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N-(2,4-Dichlorobenzylidene)-*N*′-phenylhydrazine

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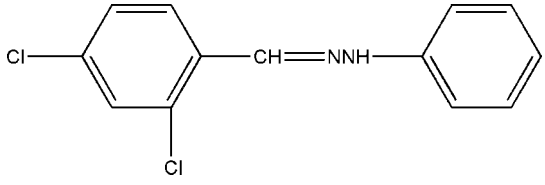
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.132; data-to-parameter ratio = 16.9.

The molecule of the title compound, $C_{13}H_{10}Cl_2N_2$, is nearly planar and adopts an E conformation about the carbon–nitrogen double bond. The dihedral angle between the two benzene rings is 6.70 (13)°. Molecules are interconnected through weak N—H$\cdots\pi$ interations.

Related literature

For related literature, see: Domino *et al.* (1984); Li *et al.* (1998); Özçelik *et al.* (2004).



Experimental

Crystal data

$C_{13}H_{10}Cl_2N_2$
M_r = 265.13
Orthorhombic, *Pbca*
a = 16.074 (3) Å
b = 8.0870 (16) Å
c = 19.333 (4) Å
V = 2513.1 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 298 (2) K
0.30 × 0.25 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.908, T_{max} = 0.908
15692 measured reflections
2599 independent reflections
2395 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.132
S = 1.22
2599 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*1 is the centroid of the benzene ring C8–C13.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$\cdots Cg1^{i}$	0.86	3.10	3.943 (2)	167

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN3063).

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supplementary materials

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N-(2,4-Dichlorobenzylidene)-*N*'-phenylhydrazine

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Comment

The chemistry of hydrazones has been widely investigated in recent years, owning to their coordinating capability, pharmacological activity, antibacterial properties and their use in analytical chemistry as highly selective extractants (Domino *et al.*, 1984; Li *et al.*, 1998).

The title molecule crystallizes in the E conformation, with an N2—N1—C7—C1 torsion angle of 179.6 (2)°. The N1—N2 and N1=C7 bond distances are comparable to those in the related hydrazones derivates (Özçelik *et al.* 2004). There is more pronounced asymmetry in the exocyclic angles at C1 and C8. The dihedral angles between the two benzene ring is 6.70 (13)°, the dichlorophenyl ring make dihedral angle with the central hydrazone bridge (N2/N1/C7) of 6.49 (11)°, while the central hydrazone bridge is co-planar. with the phenyl ring

The molecules are linked by N—H···π interaction (Table 1).

Experimental

Phenylhydrazine (1 mmol, 0.108 g) was dissolved in anhydrous methanol, H_2SO_4 (98% 0.5 ml) was added to this, the mixture was stirred for several minitutes at 351 K, 2,4-dichlorobenzyaldehyde (1 mmol 0.175 g) in methanol (8 ml) was added dropwise and the mixture was stirred at refluxing temperature for 2 h. The product was isolated and recrystallized in dichloromethane, brown single crystals of (I) was obtained after 5 d.

Refinement

All H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H=0.93Å and N—H= 0.86Å with U_{iso}(H)=1.2U_{eq}(C,*N*).

