

2-[(Z)-(2,5-Dichlorophenyl)imino-methyl]-5-(diethylamino)phenol

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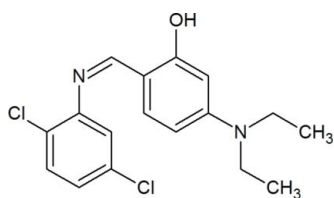
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 27.2.

In the title molecule, $\text{C}_{17}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}$, the angle between the mean planes of the 2,5-dichlorophenylimino and phenol groups is $19.5(5)^\circ$. The two ethyl groups adopt a synclinal conformation. The crystal structure is stabilized by intermolecular $\pi-\pi$ stacking interactions between adjacent 2,5-dichlorophenyl rings, the distance between the centroids of interacting rings being $3.860(8)$ Å. The molecules are stacked parallel to the a axis. In addition, an $\text{O}-\text{H}\cdots\text{N}$ intramolecular hydrogen-bonding interaction between the phenol H atom and imino N atom is observed.

Related literature

For related structures, see: Büyükgüngör *et al.* (2007); Odabaşoğlu *et al.* (2007); Yathirajan *et al.* (2007); Butcher *et al.* (2007). For related literature, see: Hodnett & Dunn (1970); Misra *et al.* (1981); Agarwal *et al.* (1983); Varma *et al.* (1986); Singh & Dash (1988); Pandey *et al.* (1999); El-Masry *et al.* (2000); Samadhiya & Halve (2001); Siddiqui *et al.* (2006).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}$
 $M_r = 337.23$
Monoclinic, $P2_1/c$
 $a = 7.1729(2)$ Å

$b = 18.6396(6)$ Å
 $c = 12.6378(4)$ Å
 $\beta = 104.157(3)^\circ$
 $V = 1638.36(9)$ Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.40$ mm⁻¹

$T = 296$ K
 $0.53 \times 0.25 \times 0.19$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\min} = 0.720$, $T_{\max} = 0.927$
17605 measured reflections
5491 independent reflections
2626 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.120$
 $S = 0.98$
5491 reflections

202 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1O}\cdots\text{N1}$	0.82	1.89	2.6139 (16)	147

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2061).

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supplementary materials

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2-[(Z)-(2,5-Dichlorophenyl)iminomethyl]-5-(diethylamino)phenol

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Comment

Schiff bases are synthesized from an aromatic amine and a carbonyl compound by a nucleophilic addition reaction. They are used as substrates in the preparation of number of biologically active compounds (Siddiqui *et al.*, 2006). Some Schiff base derivatives are also known to have activities such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh & Dash, 1988; Varma *et al.*, 1986), antitumor (Hodnett & Dunn, 1970; Misra *et al.*, 1981; Agarwal *et al.*, 1983) and as herbicides (Samadhiya & Halve, 2001). The crystal structures of (*E*)-2-hydroxy-5-methyl-3-[(4-methyl-2 pyridyl)iminomethyl] benzaldehyde (Büyükgüngör *et al.*, 2007), (*E*)-2-hydroxy-5-methyl-3-[(2-pyridylimino) methyl]benzaldehyde (Odabaşoğlu *et al.*, 2007), 1-(4-{[(*E*)-(4-diethylamino-2-hydroxy phenyl)methylene]amino} phenyl)ethanone (Yathirajan *et al.*, (2007), 2-{(E)-[(2-chloro-5-nitrophenyl)imino]methyl}-5-(diethylamino)phenol (Butcher *et al.*, 2007) have been reported. A new Schiff base, (I), C₁₇H₁₈Cl₂N₂O is prepared and its crystal structure is reported.

The angle between the mean planes of the 2,5-dichlorophenyl-imino and phenol groups is 19.5 (5)° (Fig. 1). The two ethyl groups adopt a *syn*-clinal conformation [C11—N2—C14—C15 = -87.9 (2)°; C11—N2—C16—C17 = -87.58 (19)°]. Crystal packing is stabilized by intermolecular π stacking interactions between Cg1¹- π orbitals of nearby 2,5-dichlorophenyl rings [Cg1¹...Cg1 = 3.860 (8) Å; Cg1 = center of gravity of the 2,5-dichlorophenyl ring (Fig. 2)]. The molecules are aligned in an inverted pattern along the *c* axis with the 2,5-dichlorophenyl rings stacked obliquely parallel to the *ac* face of the unit cell (Fig. 3). Intramolecular hydrogen bonding interactions [O1—H10...N1] between the phenol hydrogen atom and imino nitrogen atom provides additional crystal stability within the asymmetric unit. [*i* = 2 - *x*, -*y*, 2 - *z*].

