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N′-(2,4-Dichlorobenzylidene)benzohydrazide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.115
Data-to-parameter ratio = 18.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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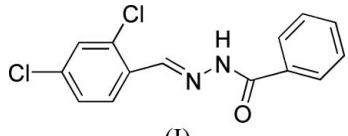
The asymmetric unit of the title compound, $C_{14}H_{10}Cl_2N_2O$, comprises two independent molecules, in which the dihedral angles between the terminal phenyl and substituted benzene rings are 21.28 (10) and 39.60 (12)°. N—H···O, C—H···O and C—H···Cl hydrogen bonds stabilize the conformations of the molecules and also stabilize the structure in the solid state.

Comment

Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). We report the synthesis and structure of the title compound, (I), as part of an investigation of its physical and chemical properties (Yu *et al.*, 2005; Deng *et al.*, 2005; Jing *et al.*, 2005*a*, 2005*b*).



(I)

The asymmetric unit comprises two independent molecules (Fig. 1 and Table 1). In molecule 1, the dihedral angle between the terminal phenyl (C2–C7) and benzene (C9–C14) rings is 21.28 (10)°, while in molecule 2 the corresponding angle is 39.60 (12). In the crystal structure, N—H···O, C—H···O and C—H···Cl hydrogen bonds stabilize the conformations of the molecules and also stabilize the structure in the solid state (Table 2 and Fig. 2).

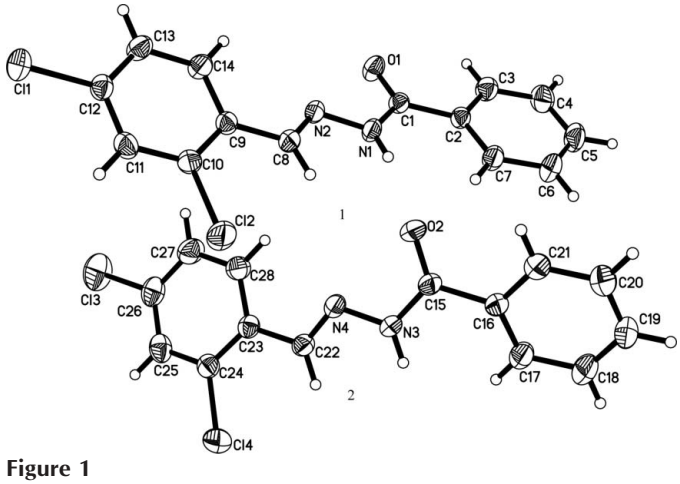


Figure 1
The structure of the asymmetric unit of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

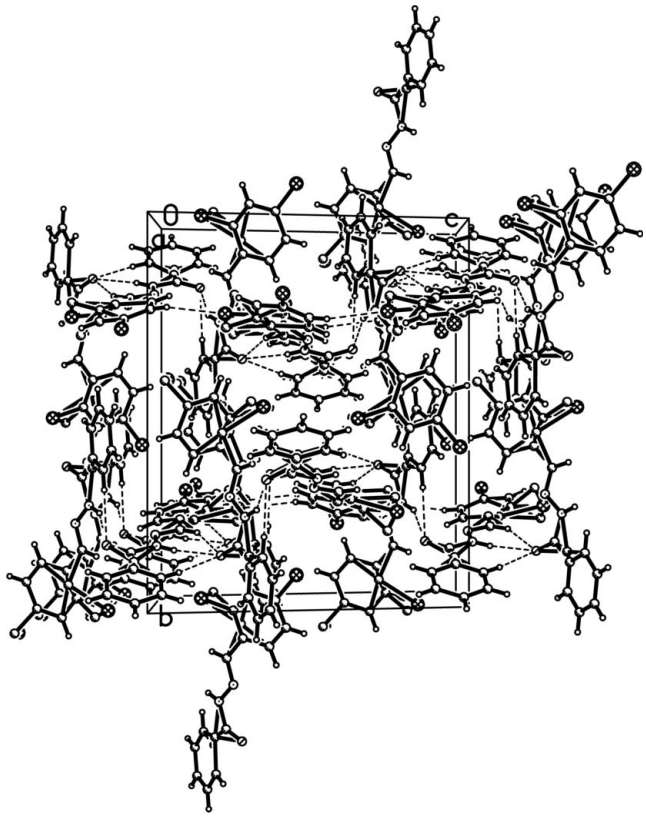


Figure 2
Packing view of (I), viewed down the *a* axis, showing intermolecular hydrogen bonds (dashed lines).

Experimental

An anhydrous ethanol solution of 2,4-dichlorobenzaldehyde (1.75 g, 10 mmol) was added to an anhydrous ethanol solution of benzohydrazide (1.36 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, whereupon a precipitate appeared. The product was isolated and recrystallized from ethanol, and then dried *in vacuo* to give pure (I) in 89% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{14}H_{10}Cl_2N_2O$
M_r = 293.14
Monoclinic, $P2_1/n$
a = 10.5668 (9) Å
b = 17.8266 (15) Å
c = 14.9814 (13) Å
β = 104.734 (1)° **[please check]**
V = 2729.3 (4) Å^3
Z = 8
D_x = 1.427 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3851 reflections
θ = 2.3–24.7°
μ = 0.47 mm^{-1}
T = 294 (2) K
Prism, colorless
0.46 × 0.34 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.822, T_{max} = 0.906
18247 measured reflections
6557 independent reflections
4110 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 28.1°
$h = -13 \rightarrow 13$
$k = -22 \rightarrow 23$
$l = -10 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.04
6557 reflections
352 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.8233P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0027 (4)

Table 1
Selected geometric parameters (°).

C1—N1—N2	119.27 (16)	C22—N4—N3	115.67 (16)
C8—N2—N1	115.09 (16)	O1—C1—N1	121.40 (17)
C15—N3—N4	117.99 (16)	O2—C15—N3	122.30 (18)
C1—N1—N2—C8	−179.31 (18)	N1—N2—C8—C9	176.43 (16)
C15—N3—N4—C22	177.48 (18)	N4—N3—C15—O2	8.9 (3)
N2—N1—C1—O1	−8.3 (3)	N4—N3—C15—C16	−169.43 (17)
N2—N1—C1—C2	170.93 (16)	N3—N4—C22—C23	−174.83 (17)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.88 (2)	2.20 (2)	3.007 (2)	153 (2)
N1—H1···O2	0.86 (2)	2.16 (2)	3.005 (2)	169 (2)
C7—H7···O2	0.93	2.45	3.372 (3)	172
C8—H8···O2	0.93	2.52	3.332 (2)	146
C11—H11···O1^{ii}	0.93	2.59	3.522 (3)	178
C13—H13···Cl2^{iii}	0.93	2.74	3.605 (2)	156
C17—H17···O1^{i}	0.93	2.50	3.416 (3)	170

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

H atoms attached to N atoms were located in a difference Fourier map and refined freely. Other H atoms were included in calculated positions (C—H = 0.93–0.96 Å) and refined using a riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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