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5-(Diethylamino)-2-[(*Z*)-(1-naphthylimino)methyl]phenol

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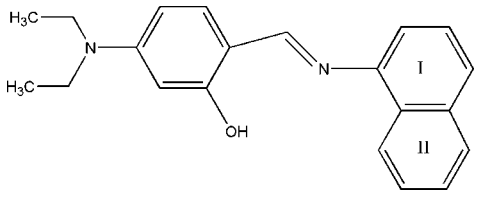
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.047; wR factor = 0.129; data-to-parameter ratio = 13.2.

In the title molecule, $C_{21}H_{22}N_2O$, the angle between the mean planes of the 1-naphthylimino and 2-methylyphenyl groups is 63.3 (2)°. The two diethyl extensions from the 5-diethylamino group are twisted in a + and − antiperiplanar conformation. One of the ethyl arms is disordered over two conformations with occupancies of 0.644 (3) and 0.356 (3). The crystal packing is stabilized by intermolecular C—H$\cdots\pi$ interactions between π orbitals of the 1-naphthyl (I/II) rings and H atoms from a nearby benzene ring as well as from an ethyl C atom of an ethylamino group. The molecules are stacked along the *b* axis in alternate inverted chains with the 1-naphthyl rings obliquely parallel to the *ab* face of the unit cell. Intramolecular interactions between the hydroxyl H atom and the imino N atom provide additional conformational stability.

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 *et al.* (1970); Misra *et al.* (1981); Agarwal *et al.* (1983); Varma *et al.* (1986); Singh *et al.* (1988); Pandey *et al.* (1999); El-Masry *et al.* (2000); Samadhiya & Halve (2001).



Experimental

Crystal data

$C_{21}H_{22}N_2O$
M_r = 318.41
Monoclinic, $P2_1$
a = 7.5329 (5) Å
b = 14.6040 (1) Å
c = 7.9904 (5) Å
β = 95.951 (6)°
V = 874.29 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.47 × 0.42 × 0.35 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.782, T_{max} = 1.000 (expected range = 0.761–0.974)
8501 measured reflections
3003 independent reflections
1651 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 0.96
3003 reflections
228 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of naphthyl rings I and II (see scheme).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1—H1*O*$\cdots$N1	0.82	1.87	2.6060 (14)	148
C16—H16*A*$\cdots$*Cg*1^{ii}	0.93	2.84	3.6475 (15)	145
C17—H17*A*$\cdots$*Cg*2^{ii}	0.93	2.85	3.6502 (15)	145
C19*A*—H19*A*$\cdots$*Cg*1^{iiii}	0.88	2.88	3.747 (7)	142
C19*B*—H19*D*$\cdots$*Cg*1^{iiii}	0.88	2.88	3.688 (4)	149

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+1$; (ii) $-x+1, y-\frac{1}{2}, -z+2$.

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro* (Oxford Diffraction, 2007); 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: BT2558).

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supplementary materials

Acta Cryst. (2007). E**63**, o4588-o4589 [**doi:10.1107/S1600536807053135**]

5-(Diethylamino)-2-[(*Z*)-(1-naphthylimino)methyl]phenol

J. P. Jasinski, R. J. Butcher, B. Narayana, M. T. Swamy and H. S. Yathirajan

Comment

Schiff bases are synthesized from an aromatic amine and a carbonyl compound by nucleophilic addition forming a hemiaminal, followed by a dehydration to generate an imine. Schiff bases are used as substrates in the preparation of number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Some Schiff base derivatives are also known to have biological activities such as antimicrobial (El-Masry *et al.* 2000; Pandey *et al.* 1999), antifungal (Singh *et al.* 1988; Varma *et al.*, 1986), antitumor (Hodnett *et al.* 1970; Misra *et al.* 1981; Agarwal *et al.*, 1983) and as herbicides (Samadhiya & Halve, 2001). The crysta 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 (Odabasoglu *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), $C_{21}H_{22}N_2O$ is prepared and its crystal structure is reported.

