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N,*N*′-Bis(2,4-dichlorobenzylidene)-ethylenediamine

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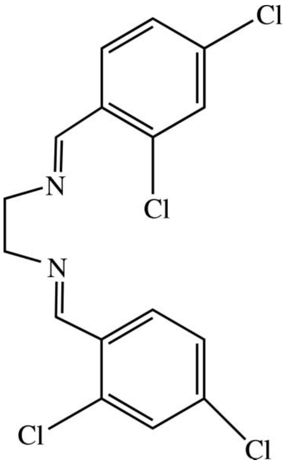
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.010 Å; R factor = 0.097; wR factor = 0.248; data-to-parameter ratio = 15.2.

The molecule of the title compound, $C_{16}H_{12}Cl_4N_2$, is located on a centre of inversion. The C—Cl bond in the *para* position is shorter than the C—Cl bond in the *ortho* position, at 1.705 (7) and 1.712 (6) Å, respectively.

Related literature

For related literature, see: Abbasi *et al.* (2007); Helldörfer *et al.* (2003); Khaniani *et al.* (2007); Richmond *et al.* (1988).



Experimental

Crystal data

$C_{16}H_{12}Cl_4N_2$
M_r = 374.08
Monoclinic, $P2_1/n$
a = 13.572 (2) Å
b = 4.4991 (7) Å
c = 14.623 (2) Å
β = 115.52 (2)°
V = 805.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 290 (2) K
0.18 × 0.10 × 0.08 mm

Data collection

STOE IPDS diffractometer
Absorption correction: numerical (*X-RED32*; Stoe & Cie, 1997)
T_{min} = 0.781, T_{max} = 0.837
5165 measured reflections
1525 independent reflections
845 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.097
$wR(F^2)$ = 0.248
S = 1.47
1525 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *IPDS Software* (Stoe & Cie, 1997); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2596).

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supplementary materials

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N,*N'*-Bis(2,4-dichlorobenzylidene)ethylenediamine

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Comment

In the current study the structure of the title compound, which can be potentially used as tetradentate ligand is investigated (Helldörfer *et al.*, 2003 & Richmond *et al.*, 1988). This structure with different chloro-substituted benzaldehyde derivative is an isomer of our previously reported structures (Abbasi *et al.*, 2007; Khaniani *et al.*, 2007). Solvatochromic phenomenon in the mixed-chelates metal complexes with similar structure has been investigated.

The moleculare structure of (I) and the atom-numbering scheme are shown in Fig. 1. The *para* chloro-substitution bond length, (Cl1–C6, 1.705 (7) Å) in (I) is significantly shorter than mean Cl–C bond distance 1.733 (4) Å and 1.732 (3) Å for the two isomers *N*,*N'*-Bis(2,*X*-dichlorobenzylidene)ethylenediamine for $X = 5$ and 3, respectively. This can be due to the conjugation between chloride electrons in *para* and benzyl ring.

The asymmetric unit contains one half-molecule in the centrosymmetric title compound with a centre of symmetry between the two central carbon atoms. Relatively weak intermolecular van der Waals interactions between the adjacent molecules are responsible to stabilize the crystal structure. Due to the center of symmetry in the middle of molecule, the two benzyl rings are located in two parallel planes with zero dihedral angle. Also, for the same reason the two carbon and two nitrogen atoms (N1–C8–C8–N1) are in a common plane with torsion angle of 180.0º. The structure of the title compound was corroborated by IR and ^{1}H NMR spectroscopy.

Experimental

The title compound was synthesized by the reaction of 2,3-dichlorobenzaldehyde (100 mmol) in absolute ethanol (30 ml) and ethylenediamine (50 mmol) followed by 24 h stirring. The colorless crystalline solid was obtained (17 mmol, 56%). The precipitates was filtered and washed with ether and hexane. Crystals suitable for crystallography were obtained by recrystallization from dichloromethane.

Refinement

All H atoms were geometrically positioned and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

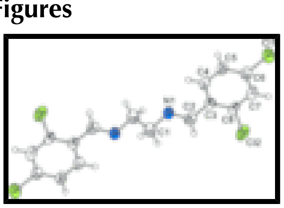
Fig. 1. Molecular structure of (I), with 50% probability displacement ellipsoids. H atoms are shown as circles of arbitrary radii.

N,*N*'-Bis(2,4-dichlorobenzylidene)ethylenediamine

Crystal data

$C_{16}H_{12}Cl_4N_2$	F_{000} = 380
M_r = 374.08	D_x = 1.542 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4934 reflections
a = 13.572 (2) Å	θ = 3.4–26.0°
b = 4.4991 (7) Å	μ = 0.73 mm^{-1}
c = 14.623 (2) Å	T = 290 (2) K
β = 115.52 (2)°	Needle, colorless
V = 805.8 (2) Å^3	0.18 × 0.10 × 0.08 mm
Z = 2	