Experimental

A mixture of 2,5-dichloroaniline (1.62 g, 0.01 mol) and 4-(diethylamino)-2-hydroxybenzaldehyde (1.93 g, 0.01 mol) in 30 ml of ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 7 h (Fig. 4). On cooling, the solid separated was filtered and recrystallized from acetone (m.p.: 397–401 K). Analysis found: C 60.46, H 5.32, N 8.24%; C₁₇H₁₈Cl₂N₂O requires: C 60.54, H 5.38, N 8.31%.

Refinement

The hydroxyl atom (H10) was located in a difference Fourier map and along with all other H atoms were placed in their calculated positions and then refined using the riding model with O—H = 0.82 Å and C—H = 0.93 to 0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.19\text{--}1.49U_{\text{eq}}(\text{C}, \text{O})$.

Figures

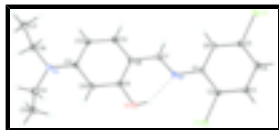


Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular O—H...N hydrogen bond.



Fig. 2. Packing diagram of the title compound, viewed down the *a* axis.

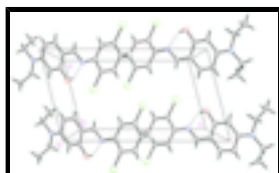


Fig. 3. Packing diagram of the title compound, viewed down the *b* axis. Dashed lines indicate intramolecular O—H...N hydrogen bonds.

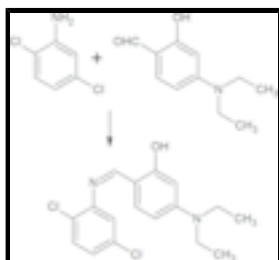


Fig. 4. Synthetic scheme for $C_{17}H_{18}Cl_2N_2O$.

2-[(Z)-(2,5-Dichlorophenyl)iminomethyl]-5-(diethylamino)phenol

Crystal data

$C_{17}H_{18}Cl_2N_2O$

$M_r = 337.23$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.1729$ (2) Å

$b = 18.6396$ (6) Å

$c = 12.6378$ (4) Å

$\beta = 104.157$ (3)°

$V = 1638.36$ (9) Å³

$Z = 4$

$F_{000} = 704$

$D_x = 1.367$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4869 reflections

$\theta = 4.7$ – 32.5 °

$\mu = 0.40$ mm⁻¹

$T = 296$ K

Thick needle, pale yellow

$0.53 \times 0.25 \times 0.19$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer

5491 independent reflections

Radiation source: fine-focus sealed tube	2626 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.034$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{\text{max}} = 32.5^\circ$
$T = 296 \text{ K}$	$\theta_{\text{min}} = 4.7^\circ$
φ and ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -27 \rightarrow 27$
$T_{\text{min}} = 0.720$, $T_{\text{max}} = 0.927$	$l = -18 \rightarrow 19$
17605 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$
$S = 0.98$	where $P = (F_o^2 + 2F_c^2)/3$
5491 reflections	$(\Delta/\sigma)_{\text{max}} = 0.003$
202 parameters	$\Delta\rho_{\text{max}} = 0.28 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.31 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.43274 (6)	0.45456 (3)	0.77923 (4)	0.06735 (16)
C12	-0.37011 (6)	0.41423 (3)	0.46310 (4)	0.06539 (16)
O1	0.30792 (15)	0.59856 (7)	0.95939 (10)	0.0573 (3)
H1O	0.2780	0.5722	0.9060	0.069*
N1	0.07935 (18)	0.52207 (6)	0.80838 (10)	0.0435 (3)
N2	0.0292 (2)	0.73892 (7)	1.19527 (11)	0.0532 (3)
C1	0.0490 (2)	0.47783 (7)	0.71617 (12)	0.0398 (3)
C2	0.2079 (2)	0.44459 (8)	0.69148 (13)	0.0443 (4)
C3	0.1895 (3)	0.40261 (9)	0.59958 (14)	0.0547 (4)