The angle between the mean planes of the 1-naphthylimino and 2-methylyphenyl groups is 63.3 (2)° (Fig. 1). The two diethyl extensions from the 5-diethylamino group are twisted in a + and - antiperiplanar conformation. One of the ethyl arms C19—C19 is disordered over two conformations which are constrained to have similar metrical parameters with occupancies of 0.644 (3) [C18B & C19B)] and 0.356 (3) [C18A & C19A], respectively. Crystal packing is stabilized by intermolecular C—H···*Cg*1/*Cg*2 packing interactions between *Cg*1/*Cg*2-π orbitals of the 1-naphthyl (I/II) rings and hydrogen atoms from a nearby phenyl ring [*Cg*1/*Cg*2 = center of gravity of the 1-naphthyl (I/II) rings, respectively] as well as between a disordered ethyl carbon from an ethylamino group and *Cg*1 (Fig. 2). The molecules are stacked along the *b* axis in alternate, inverted chains with the 1-naphthyl rings obliquely parallel to the *ab* face of the unit cell (Fig. 3). Intramolecular interactions between the hydroxyl hydrogen atom and the imino nitrogen atom [O1—H10···N1 = 2.6060 (14) Å] in the asymmetric unit provide additional crystal stability.

Experimental

A mixture of naphthalen-1-amine (1.43 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 5 h (Fig. 4). On cooling, the solid separated was filtered and recrystallized from acetone (m.p.: 371–373 K). Analysis found: C 79.11, H 6.89, N 8.72%; $C_{21}H_{22}N_2O$ requires: C 79.21, H 6.96, N 8.80%.

Refinement

In the absence of anomalous scatterers Friedel pairs had been merged. The hydroxyl hydrogen atom (H10) was located in a difference Fourier map and along with all other all other H atoms placed in their calculated positions and then refined using the riding model with O—H = 0.82Å and C—H = 0.93 to 0.97 Å, and with U_{iso}(H) = 1.19–1.49U_{eq}(C, O). Atoms C17 and C18 are disordered with refined occupancies of 0.4267 (14) [A] and 0.5733 (14) [B], respectively.

Figures

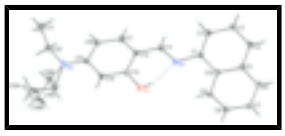

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids. Atoms C18 and C19 are disordered over two conformations which are constrained to have similar metrical parameters with occupanicies of 0.644 (3) [C18B & C19B)] and 0.356 (3) [C18A & C19A], respectively. Dashed lines indicate intramolecular O1—H10···N1 hydrogen bonds.

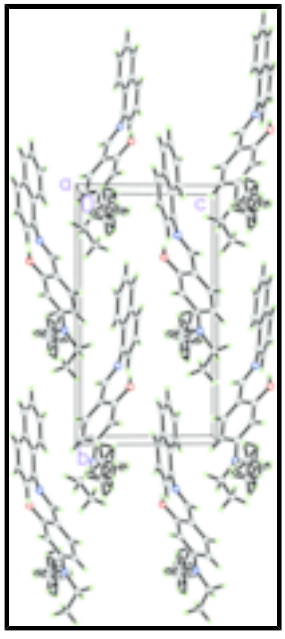

Fig. 2. Packing diagram of the title compound, viewed down the *a* axis.

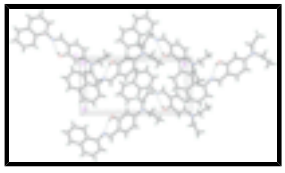

Fig. 3. Packing diagram of the title compound, viewed down the *c* axis. Dashed lines indicate intramolecular O1—H10···N1 hydrogen bonds.

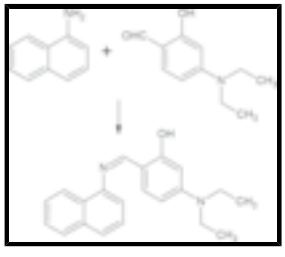

Fig. 4. Synthetic scheme for $C_{21}H_{22}N_2O$.

5-(Diethylamino)-2-[(*Z*)-(1-naphthylimino)methyl]phenol

Crystal data

$C_{21}H_{22}N_2O$	F_{000} = 340
M_r = 318.41	D_x = 1.209 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 3058 reflections
a = 7.5329 (5) Å	θ = 4.8–32.5º

b = 14.6040 (1) Å	μ = 0.08 mm^{-1}
c = 7.9904 (5) Å	T = 296 K
β = 95.951 (6)º	Prism, pale yellow
V = 874.29 (10) Å^3	0.47 × 0.42 × 0.35 mm
Z = 2	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	3003 independent reflections
Radiation source: fine-focus sealed tube	1651 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
Detector resolution: 10.5081 pixels mm^{-1}	θ_{max} = 32.5º
T = 296 K	θ_{min} = 4.8º
φ and ω scans	h = −11→11
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	k = −21→21
T_{min} = 0.782, T_{max} = 1.000	l = −11→11
8501 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.129	$(\Delta/\sigma)_{max}$ = 0.036
S = 0.96	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
3003 reflections	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
228 parameters	Extinction correction: none
1 restraint	Absolute structure:
Primary atom site location: structure-invariant direct methods	Flack parameter:
Secondary atom site location: difference Fourier map	Rogers parameter: ?

