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

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Key indicators

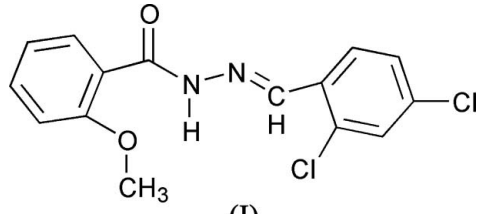
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.093
Data-to-parameter ratio = 13.3

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

In the crystal structure of the title compound, $C_{15}H_{12}Cl_2N_2O_2$, molecules are connected *via* weak intermolecular C—H···O hydrogen bonds, forming a two-dimensional network.

Comment

Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centers in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). Important to the understanding of the coordination potential of these ligands is a knowledge of ligand structure. Investigation of their crystal structures may provide useful information concerning their physical and chemical properties (Yu *et al.*, 2005; Deng *et al.*, 2005; Jing, Fan *et al.*, 2005*a*, 2005*b*; Jing, Wang *et al.*, 2005; Jing *et al.*, 2006; Guo *et al.*, 2006). In the present study, we report the synthesis and structure of the title compound, (I) (Fig. 1).



(I)

The Schiff base is approximately planar; the C8–C14 portion and the benzaldehyde group (C1–C7) are each planar, with r.m.s. deviations of 0.0148 (5) and 0.0017 (2) Å, respectively, and the dihedral angle between these planes is 4.23 (6)°. An intramolecular N—H···O hydrogen bond stabilizes the molecular conformation, while an intermolecular C—H···O hydrogen bond stabilizes the crystal structure (Table 2). The molecules associate in a two-dimensional pattern parallel to the (100) plane (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 2,4-dichlorobenzaldehyde (1.75 g, 10 mmol) was added to an anhydrous ethanol solution of (50 ml) 2-methoxybenzhydrazide (1.66 g, 10 mmol) and the mixture was stirred at 330 K for 8 h under N_2, whereupon a colorless solution was obtained. The solvent was removed and the residue recrystallized from *N*,*N*-dimethylformamide. The product was isolated and then dried *in vacuo* to give pure (I) in 73% yield. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution of (I).

Crystal data

$C_{15}H_{12}Cl_2N_2O_2$
M_r = 323.17
Triclinic, $P\overline{1}$
a = 7.389 (3) Å
b = 7.908 (3) Å
c = 13.575 (5) Å
α = 80.877 (5)°
β = 79.738 (5)°
γ = 70.002 (5)°
V = 729.3 (5) Å^3
Z = 2
D_x = 1.472 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 293 (2) K
Prism, colorless
0.22 × 0.16 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.901, T_{max} = 0.939
4004 measured reflections
2545 independent reflections
1968 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.03
2545 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.0881P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.208 (2)	C5—C6	1.396 (2)
N1—C7	1.274 (2)	C6—C7	1.458 (2)
N1—N2	1.3708 (19)	C8—C9	1.504 (2)
N2—C8	1.357 (2)	C9—C14	1.391 (2)
C1—C6	1.394 (2)	C9—C10	1.400 (2)
C7—N1—N2	115.05 (15)	O1—C8—N2	122.45 (16)
C8—N2—N1	121.24 (15)	O1—C8—C9	121.68 (16)
C1—C6—C7	122.09 (15)	N2—C8—C9	115.87 (15)
C5—C6—C7	121.22 (15)	C14—C9—C8	115.40 (16)
N1—C7—C6	121.32 (16)	C10—C9—C8	126.71 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2	0.86	1.96	2.627 (2)	134
C15—H15C···O1^{i}	0.96	2.52	3.359 (3)	146

Symmetry code: (i) $x, y+1, z$.

H atoms were included in calculated positions (C—H = 0.9–0.96 Å and N—H = 0.86 Å) and refined using a riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C,N) 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, 1997); software used to prepare material for publication: *SHELXTL*.

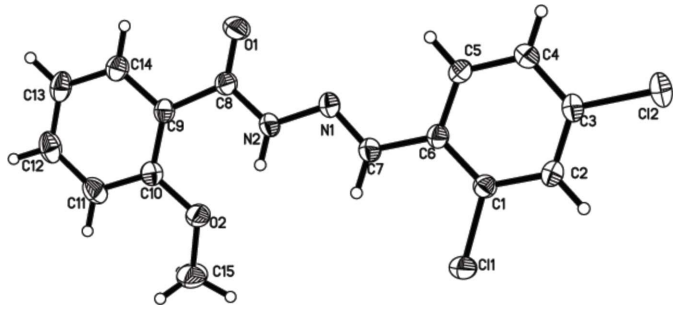


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

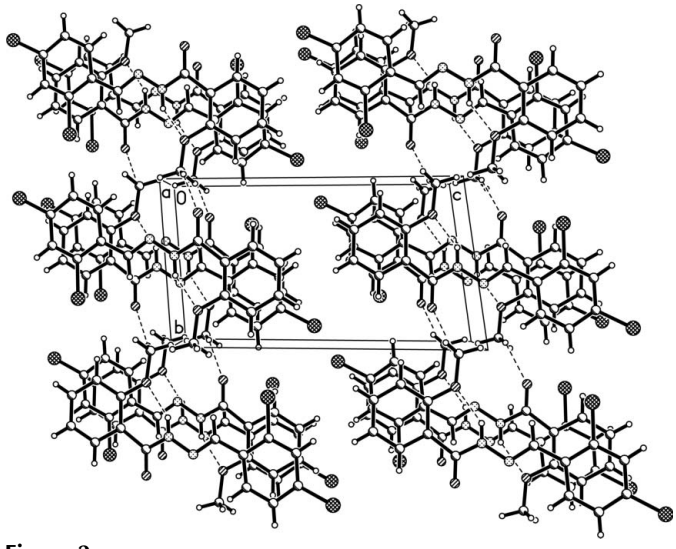


Figure 2
Packing view of (I) along the *a* axis, showing inter- and intermolecular hydrogen bonds as dashed lines.

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