supplementary materials

H3A	0.2976	0.3812	0.5849	0.066*
C4	0.0108 (3)	0.39229 (9)	0.52911 (14)	0.0539 (4)
H4A	-0.0033	0.3636	0.4674	0.065*
C5	-0.1452 (2)	0.42544 (8)	0.55252 (12)	0.0458 (4)
C6	-0.1297 (2)	0.46767 (8)	0.64337 (12)	0.0433 (3)
H6A	-0.2385	0.4895	0.6564	0.052*
C7	-0.0578 (2)	0.53797 (8)	0.85377 (12)	0.0441 (4)
H7A	-0.1774	0.5166	0.8277	0.053*
C8	-0.0324 (2)	0.58710 (8)	0.94251 (12)	0.0411 (3)
C9	0.1485 (2)	0.61728 (8)	0.99181 (12)	0.0422 (3)
C10	0.1682 (2)	0.66657 (8)	1.07560 (13)	0.0474 (4)
H10A	0.2889	0.6856	1.1070	0.057*
C11	0.0095 (2)	0.68848 (8)	1.11419 (12)	0.0439 (4)
C12	-0.1712 (2)	0.65751 (8)	1.06588 (13)	0.0484 (4)
H12A	-0.2790	0.6707	1.0899	0.058*
C13	-0.1882 (2)	0.60832 (8)	0.98419 (13)	0.0474 (4)
H13A	-0.3081	0.5880	0.9548	0.057*
C14	0.2107 (3)	0.77568 (9)	1.24016 (14)	0.0550 (4)
H14A	0.1839	0.8229	1.2650	0.066*
H14B	0.2776	0.7820	1.1828	0.066*
C15	0.3403 (3)	0.73581 (11)	1.33400 (16)	0.0708 (5)
H15A	0.4551	0.7632	1.3618	0.106*
H15B	0.3737	0.6901	1.3090	0.106*
H15C	0.2746	0.7288	1.3909	0.106*
C16	-0.1285 (3)	0.75621 (9)	1.24523 (14)	0.0548 (4)
H16A	-0.0757	0.7719	1.3197	0.066*
H16B	-0.2035	0.7132	1.2477	0.066*
C17	-0.2591 (3)	0.81395 (10)	1.18432 (16)	0.0647 (5)
H17A	-0.3574	0.8245	1.2217	0.097*
H17B	-0.3177	0.7976	1.1117	0.097*
H17C	-0.1855	0.8565	1.1807	0.097*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0356 (2)	0.1007 (4)	0.0625 (3)	0.0009 (2)	0.00571 (19)	-0.0005 (2)
C12	0.0521 (3)	0.0786 (3)	0.0573 (3)	-0.0096 (2)	-0.0023 (2)	-0.0120 (2)
O1	0.0354 (6)	0.0763 (8)	0.0580 (8)	0.0022 (5)	0.0073 (5)	-0.0187 (6)
N1	0.0392 (7)	0.0453 (7)	0.0430 (7)	0.0010 (6)	0.0047 (5)	-0.0007 (5)
N2	0.0458 (8)	0.0567 (8)	0.0551 (9)	0.0044 (6)	0.0086 (6)	-0.0122 (6)
C1	0.0394 (8)	0.0400 (7)	0.0390 (8)	-0.0030 (6)	0.0077 (6)	0.0033 (6)
C2	0.0343 (8)	0.0548 (9)	0.0433 (9)	-0.0019 (7)	0.0088 (6)	0.0063 (7)
C3	0.0462 (10)	0.0688 (11)	0.0533 (10)	0.0061 (8)	0.0202 (8)	0.0015 (8)
C4	0.0577 (11)	0.0601 (10)	0.0461 (10)	-0.0042 (9)	0.0170 (8)	-0.0085 (7)
C5	0.0420 (9)	0.0507 (9)	0.0420 (9)	-0.0074 (7)	0.0048 (7)	0.0000 (7)
C6	0.0381 (8)	0.0455 (8)	0.0455 (9)	0.0012 (7)	0.0088 (6)	0.0006 (6)
C7	0.0380 (8)	0.0453 (8)	0.0455 (9)	-0.0056 (7)	0.0038 (6)	0.0021 (7)
C8	0.0370 (8)	0.0433 (8)	0.0412 (8)	-0.0031 (6)	0.0065 (6)	0.0035 (6)