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)
O1	0.44021 (13)	0.32600 (7)	0.87995 (13)	0.0690 (3)	
H1O	0.3569	0.3617	0.8848	0.083*	
N1	0.13393 (14)	0.40391 (7)	0.78988 (14)	0.0514 (3)	
N2	0.57713 (17)	0.04299 (9)	0.62685 (14)	0.0650 (4)	
C1	0.00190 (15)	0.46814 (9)	0.82282 (15)	0.0465 (3)	
C2	−0.16455 (18)	0.44247 (11)	0.86254 (17)	0.0557 (4)	
H2A	−0.1983	0.3812	0.8548	0.067*	
C3	−0.28310 (18)	0.50751 (11)	0.91432 (17)	0.0597 (4)	
H3A	−0.3944	0.4887	0.9420	0.072*	
C4	−0.23931 (19)	0.59759 (12)	0.92512 (18)	0.0618 (4)	
H4A	−0.3197	0.6398	0.9609	0.074*	
C5	−0.06962 (18)	0.62741 (10)	0.88146 (15)	0.0503 (3)	
C6	−0.0191 (2)	0.72118 (11)	0.88894 (19)	0.0647 (4)	
H6A	−0.0978	0.7647	0.9234	0.078*	
C7	0.1446 (2)	0.74816 (11)	0.8459 (2)	0.0677 (5)	
H7A	0.1769	0.8096	0.8518	0.081*	
C8	0.2618 (2)	0.68327 (11)	0.79346 (18)	0.0621 (4)	
H8A	0.3719	0.7020	0.7628	0.074*	
C9	0.21839 (18)	0.59312 (10)	0.78615 (17)	0.0528 (4)	
H9A	0.2997	0.5510	0.7517	0.063*	
C10	0.05183 (17)	0.56224 (9)	0.82993 (14)	0.0448 (3)	
C11	0.09765 (17)	0.33416 (9)	0.69144 (16)	0.0502 (3)	
H11A	−0.0150	0.3305	0.6321	0.060*	
C12	0.22364 (17)	0.26267 (9)	0.67030 (15)	0.0470 (3)	
C13	0.39169 (16)	0.25952 (9)	0.76692 (15)	0.0478 (3)	
C14	0.50757 (17)	0.18848 (10)	0.75195 (16)	0.0516 (4)	
H14A	0.6171	0.1883	0.8174	0.062*	
C15	0.46460 (17)	0.11565 (10)	0.63957 (15)	0.0494 (3)	
C16	0.29674 (19)	0.12017 (11)	0.53899 (17)	0.0610 (4)	
H16A	0.2639	0.0741	0.4616	0.073*	
C17	0.18444 (19)	0.19213 (10)	0.55627 (17)	0.0591 (4)	
H17A	0.0765	0.1939	0.4883	0.071*	
C18A	0.7636 (6)	0.0545 (4)	0.7223 (6)	0.0672 (7)	0.356 (3)
H18A	0.8217	0.1071	0.6778	0.081*	0.356 (3)
H18B	0.7516	0.0662	0.8401	0.081*	0.356 (3)
C19A	0.8621 (6)	−0.0171 (10)	0.7100 (9)	0.187 (3)	0.356 (3)
H19A	0.9649	−0.0136	0.7915	0.280*	0.356 (3)
H19B	0.8999	−0.0200	0.5990	0.280*	0.356 (3)
H19C	0.7947	−0.0711	0.7304	0.280*	0.356 (3)
C18B	0.7214 (3)	0.0213 (2)	0.7592 (3)	0.0672 (7)	0.644 (3)
H18C	0.7000	−0.0386	0.8058	0.081*	0.644 (3)
H18D	0.7214	0.0659	0.8491	0.081*	0.644 (3)
C19B	0.9046 (4)	0.0216 (6)	0.6908 (5)	0.187 (3)	0.644 (3)
H19D	0.9947	0.0035	0.7782	0.280*	0.644 (3)
H19E	0.9303	0.0821	0.6529	0.280*	0.644 (3)