Figures

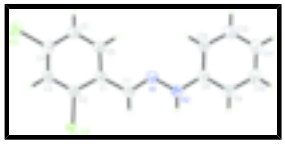

Fig. 1. Molecular view of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

N-(2,4-Dichlorobenzylidene)-*N*'-phenylhydrazine

Crystal data

$C_{13}H_{10}Cl_2N_2$	F_{000} = 1088
M_r = 265.13	D_x = 1.401 Mg m^{-3}

Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1225 reflections
a = 16.074 (3) Å	θ = 2.5–24.1º
b = 8.0870 (16) Å	μ = 0.49 mm^{-1}
c = 19.333 (4) Å	*T* = 298 (2) K
V = 2513.1 (9) $Å^3$	Block, brown
Z = 8	0.30 × 0.25 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2599 independent reflections
Radiation source: fine-focus sealed tube	2395 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 26.5º
ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→20
T_{min} = 0.908, T_{max} = 0.908	*k* = −10→8
15692 measured reflections	*l* = −22→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H-atom parameters constrained
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 1.2232P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.22	$(\Delta/\sigma)_{max} < 0.001$
2599 reflections	$\Delta\rho_{max}$ = 0.28 e $Å^{-3}$
154 parameters	$\Delta\rho_{min}$ = −0.26 e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Cl1	0.30414 (6)	0.64104 (12)	0.50050 (4)	0.0915 (3)	
Cl2	0.36390 (6)	0.12890 (10)	0.33193 (4)	0.0806 (3)	
N1	0.49038 (12)	0.4273 (2)	0.63809 (10)	0.0488 (5)	
N2	0.50608 (13)	0.5073 (3)	0.69797 (10)	0.0549 (5)	
H2	0.4763	0.5911	0.7096	0.066*	
C1	0.41639 (14)	0.4009 (3)	0.53262 (12)	0.0466 (5)	
C2	0.35838 (14)	0.4587 (3)	0.48464 (12)	0.0503 (6)	
C3	0.34205 (15)	0.3774 (3)	0.42305 (13)	0.0546 (6)	
H3	0.3028	0.4188	0.3922	0.066*	
C4	0.38476 (16)	0.2352 (3)	0.40837 (13)	0.0539 (6)	
C5	0.44459 (19)	0.1751 (3)	0.45313 (14)	0.0632 (7)	
H5	0.4746	0.0804	0.4421	0.076*	
C6	0.45912 (17)	0.2577 (3)	0.51431 (13)	0.0580 (6)	
H6	0.4990	0.2162	0.5445	0.070*	
C7	0.43389 (15)	0.4853 (3)	0.59798 (12)	0.0501 (6)	
H7	0.4044	0.5798	0.6103	0.060*	
C8	0.57047 (15)	0.4544 (3)	0.74095 (11)	0.0479 (5)	
C9	0.58364 (17)	0.5361 (3)	0.80344 (13)	0.0602 (7)	
H9	0.5495	0.6240	0.8160	0.072*	
C10	0.64752 (19)	0.4865 (4)	0.84683 (14)	0.0686 (8)	
H10	0.6561	0.5421	0.8883	0.082*	
C11	0.69857 (17)	0.3561 (4)	0.82948 (15)	0.0663 (8)	
H11	0.7414	0.3236	0.8588	0.080*	
C12	0.68496 (16)	0.2745 (4)	0.76772 (14)	0.0640 (7)	
H12	0.7189	0.1859	0.7557	0.077*	
C13	0.62166 (16)	0.3221 (3)	0.72330 (13)	0.0546 (6)	
H13	0.6134	0.2659	0.6819	0.066*	
CG1	0.6345	0.4049	0.7853	0.010*	0.00

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0915 (6)	0.1023 (7)	0.0807 (5)	0.0577 (5)	−0.0167 (4)	−0.0143 (4)
Cl2	0.0948 (6)	0.0796 (5)	0.0673 (5)	−0.0035 (4)	−0.0170 (4)	−0.0152 (4)
N1	0.0540 (11)	0.0473 (10)	0.0452 (11)	0.0003 (9)	0.0038 (9)	0.0036 (9)
N2	0.0637 (12)	0.0536 (11)	0.0473 (11)	0.0126 (10)	−0.0010 (9)	−0.0038 (9)
C1	0.0452 (12)	0.0473 (12)	0.0473 (13)	−0.0006 (10)	0.0037 (10)	0.0079 (10)
C2	0.0419 (12)	0.0555 (14)	0.0535 (14)	0.0061 (10)	0.0045 (10)	0.0046 (11)
C3	0.0421 (12)	0.0691 (16)	0.0528 (14)	0.0010 (12)	−0.0036 (11)	0.0080 (12)
C4	0.0589 (14)	0.0528 (14)	0.0500 (13)	−0.0094 (12)	−0.0002 (11)	0.0019 (11)
C5	0.0787 (18)	0.0467 (13)	0.0642 (16)	0.0103 (13)	−0.0102 (14)	−0.0012 (12)
C6	0.0686 (16)	0.0482 (13)	0.0573 (15)	0.0107 (12)	−0.0099 (12)	0.0056 (11)
C7	0.0514 (13)	0.0491 (13)	0.0497 (13)	0.0071 (11)	0.0061 (11)	0.0047 (10)
C8	0.0506 (13)	0.0491 (12)	0.0439 (12)	−0.0032 (11)	0.0055 (10)	0.0059 (10)