C9	0.0349 (8)	0.0453 (8)	0.0436 (8)	0.0038 (7)	0.0043 (6)	0.0028 (6)
C10	0.0358 (8)	0.0533 (9)	0.0486 (9)	−0.0021 (7)	0.0017 (7)	−0.0024 (7)
C11	0.0425 (9)	0.0440 (8)	0.0424 (9)	0.0035 (7)	0.0048 (7)	0.0021 (6)
C12	0.0396 (9)	0.0541 (9)	0.0526 (10)	0.0017 (7)	0.0134 (7)	0.0006 (7)
C13	0.0382 (8)	0.0518 (9)	0.0518 (10)	−0.0090 (7)	0.0103 (7)	−0.0022 (7)
C14	0.0587 (11)	0.0498 (9)	0.0528 (10)	−0.0009 (8)	0.0065 (8)	−0.0075 (7)
C15	0.0641 (12)	0.0752 (12)	0.0644 (12)	0.0043 (10)	−0.0014 (10)	−0.0011 (10)
C16	0.0593 (11)	0.0566 (10)	0.0490 (10)	0.0041 (8)	0.0144 (8)	−0.0022 (7)
C17	0.0571 (11)	0.0673 (11)	0.0693 (12)	0.0124 (9)	0.0149 (9)	0.0008 (9)

Geometric parameters (Å, °)

C11—C2	1.7293 (16)	C8—C9	1.411 (2)
C12—C5	1.7412 (16)	C9—C10	1.383 (2)
O1—C9	1.3516 (17)	C10—C11	1.404 (2)
O1—H10	0.8200	C10—H10A	0.9300
N1—C7	1.2885 (19)	C11—C12	1.414 (2)
N1—C1	1.4005 (18)	C12—C13	1.364 (2)
N2—C11	1.372 (2)	C12—H12A	0.9300
N2—C14	1.457 (2)	C13—H13A	0.9300
N2—C16	1.461 (2)	C14—C15	1.511 (2)
C1—C6	1.396 (2)	C14—H14A	0.9700
C1—C2	1.398 (2)	C14—H14B	0.9700
C2—C3	1.380 (2)	C15—H15A	0.9600
C3—C4	1.384 (2)	C15—H15B	0.9600
C3—H3A	0.9300	C15—H15C	0.9600
C4—C5	1.372 (2)	C16—C17	1.508 (2)
C4—H4A	0.9300	C16—H16A	0.9700
C5—C6	1.374 (2)	C16—H16B	0.9700
C6—H6A	0.9300	C17—H17A	0.9600
C7—C8	1.425 (2)	C17—H17B	0.9600
C7—H7A	0.9300	C17—H17C	0.9600
C8—C13	1.404 (2)		
C9—O1—H10	109.5	C11—C10—H10A	119.4
C7—N1—C1	121.73 (13)	N2—C11—C10	120.95 (14)
C11—N2—C14	122.14 (14)	N2—C11—C12	121.22 (14)
C11—N2—C16	121.65 (14)	C10—C11—C12	117.83 (14)
C14—N2—C16	116.15 (14)	C13—C12—C11	120.25 (15)
C6—C1—C2	117.40 (14)	C13—C12—H12A	119.9
C6—C1—N1	123.98 (13)	C11—C12—H12A	119.9
C2—C1—N1	118.53 (13)	C12—C13—C8	122.81 (15)
C3—C2—C1	121.60 (15)	C12—C13—H13A	118.6
C3—C2—C11	118.88 (12)	C8—C13—H13A	118.6
C1—C2—C11	119.51 (12)	N2—C14—C15	113.20 (15)
C2—C3—C4	120.22 (15)	N2—C14—H14A	108.9
C2—C3—H3A	119.9	C15—C14—H14A	108.9
C4—C3—H3A	119.9	N2—C14—H14B	108.9
C5—C4—C3	118.33 (15)	C15—C14—H14B	108.9
C5—C4—H4A	120.8	H14A—C14—H14B	107.8