H19F	0.9032	−0.0205	0.5984	0.280*	0.644 (3)
C20	0.5237 (2)	−0.03633 (11)	0.52343 (19)	0.0613 (4)	
H20A	0.6303	−0.0672	0.4942	0.074*	
H20B	0.4581	−0.0153	0.4197	0.074*	
C21	0.4101 (3)	−0.10460 (16)	0.6054 (3)	0.1049 (7)	
H21A	0.3791	−0.1541	0.5289	0.157*	
H21B	0.3033	−0.0751	0.6337	0.157*	
H21C	0.4756	−0.1281	0.7058	0.157*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0547 (5)	0.0600 (6)	0.0886 (7)	−0.0032 (5)	−0.0097 (5)	−0.0216 (6)
N1	0.0516 (5)	0.0430 (6)	0.0596 (6)	−0.0019 (5)	0.0053 (5)	0.0035 (5)
N2	0.0665 (7)	0.0656 (8)	0.0596 (6)	0.0245 (6)	−0.0088 (6)	−0.0160 (6)
C1	0.0457 (6)	0.0477 (7)	0.0455 (6)	0.0015 (6)	0.0024 (5)	0.0017 (6)
C2	0.0539 (7)	0.0546 (8)	0.0587 (7)	−0.0051 (6)	0.0060 (6)	0.0070 (6)
C3	0.0477 (7)	0.0759 (10)	0.0560 (7)	−0.0026 (7)	0.0078 (6)	−0.0003 (7)
C4	0.0571 (7)	0.0722 (10)	0.0568 (7)	0.0105 (8)	0.0089 (6)	−0.0107 (7)
C5	0.0581 (7)	0.0513 (7)	0.0416 (6)	0.0013 (6)	0.0063 (5)	−0.0057 (5)
C6	0.0795 (9)	0.0520 (8)	0.0633 (8)	0.0069 (8)	0.0101 (7)	−0.0139 (7)
C7	0.0882 (10)	0.0440 (7)	0.0707 (9)	−0.0110 (8)	0.0076 (8)	−0.0068 (7)
C8	0.0638 (8)	0.0569 (9)	0.0658 (8)	−0.0109 (8)	0.0082 (7)	−0.0003 (7)
C9	0.0526 (7)	0.0496 (8)	0.0559 (7)	0.0010 (6)	0.0048 (6)	0.0003 (6)
C10	0.0471 (6)	0.0496 (7)	0.0368 (5)	0.0002 (6)	0.0006 (5)	−0.0023 (5)
C11	0.0532 (7)	0.0469 (7)	0.0493 (6)	0.0032 (6)	−0.0010 (5)	0.0041 (6)
C12	0.0514 (6)	0.0430 (7)	0.0454 (6)	0.0007 (6)	−0.0001 (5)	0.0051 (5)
C13	0.0495 (7)	0.0433 (7)	0.0500 (6)	−0.0092 (6)	0.0030 (6)	−0.0043 (6)
C14	0.0429 (6)	0.0588 (8)	0.0518 (7)	−0.0026 (6)	−0.0013 (5)	−0.0021 (6)
C15	0.0494 (7)	0.0522 (8)	0.0464 (6)	0.0020 (6)	0.0045 (5)	−0.0025 (6)
C16	0.0621 (8)	0.0622 (8)	0.0557 (7)	0.0087 (7)	−0.0086 (6)	−0.0145 (7)
C17	0.0571 (7)	0.0624 (9)	0.0536 (7)	0.0105 (7)	−0.0143 (6)	−0.0084 (7)
C18A	0.0683 (12)	0.0760 (17)	0.0551 (11)	0.0169 (12)	−0.0047 (9)	−0.0071 (11)
C19A	0.0287 (12)	0.443 (9)	0.0883 (16)	−0.048 (3)	0.0068 (12)	0.020 (3)
C18B	0.0683 (12)	0.0760 (17)	0.0551 (11)	0.0169 (12)	−0.0047 (9)	−0.0071 (11)
C19B	0.0287 (12)	0.443 (9)	0.0883 (16)	−0.048 (3)	0.0068 (12)	0.020 (3)
C20	0.0633 (7)	0.0632 (9)	0.0583 (8)	0.0090 (8)	0.0102 (6)	−0.0095 (7)
C21	0.1101 (14)	0.0808 (14)	0.1280 (16)	−0.0032 (13)	0.0325 (12)	0.0187 (13)

