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(*E*)-1-(2,4-Dichlorobenzylidene)thiosemicarbazide

Zuo-Liang Jing,* Qiao-Zhen Zhang, Ming Yu and Xin Chen

College of Sciences, Tianjin University of Science and Technology, Tianjin 300222, People's Republic of China

Correspondence e-mail: jzl74@tust.edu.cn

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Key indicators

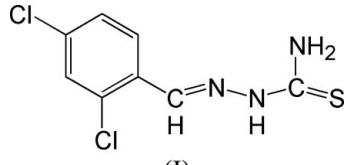
Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.072
Data-to-parameter ratio = 17.1

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, $C_8H_7Cl_2N_3S$, the Schiff base is approximately planar. An intramolecular N—H···S hydrogen bond stabilizes the molecular structure. The molecules are linked by N—H···S and N—H···Cl hydrogen bonds, forming a chain along the *c* axis.

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). A knowledge of the ligand structure is important in understanding the coordination potential of these ligands. Investigation of their crystal structures may provide useful information concerning their physical and chemical properties. In the present study, we report the synthesis and structure of the title compound, (I). In the molecular structure of (I) (Fig. 1), the expected geometric parameters are observed.



(I)

Intermolecular N—H···S and N—H···Cl hydrogen-bonding interactions stabilize the crystal structure (details are given in Table 1). Screw-related Schiff base molecules are linked *via* N—H···S and N—H···Cl hydrogen bonds involving the thiosemicarbazide and hydroxyl groups, forming zigzag chains along the *c* axis, as illustrated in Fig. 2.

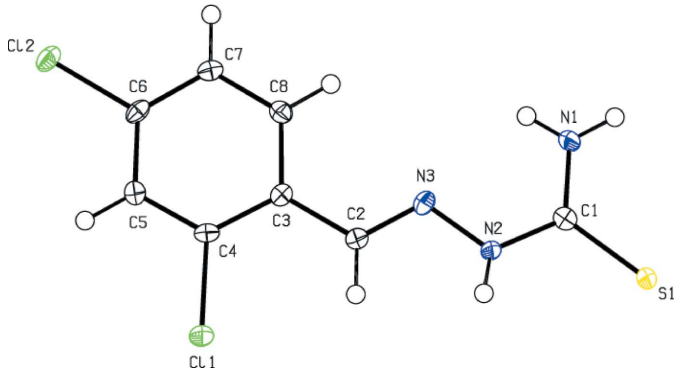


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

Experimental

An anhydrous ethanol solution (50 ml) of 2,4-dichlorobenzaldehyde (1.73 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of thiosemicarbazide (0.75 g, 10 mmol) and the mixture was stirred at 330 K for 8 h under N_2, whereupon a colourless solution appeared. The solvent was removed and the residue recrystallized from dimethylformamide. The product was isolated and then dried *in vacuo* to give pure (I) in 95% yield. Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution of (I).

Crystal data

$C_8H_7Cl_2N_3S$
M_r = 248.13
Triclinic, $P\overline{1}$
a = 7.8840 (12) Å
b = 8.1407 (13) Å
c = 8.3101 (14) Å
α = 100.603 (8)°
β = 101.290 (8)°
γ = 93.550 (9)°
V = 511.44 (14) Å^3
Z = 2
D_x = 1.611 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 113 (2) K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.844, T_{max} = 0.883
6307 measured reflections
2411 independent reflections
1860 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.072
S = 0.99
2411 reflections
141 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.058 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···S1^{i}	0.846 (19)	2.534 (19)	3.3685 (15)	169.0 (16)
N1—H3···Cl1^{ii}	0.826 (18)	2.955 (17)	3.5331 (15)	128.9 (15)
N2—H4···S1^{iii}	0.783 (17)	2.574 (17)	3.3372 (14)	165.1 (17)

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

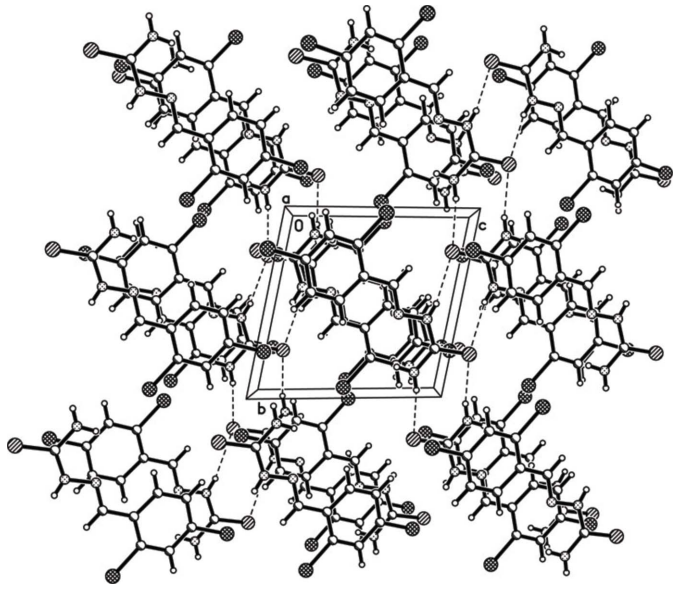


Figure 2
The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are indicated by dashed lines.

H atoms bonded to N atoms were found in a difference Fourier map and their positions were refined freely. The other H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.95 Å; U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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