max} = 0.20$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.34$ 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 $F^2 > \sigma(F^2)$ 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	0.08171 (10)	0.072034 (18)	0.35298 (7)	0.0675 (2)
Cl2	0.28271 (12)	0.02969 (2)	1.04608 (9)	0.0896 (3)
N1	0.2165 (2)	0.21754 (5)	0.51447 (19)	0.0456 (3)
N2	0.1732 (2)	0.24652 (5)	0.36590 (19)	0.0461 (4)
O1	0.2584 (2)	0.39071 (4)	0.38436 (19)	0.0607 (4)
H1	0.3024	0.3723	0.4706	0.091*
O2	0.3710 (2)	0.30580 (5)	0.54178 (17)	0.0612 (4)
C1	0.1840 (3)	0.13994 (6)	0.6149 (2)	0.0418 (4)
C2	0.1588 (3)	0.09173 (6)	0.5740 (2)	0.0456 (4)
C3	0.1937 (3)	0.05770 (7)	0.7075 (3)	0.0532 (5)
H3	0.1815	0.0255	0.6790	0.064*
C4	0.2466 (3)	0.07250 (7)	0.8822 (3)	0.0564 (5)
C5	0.2684 (3)	0.11985 (7)	0.9281 (3)	0.0571 (5)
H5	0.3025	0.1293	1.0470	0.068*
C6	0.2390 (3)	0.15312 (7)	0.7953 (2)	0.0507 (4)
H6	0.2562	0.1851	0.8263	0.061*
C7	0.1512 (3)	0.17531 (6)	0.4737 (2)	0.0447 (4)
H7	0.0814	0.1667	0.3522	0.054*
C8	0.2616 (3)	0.28989 (6)	0.3889 (2)	0.0440 (4)
C9	0.2212 (2)	0.31687 (6)	0.2219 (2)	0.0412 (4)
C10	0.2190 (3)	0.36649 (6)	0.2284 (2)	0.0458 (4)
C11	0.1737 (3)	0.39357 (7)	0.0725 (3)	0.0530 (5)
C12	0.1414 (3)	0.36996 (7)	−0.0855 (3)	0.0598 (5)
H12	0.1124	0.3876	−0.1902	0.072*
C13	0.1503 (3)	0.32088 (8)	−0.0946 (3)	0.0595 (5)
H13	0.1306	0.3060	−0.2028	0.071*
C14	0.1888 (3)	0.29443 (6)	0.0593 (2)	0.0487 (4)
H14	0.1932	0.2615	0.0544	0.058*
C15	0.1625 (4)	0.44689 (7)	0.0806 (4)	0.0719 (6)
H15A	0.1534	0.4603	−0.0312	0.108*
H15B	0.2845	0.4586	0.1797	0.108*
H15C	0.0425	0.4558	0.0983	0.108*
H2	0.077 (3)	0.2377 (8)	0.2565 (18)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cl1	0.1002 (5)	0.0532 (3)	0.0537 (3)	−0.0007 (3)	0.0369 (3)	−0.0057 (2)
Cl2	0.1246 (6)	0.0848 (5)	0.0756 (4)	0.0201 (4)	0.0580 (4)	0.0368 (3)
N1	0.0454 (8)	0.0445 (8)	0.0405 (7)	−0.0003 (6)	0.0122 (6)	0.0052 (6)
N2	0.0480 (9)	0.0424 (8)	0.0379 (7)	−0.0048 (6)	0.0083 (6)	0.0040 (6)
O1	0.0731 (10)	0.0438 (7)	0.0648 (9)	−0.0015 (6)	0.0290 (8)	−0.0077 (6)
O2	0.0725 (9)	0.0499 (8)	0.0422 (7)	−0.0099 (6)	0.0060 (7)	−0.0029 (6)
C1	0.0380 (9)	0.0467 (9)	0.0401 (9)	0.0001 (7)	0.0158 (7)	0.0036 (7)
C2	0.0472 (10)	0.0483 (10)	0.0472 (9)	0.0026 (7)	0.0256 (8)	0.0032 (7)
C3	0.0599 (12)	0.0453 (10)	0.0631 (12)	0.0056 (8)	0.0344 (10)	0.0104 (9)
C4	0.0585 (12)	0.0638 (13)	0.0545 (11)	0.0116 (9)	0.0312 (10)	0.0189 (9)
C5	0.0597 (12)	0.0695 (13)	0.0416 (9)	0.0060 (9)	0.0211 (9)	0.0056 (9)
C6	0.0516 (11)	0.0515 (11)	0.0451 (10)	−0.0009 (8)	0.0168 (9)	0.0011 (8)
C7	0.0437 (10)	0.0457 (10)	0.0409 (9)	−0.0019 (7)	0.0143 (8)	0.0015 (7)
C8	0.0411 (9)	0.0408 (9)	0.0436 (9)	0.0018 (7)	0.0118 (8)	0.0015 (7)
C9	0.0346 (8)	0.0412 (9)	0.0425 (9)	−0.0015 (6)	0.0111 (7)	0.0013 (7)
C10	0.0369 (9)	0.0419 (9)	0.0550 (11)	0.0006 (7)	0.0159 (8)	0.0032 (8)
C11	0.0398 (10)	0.0487 (10)	0.0666 (12)	0.0021 (7)	0.0188 (9)	0.0103 (9)
C12	0.0507 (12)	0.0641 (13)	0.0593 (12)	−0.0033 (9)	0.0181 (10)	0.0198 (10)
C13	0.0579 (12)	0.0746 (14)	0.0435 (10)	−0.0112 (10)	0.0191 (9)	−0.0023 (9)
C14	0.0467 (10)	0.0469 (10)	0.0489 (10)	−0.0041 (8)	0.0167 (8)	−0.0011 (8)
C15	0.0662 (14)	0.0479 (12)	0.0980 (17)	0.0069 (9)	0.0313 (13)	0.0206 (11)