Geometric parameters (Å, °)

O1—C13	1.3503 (16)	C12—C17	1.3867 (19)
O1—H1O	0.8200	C12—C13	1.4135 (17)
N1—C11	1.2987 (17)	C13—C14	1.3691 (19)
N1—C1	1.4116 (17)	C14—C15	1.4080 (19)
N2—C15	1.3684 (19)	C14—H14A	0.9300
N2—C20	1.455 (2)	C15—C16	1.4277 (19)
N2—C18B	1.470 (3)	C16—C17	1.365 (2)
N2—C18A	1.537 (5)	C16—H16A	0.9300

C1—C2	1.3769 (18)	C17—H17A	0.9300
C1—C10	1.4244 (19)	C18A—C19A	1.293 (13)
C2—C3	1.396 (2)	C18A—H18A	0.9700
C2—H2A	0.9300	C18A—H18B	0.9700
C3—C4	1.357 (2)	C19A—H19A	0.9600
C3—H3A	0.9300	C19A—H19B	0.9600
C4—C5	1.427 (2)	C19A—H19C	0.9600
C4—H4A	0.9300	C18B—C19B	1.536 (4)
C5—C10	1.4108 (19)	C18B—H18C	0.9700
C5—C6	1.421 (2)	C18B—H18D	0.9700
C6—C7	1.371 (2)	C19B—H19D	0.9600
C6—H6A	0.9300	C19B—H19E	0.9600
C7—C8	1.389 (2)	C19B—H19F	0.9600
C7—H7A	0.9300	C20—C21	1.507 (3)
C8—C9	1.356 (2)	C20—H20A	0.9700
C8—H8A	0.9300	C20—H20B	0.9700
C9—C10	1.4110 (19)	C21—H21A	0.9600
C9—H9A	0.9300	C21—H21B	0.9600
C11—C12	1.4327 (19)	C21—H21C	0.9600
C11—H11A	0.9300		

C13—O1—H1O	109.5	O1—C13—C12	120.46 (12)
C11—N1—C1	121.73 (11)	C14—C13—C12	121.33 (11)
C15—N2—C20	121.50 (12)	C13—C14—C15	121.45 (11)
C15—N2—C18B	122.08 (15)	C13—C14—H14A	119.3
C20—N2—C18B	112.15 (16)	C15—C14—H14A	119.3
C15—N2—C18A	114.8 (2)	N2—C15—C14	122.00 (11)
C20—N2—C18A	123.6 (2)	N2—C15—C16	120.89 (12)
C18B—N2—C18A	25.5 (2)	C14—C15—C16	117.11 (12)
C2—C1—N1	122.56 (13)	C17—C16—C15	120.05 (13)
C2—C1—C10	119.77 (12)	C17—C16—H16A	120.0
N1—C1—C10	117.40 (11)	C15—C16—H16A	120.0
C1—C2—C3	120.60 (14)	C16—C17—C12	123.12 (13)
C1—C2—H2A	119.7	C16—C17—H17A	118.4
C3—C2—H2A	119.7	C12—C17—H17A	118.4
C4—C3—C2	121.33 (13)	C19A—C18A—N2	112.1 (5)
C4—C3—H3A	119.3	C19A—C18A—H18A	109.2
C2—C3—H3A	119.3	N2—C18A—H18A	109.2
C3—C4—C5	119.88 (14)	C19A—C18A—H18B	109.2
C3—C4—H4A	120.1	N2—C18A—H18B	109.2
C5—C4—H4A	120.1	H18A—C18A—H18B	107.9
C10—C5—C6	118.91 (13)	N2—C18B—C19B	111.6 (2)
C10—C5—C4	119.32 (13)	N2—C18B—H18C	109.3
C6—C5—C4	121.77 (14)	C19B—C18B—H18C	109.3
C7—C6—C5	120.68 (15)	N2—C18B—H18D	109.3
C7—C6—H6A	119.7	C19B—C18B—H18D	109.3
C5—C6—H6A	119.7	H18C—C18B—H18D	108.0
C6—C7—C8	119.71 (15)	C18B—C19B—H19D	109.5
C6—C7—H7A	120.1	C18B—C19B—H19E	109.5
C8—C7—H7A	120.1	H19D—C19B—H19E	109.5