Data collection

STOE IPDS diffractometer	1525 independent reflections
Radiation source: fine-focus sealed tube	845 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 290(2) K	θ_{max} = 26.0°
Area detector – phi oscillation scans	θ_{min} = 4.2°
Absorption correction: numerical (X-RED32; Stoe & Cie, 1997)	$h = -16 \rightarrow 16$
T_{min} = 0.781, T_{max} = 0.837	$k = -2 \rightarrow 5$
5165 measured reflections	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.097	H-atom parameters constrained
$wR(F^2)$ = 0.248	$w = 1/[\sigma^2(F_o^2) + (0.090P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.47	$(\Delta/\sigma)_{max}$ < 0.001
1525 reflections	$\Delta\rho_{max}$ = 0.98 e Å^{-3}
100 parameters	$\Delta\rho_{min}$ = −0.40 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}
Cl1	−0.20151 (17)	−0.0529 (5)	−0.02731 (15)	0.0671 (8)
Cl2	0.13294 (15)	0.6230 (5)	0.20624 (15)	0.0658 (8)
N1	−0.0545 (5)	0.8441 (12)	0.3714 (4)	0.0501 (15)
C1	−0.0077 (7)	1.0651 (15)	0.4500 (5)	0.056 (2)
H1A	−0.0558	1.2362	0.4343	0.067*
H1B	0.0620	1.1305	0.4539	0.067*
C2	−0.0076 (6)	0.7871 (14)	0.3163 (5)	0.0463 (17)
H2	0.0575	0.8840	0.3290	0.056*
C3	−0.0506 (5)	0.5762 (13)	0.2336 (5)	0.0372 (15)
C4	−0.1551 (5)	0.4606 (14)	0.2042 (5)	0.0423 (16)
H4	−0.1949	0.5189	0.2394	0.051*
C5	−0.2006 (6)	0.2677 (14)	0.1269 (5)	0.0442 (17)
H5	−0.2702	0.1928	0.1097	0.053*
C6	−0.1431 (6)	0.1822 (14)	0.0733 (5)	0.0443 (16)
C7	−0.0405 (6)	0.2928 (14)	0.1000 (5)	0.0482 (18)
H7	−0.0011	0.2337	0.0646	0.058*
C8	0.0049 (5)	0.4922 (13)	0.1794 (4)	0.0355 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0817 (16)	0.0768 (14)	0.0482 (12)	−0.0135 (11)	0.0330 (11)	−0.0191 (10)
Cl2	0.0442 (11)	0.0989 (17)	0.0649 (14)	−0.0075 (10)	0.0333 (10)	−0.0062 (11)
N1	0.058 (4)	0.059 (3)	0.038 (3)	−0.010 (3)	0.025 (3)	−0.009 (3)
C1	0.071 (5)	0.061 (5)	0.038 (4)	−0.012 (4)	0.024 (4)	−0.007 (3)
C2	0.050 (4)	0.050 (4)	0.040 (4)	0.000 (3)	0.021 (4)	0.006 (3)
C3	0.037 (4)	0.041 (3)	0.036 (4)	0.004 (3)	0.017 (3)	0.004 (3)
C4	0.045 (4)	0.052 (4)	0.035 (4)	0.003 (3)	0.022 (3)	0.001 (3)
C5	0.044 (4)	0.055 (4)	0.036 (4)	−0.003 (3)	0.020 (3)	−0.002 (3)
C6	0.053 (4)	0.045 (4)	0.039 (4)	−0.001 (3)	0.023 (3)	0.003 (3)
C7	0.049 (4)	0.064 (4)	0.039 (4)	0.009 (4)	0.027 (4)	0.003 (4)
C8	0.031 (3)	0.046 (4)	0.033 (4)	0.010 (3)	0.018 (3)	0.013 (3)

Geometric parameters (Å, °)

Cl1—C6	1.705 (7)	C3—C8	1.361 (9)
Cl2—C8	1.712 (6)	C3—C4	1.393 (9)
N1—C2	1.248 (8)	C4—C5	1.347 (9)
N1—C1	1.444 (8)	C4—H4	0.9300
C1—C1^{i}	1.503 (13)	C5—C6	1.377 (9)
C1—H1A	0.9700	C5—H5	0.9300
C1—H1B	0.9700	C6—C7	1.367 (9)
C2—C3	1.448 (9)	C7—C8	1.384 (9)
C2—H2	0.9300	C7—H7	0.9300
C2—N1—C1	118.9 (6)	C5—C4—H4	118.8
N1—C1—C1^{i}	109.6 (7)	C3—C4—H4	118.8
N1—C1—H1A	109.8	C4—C5—C6	119.4 (6)
C1^{i}—C1—H1A	109.8	C4—C5—H5	120.3
N1—C1—H1B	109.8	C6—C5—H5	120.3
C1^{i}—C1—H1B	109.8	C7—C6—C5	119.5 (6)
H1A—C1—H1B	108.2	C7—C6—Cl1	120.6 (5)
N1—C2—C3	122.7 (6)	C5—C6—Cl1	119.8 (5)
N1—C2—H2	118.7	C6—C7—C8	120.4 (6)
C3—C2—H2	118.7	C6—C7—H7	119.8
C8—C3—C4	117.6 (6)	C8—C7—H7	119.8
C8—C3—C2	122.9 (6)	C3—C8—C7	120.6 (6)
C4—C3—C2	119.5 (6)	C3—C8—Cl2	122.2 (5)
C5—C4—C3	122.5 (6)	C7—C8—Cl2	117.2 (5)
C2—N1—C1—C1^{i}	−126.3 (9)	C5—C6—C7—C8	−0.8 (10)
C1—N1—C2—C3	−177.9 (6)	Cl1—C6—C7—C8	177.6 (5)
N1—C2—C3—C8	−173.6 (6)	C4—C3—C8—C7	−1.7 (9)
N1—C2—C3—C4	9.0 (9)	C2—C3—C8—C7	−179.1 (5)
C8—C3—C4—C5	1.4 (10)	C4—C3—C8—Cl2	178.9 (4)
C2—C3—C4—C5	178.9 (6)	C2—C3—C8—Cl2	1.5 (9)
C3—C4—C5—C6	−0.8 (10)	C6—C7—C8—C3	1.5 (9)
C4—C5—C6—C7	0.5 (10)	C6—C7—C8—Cl2	−179.1 (5)
C4—C5—C6—Cl1	−177.9 (5)		

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

Fig. 1