supplementary materials

C3—C4—H4A	120.8	C14—C15—H15A	109.5
C4—C5—C6	122.32 (15)	C14—C15—H15B	109.5
C4—C5—C12	118.75 (13)	H15A—C15—H15B	109.5
C6—C5—C12	118.93 (12)	C14—C15—H15C	109.5
C5—C6—C1	120.12 (14)	H15A—C15—H15C	109.5
C5—C6—H6A	119.9	H15B—C15—H15C	109.5
C1—C6—H6A	119.9	N2—C16—C17	112.77 (14)
N1—C7—C8	122.27 (14)	N2—C16—H16A	109.0
N1—C7—H7A	118.9	C17—C16—H16A	109.0
C8—C7—H7A	118.9	N2—C16—H16B	109.0
C13—C8—C9	116.88 (14)	C17—C16—H16B	109.0
C13—C8—C7	121.09 (14)	H16A—C16—H16B	107.8
C9—C8—C7	122.03 (14)	C16—C17—H17A	109.5
O1—C9—C10	117.90 (13)	C16—C17—H17B	109.5
O1—C9—C8	121.19 (13)	H17A—C17—H17B	109.5
C10—C9—C8	120.91 (14)	C16—C17—H17C	109.5
C9—C10—C11	121.29 (14)	H17A—C17—H17C	109.5
C9—C10—H10A	119.4	H17B—C17—H17C	109.5
C7—N1—C1—C6	23.4 (2)	C13—C8—C9—C10	-1.4 (2)
C7—N1—C1—C2	-160.16 (14)	C7—C8—C9—C10	177.95 (14)
C6—C1—C2—C3	-0.7 (2)	O1—C9—C10—C11	-179.71 (14)
N1—C1—C2—C3	-177.40 (14)	C8—C9—C10—C11	-0.2 (2)
C6—C1—C2—C11	-179.43 (11)	C14—N2—C11—C10	4.2 (2)
N1—C1—C2—C11	3.92 (18)	C16—N2—C11—C10	-172.72 (15)
C1—C2—C3—C4	-0.2 (2)	C14—N2—C11—C12	-175.03 (15)
C11—C2—C3—C4	178.53 (13)	C16—N2—C11—C12	8.0 (2)
C2—C3—C4—C5	0.8 (2)	C9—C10—C11—N2	-178.16 (14)
C3—C4—C5—C6	-0.5 (2)	C9—C10—C11—C12	1.1 (2)
C3—C4—C5—C12	178.80 (12)	N2—C11—C12—C13	178.94 (15)
C4—C5—C6—C1	-0.4 (2)	C10—C11—C12—C13	-0.3 (2)
C12—C5—C6—C1	-179.72 (11)	C11—C12—C13—C8	-1.4 (2)
C2—C1—C6—C5	1.0 (2)	C9—C8—C13—C12	2.2 (2)
N1—C1—C6—C5	177.46 (13)	C7—C8—C13—C12	-177.13 (15)
C1—N1—C7—C8	-175.23 (13)	C11—N2—C14—C15	-87.9 (2)
N1—C7—C8—C13	174.32 (14)	C16—N2—C14—C15	89.23 (18)
N1—C7—C8—C9	-5.0 (2)	C11—N2—C16—C17	-87.58 (19)
C13—C8—C9—O1	178.08 (14)	C14—N2—C16—C17	95.31 (19)
C7—C8—C9—O1	-2.6 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H10 \cdots N1	0.82	1.89	2.6139 (16)	147