Geometric parameters (Å, °)

Cl1—C2	1.7319 (18)	C5—H5	0.93
Cl2—C4	1.7323 (18)	C6—H6	0.93
N1—C7	1.268 (2)	C7—H7	0.93
N1—N2	1.3795 (19)	C8—C9	1.474 (2)
N2—C8	1.350 (2)	C9—C14	1.393 (2)
N2—H2	0.898 (10)	C9—C10	1.398 (2)
O1—C10	1.360 (2)	C10—C11	1.394 (3)
O1—H1	0.82	C11—C12	1.376 (3)
O2—C8	1.2376 (19)	C11—C15	1.506 (3)
C1—C2	1.391 (3)	C12—C13	1.386 (3)
C1—C6	1.398 (2)	C12—H12	0.93
C1—C7	1.461 (2)	C13—C14	1.379 (3)
C2—C3	1.389 (2)	C13—H13	0.93
C3—C4	1.371 (3)	C14—H14	0.93
C3—H3	0.93	C15—H15A	0.96
C4—C5	1.375 (3)	C15—H15B	0.96
C5—C6	1.376 (3)	C15—H15C	0.96
C7—N1—N2	113.86 (14)	O2—C8—C9	122.17 (16)
C8—N2—N1	119.69 (14)	N2—C8—C9	116.17 (14)
C8—N2—H2	120.2 (15)	C14—C9—C10	119.26 (16)
N1—N2—H2	119.8 (15)	C14—C9—C8	121.98 (16)
C10—O1—H1	109.5	C10—C9—C8	118.75 (15)
C2—C1—C6	117.41 (16)	O1—C10—C11	116.74 (17)
C2—C1—C7	121.03 (15)	O1—C10—C9	122.35 (16)
C6—C1—C7	121.56 (16)	C11—C10—C9	120.91 (17)

C3—C2—C1	121.58 (17)	C12—C11—C10	117.83 (17)
C3—C2—Cl1	117.58 (14)	C12—C11—C15	122.08 (19)
C1—C2—Cl1	120.84 (13)	C10—C11—C15	120.09 (19)
C4—C3—C2	118.68 (18)	C11—C12—C13	122.54 (18)
C4—C3—H3	120.7	C11—C12—H12	118.7
C2—C3—H3	120.7	C13—C12—H12	118.7
C3—C4—C5	121.67 (17)	C14—C13—C12	119.04 (19)
C3—C4—Cl2	118.12 (16)	C14—C13—H13	120.5
C5—C4—Cl2	120.20 (15)	C12—C13—H13	120.5
C4—C5—C6	119.02 (18)	C13—C14—C9	120.33 (18)
C4—C5—H5	120.5	C13—C14—H14	119.8
C6—C5—H5	120.5	C9—C14—H14	119.8
C5—C6—C1	121.58 (17)	C11—C15—H15A	109.5
C5—C6—H6	119.2	C11—C15—H15B	109.5
C1—C6—H6	119.2	H15A—C15—H15B	109.5
N1—C7—C1	120.98 (16)	C11—C15—H15C	109.5
N1—C7—H7	119.5	H15A—C15—H15C	109.5
C1—C7—H7	119.5	H15B—C15—H15C	109.5
O2—C8—N2	121.66 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.96	2.6689 (19)	144
N2—H2···O2^{i}	0.90 (1)	2.13 (1)	2.9905 (19)	161 (2)
C7—H7···O2^{i}	0.93	2.45	3.264 (2)	146

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

Fig. 1

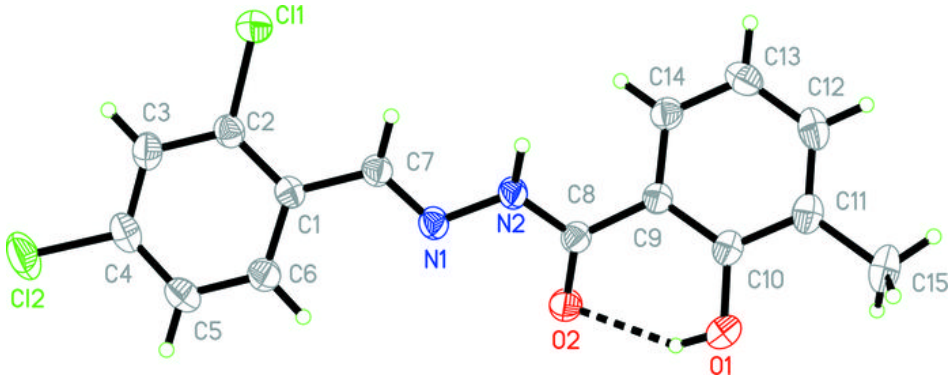
Cl1
C3
C2
C7
C1
N1
N2
C8
C14
C13
C12
C11
C9
C10
C15
Cl2
C4
C6
C5
O2
O1

Fig. 2