C9	0.0683 (16)	0.0602 (15)	0.0521 (14)	0.0004 (13)	0.0036 (12)	−0.0047 (12)
C10	0.0743 (18)	0.0794 (19)	0.0521 (15)	−0.0137 (16)	−0.0063 (14)	−0.0038 (14)
C11	0.0558 (15)	0.0811 (19)	0.0619 (17)	−0.0080 (14)	−0.0077 (13)	0.0158 (15)
C12	0.0591 (15)	0.0633 (16)	0.0697 (17)	0.0047 (13)	0.0031 (13)	0.0108 (14)
C13	0.0588 (15)	0.0555 (14)	0.0495 (13)	0.0025 (12)	0.0040 (11)	0.0000 (11)

Geometric parameters (Å, °)

Cl1—C2	1.741 (2)	C6—H6	0.9300
Cl2—C4	1.742 (3)	C7—H7	0.9300
N1—C7	1.283 (3)	C8—C13	1.392 (3)
N1—N2	1.350 (3)	C8—C9	1.393 (3)
N2—C8	1.395 (3)	C8—CG1	1.397 (2)
N2—H2	0.8600	C9—C10	1.385 (4)
C1—C6	1.392 (3)	C9—H9	0.9300
C1—C2	1.396 (3)	C10—C11	1.377 (4)
C1—C7	1.463 (3)	C10—H10	0.9300
C2—C3	1.385 (3)	C11—C12	1.382 (4)
C3—C4	1.369 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.386 (4)
C4—C5	1.382 (4)	C12—H12	0.9300
C5—C6	1.378 (4)	C13—H13	0.9300
C5—H5	0.9300		
C7—N1—N2	118.4 (2)	N1—C7—H7	120.4
N1—N2—C8	120.2 (2)	C1—C7—H7	120.4
N1—N2—H2	119.9	C13—C8—C9	119.2 (2)
C8—N2—H2	119.9	C13—C8—N2	121.9 (2)
C6—C1—C2	116.0 (2)	C9—C8—N2	118.9 (2)
C6—C1—C7	120.9 (2)	C13—C8—CG1	59.69 (14)
C2—C1—C7	123.1 (2)	C9—C8—CG1	59.47 (15)
C3—C2—C1	122.6 (2)	N2—C8—CG1	178.4 (2)
C3—C2—Cl1	117.29 (18)	C10—C9—C8	120.0 (3)
C1—C2—Cl1	120.08 (19)	C10—C9—H9	120.0
C4—C3—C2	118.8 (2)	C8—C9—H9	120.0
C4—C3—H3	120.6	C11—C10—C9	121.1 (3)
C2—C3—H3	120.6	C11—C10—H10	119.5
C3—C4—C5	121.0 (2)	C9—C10—H10	119.5
C3—C4—Cl2	119.6 (2)	C10—C11—C12	118.8 (3)
C5—C4—Cl2	119.4 (2)	C10—C11—H11	120.6
C6—C5—C4	119.0 (2)	C12—C11—H11	120.6
C6—C5—H5	120.5	C11—C12—C13	121.3 (3)
C4—C5—H5	120.5	C11—C12—H12	119.4
C5—C6—C1	122.5 (2)	C13—C12—H12	119.4
C5—C6—H6	118.7	C12—C13—C8	119.7 (2)
C1—C6—H6	118.7	C12—C13—H13	120.1
N1—C7—C1	119.2 (2)	C8—C13—H13	120.1

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cg1^{i}	0.86	3.10	3.943 (2)	167

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1