Fig. 1

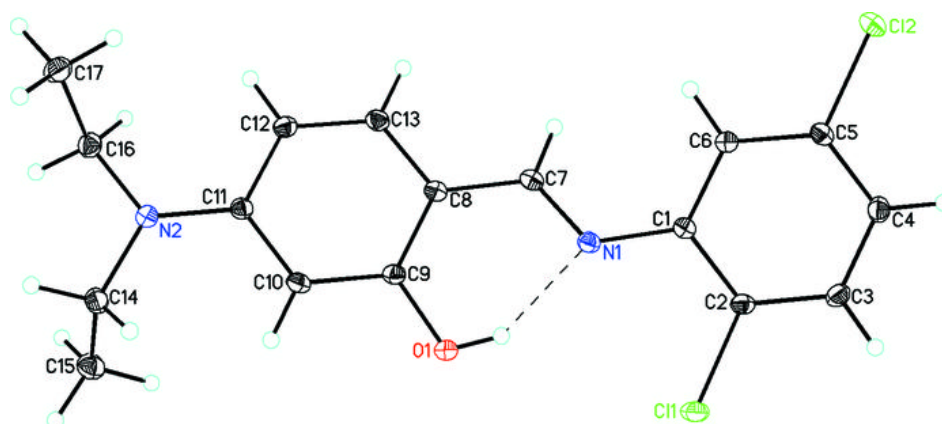


Fig. 2

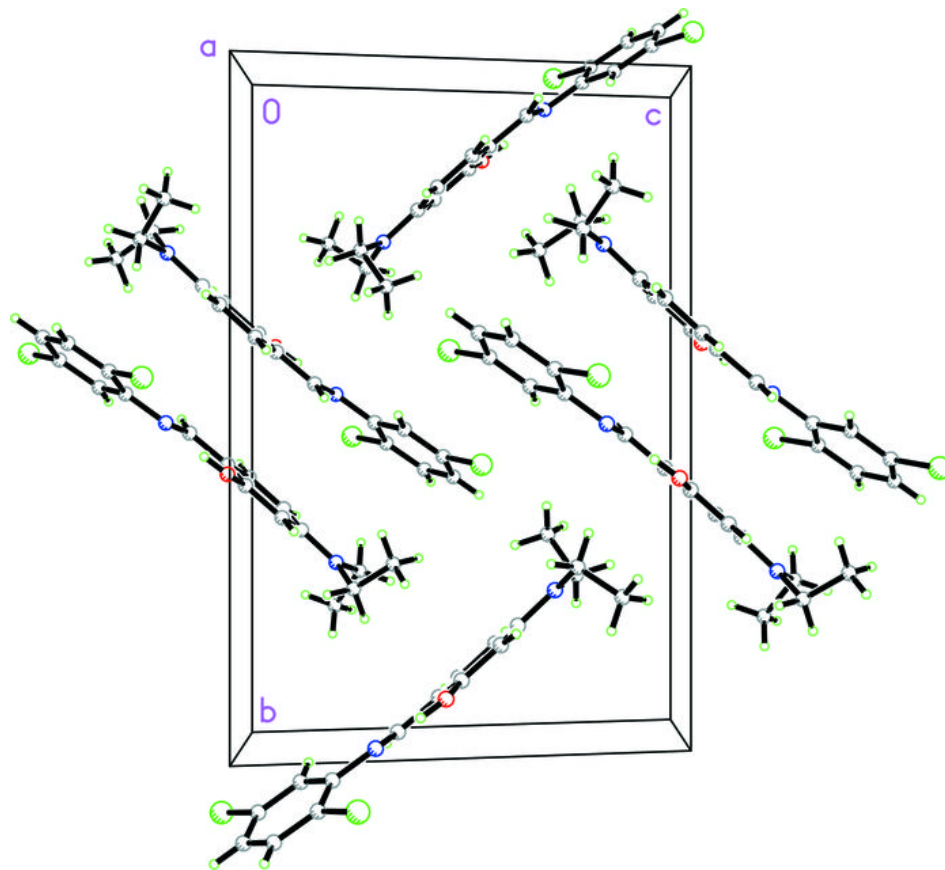


Fig. 3

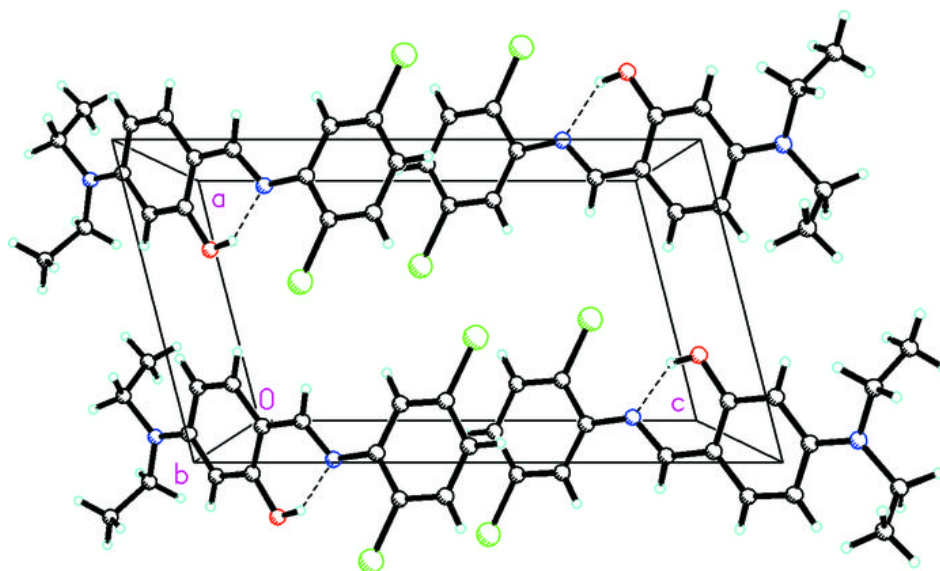


Fig. 4

