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Key indicators

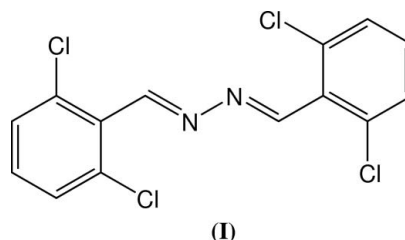
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.040
 wR factor = 0.105
Data-to-parameter ratio = 16.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N,N'*-Bis(2,6-dichlorobenzylidene)hydrazine

The title compound, $\text{C}_{14}\text{H}_8\text{Cl}_4\text{N}_2$, was synthesized by the reaction of 2,6-dichlorobenzaldehyde with hydrazine hydrate. The two benzene rings are nearly parallel, forming a dihedral angle of $2.9(4)^\circ$. A weak intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bond links the molecules into an infinite chain running along $[100]$.

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Comment

Recently, a number of azine compounds containing both a diimine linkage and an $\text{N}-\text{N}$ bond have been investigated in terms of their solid state structures and coordination chemistry (Xu *et al.*, 1997; Armstrong *et al.*, 1998; Kesslen *et al.*, 1999; Duan *et al.*, 2005; Kundu *et al.*, 2005; Zheng *et al.*, 2005*a,b*). We report here the crystal structure of the title compound, (I), where two 2,6-dichlorobenzylidene units are directly linked through the imine N atoms.



The title molecule crystallizes in an *E,E* configuration but is not centrosymmetric (Fig. 1). The molecule is not planar, the mean deviation being $0.1586(3)$ Å, while a planar molecule is observed for benzalazine (Burke-Laing & Laing, 1976). This configuration is different from that found in a number of analogous azine compounds in which there is a crystallographically imposed centre of symmetry at the mid-point of the $\text{N}-\text{N}$ bond (Liu *et al.*, 2004; Şengül *et al.*, 2004; Duan *et al.*, 2005; Zheng *et al.*, 2005*a,b*). The two benzene rings in (I) are nearly parallel, making a dihedral angle of $2.9(4)^\circ$. The $\text{N}-\text{N}$ bond length (Table 1) is slightly longer than that observed in related azine compounds (Liu *et al.*, 2004; Şengül *et al.*, 2004; Duan *et al.*, 2005; Xu *et al.*, 2005; Zheng *et al.*, 2005*a,b*). The $\text{C}7-\text{N}1-\text{N}2-\text{C}8$ torsion angle indicates that the $\text{C}=\text{N}-\text{N}=\text{C}$ linkage is not a planar system. The $\text{C}=\text{N}-\text{N}$ angles are significantly smaller than the ideal value of 120° expected for sp^2 -hybridized N atoms. This is probably a consequence of repulsion between the nitrogen lone pairs and the adjacent $\text{C}=\text{N}$ bonds. The four $\text{C}-\text{Cl}$ bond lengths are slightly different but are similar to those of $\text{C}sp^2-\text{Cl}$ bonds in related compounds (Jiang & Hu, 2004; Zheng *et al.*, 2005*a*).

In the crystal structure, a weak intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bond (Table 2 and Fig. 2) leads to an infinite chain

running along [100]. Furthermore, a weak Clⁱ⋯Clⁱⁱ contact is observed between chains [Clⁱ⋯Clⁱⁱ = 3.356 (3) Å; van der Waals radii for Cl = 1.75 Å; symmetry code: (ii) 1 - x, -y, -z].

Experimental

The title compound was synthesized by the reaction of 2,6-dichlorobenzaldehyde with hydrazine hydrate in refluxing ethanol (Liu *et al.*, 2004). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a tetrahydrofuran solution.

Crystal data

C ₁₄ H ₈ Cl ₄ N ₂	Z = 4
M _r = 346.02	D _x = 1.558 Mg m ⁻³
Monoclinic, P2 ₁ /n	Mo Kα radiation
a = 4.265 (3) Å	μ = 0.79 mm ⁻¹
b = 13.548 (9) Å	T = 294 (2) K
c = 25.593 (17) Å	Block, light yellow
β = 94.008 (12)°	0.20 × 0.10 × 0.06 mm
V = 1475.2 (17) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	8021 measured reflections
φ and ω scans	2999 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1718 reflections with I > 2σ(I)
T _{min} = 0.902, T _{max} = 0.954	R _{int} = 0.041
	θ _{max} = 26.3°

Refinement

Refinement on F ²	w = 1/[σ ² (F _o ²) + (0.0382P) ² + 0.7304P]
R[F ² > 2σ(F ²)] = 0.040	where P = (F _o ² + 2F _c ²)/3
wR(F ²) = 0.105	(Δ/σ) _{max} < 0.001
S = 0.99	Δρ _{max} = 0.28 e Å ⁻³
2999 reflections	Δρ _{min} = -0.34 e Å ⁻³
181 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

C1—C1	1.732 (3)	N1—C7	1.248 (3)
C12—C5	1.745 (3)	N1—N2	1.424 (3)
C13—C10	1.737 (3)	N2—C8	1.242 (3)
C14—C14	1.739 (3)		
C7—N1—N2	112.2 (2)	C8—N2—N1	112.7 (2)
C7—N1—N2—C8	-166.3 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C8—H8⋯N2 ⁱ	0.93	2.58	3.487 (3)	166

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

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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.

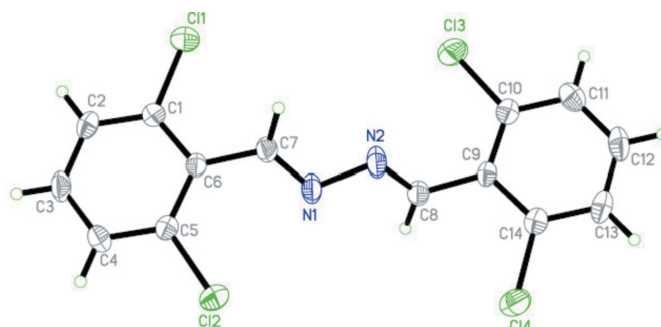


Figure 1

View of the molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

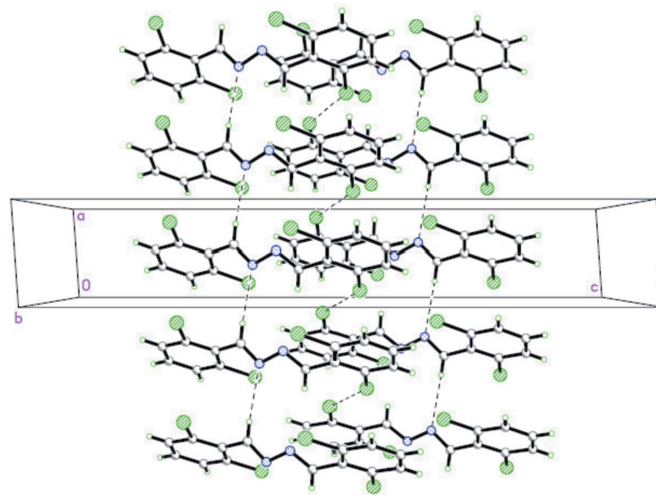


Figure 2

The packing of (I), viewed down the b axis, showing the intermolecular hydrogen-bonding extended network and Cl⋯Cl contacts (dashed lines).

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