C9—C8—C7	121.14 (14)	C18B—C19B—H19F	109.5
C9—C8—H8A	119.4	H19D—C19B—H19F	109.5
C7—C8—H8A	119.4	H19E—C19B—H19F	109.5
C8—C9—C10	121.07 (14)	N2—C20—C21	114.57 (15)
C8—C9—H9A	119.5	N2—C20—H20A	108.6
C10—C9—H9A	119.5	C21—C20—H20A	108.6
C5—C10—C9	118.49 (12)	N2—C20—H20B	108.6
C5—C10—C1	119.08 (12)	C21—C20—H20B	108.6
C9—C10—C1	122.44 (12)	H20A—C20—H20B	107.6
N1—C11—C12	122.86 (11)	C20—C21—H21A	109.5
N1—C11—H11A	118.6	C20—C21—H21B	109.5
C12—C11—H11A	118.6	H21A—C21—H21B	109.5
C17—C12—C13	116.90 (12)	C20—C21—H21C	109.5
C17—C12—C11	121.35 (12)	H21A—C21—H21C	109.5
C13—C12—C11	121.74 (11)	H21B—C21—H21C	109.5
O1—C13—C14	118.19 (11)		
C11—N1—C1—C2	46.16 (18)	C11—C12—C13—O1	−1.77 (19)
C11—N1—C1—C10	−139.83 (12)	C17—C12—C13—C14	−2.00 (19)
N1—C1—C2—C3	172.06 (12)	C11—C12—C13—C14	176.64 (12)
C10—C1—C2—C3	−1.81 (19)	O1—C13—C14—C15	178.56 (12)
C1—C2—C3—C4	0.8 (2)	C12—C13—C14—C15	0.1 (2)
C2—C3—C4—C5	0.6 (2)	C20—N2—C15—C14	173.50 (13)
C3—C4—C5—C10	−0.97 (19)	C18B—N2—C15—C14	18.5 (2)
C3—C4—C5—C6	179.22 (14)	C18A—N2—C15—C14	−9.3 (3)
C10—C5—C6—C7	0.4 (2)	C20—N2—C15—C16	−6.1 (2)
C4—C5—C6—C7	−179.83 (13)	C18B—N2—C15—C16	−161.04 (18)
C5—C6—C7—C8	0.4 (2)	C18A—N2—C15—C16	171.1 (2)
C6—C7—C8—C9	−0.9 (2)	C13—C14—C15—N2	−178.13 (12)
C7—C8—C9—C10	0.7 (2)	C13—C14—C15—C16	1.5 (2)
C6—C5—C10—C9	−0.63 (17)	N2—C15—C16—C17	178.46 (14)
C4—C5—C10—C9	179.56 (12)	C14—C15—C16—C17	−1.1 (2)
C6—C5—C10—C1	179.79 (12)	C15—C16—C17—C12	−0.8 (2)
C4—C5—C10—C1	−0.02 (17)	C13—C12—C17—C16	2.3 (2)
C8—C9—C10—C5	0.12 (19)	C11—C12—C17—C16	−176.30 (14)
C8—C9—C10—C1	179.69 (13)	C15—N2—C18A—C19A	178.1 (5)
C2—C1—C10—C5	1.40 (17)	C20—N2—C18A—C19A	−4.8 (6)
N1—C1—C10—C5	−172.78 (10)	C18B—N2—C18A—C19A	65.1 (6)
C2—C1—C10—C9	−178.16 (12)	C15—N2—C18B—C19B	−121.8 (4)
N1—C1—C10—C9	7.66 (17)	C20—N2—C18B—C19B	81.2 (4)
C1—N1—C11—C12	−172.94 (12)	C18A—N2—C18B—C19B	−41.2 (6)
N1—C11—C12—C17	−175.92 (13)	C15—N2—C20—C21	−81.05 (19)
N1—C11—C12—C13	5.5 (2)	C18B—N2—C20—C21	76.2 (2)
C17—C12—C13—O1	179.60 (12)	C18A—N2—C20—C21	102.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···N1	0.82	1.87	2.6060 (14)	148
C16—H16A···Cg1^{ii}	0.93	2.84	3.6475 (15)	145

C17—H17A···Cg2^{ii}	0.93	2.85	3.6502 (15)	145
C19A—H19A···Cg1^{iiii}	0.88	2.88	3.747 (7)	142
C19B—H19D···Cg1^{iiii}	0.88	2.88	3.688 (4)	149

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

Fig. 1

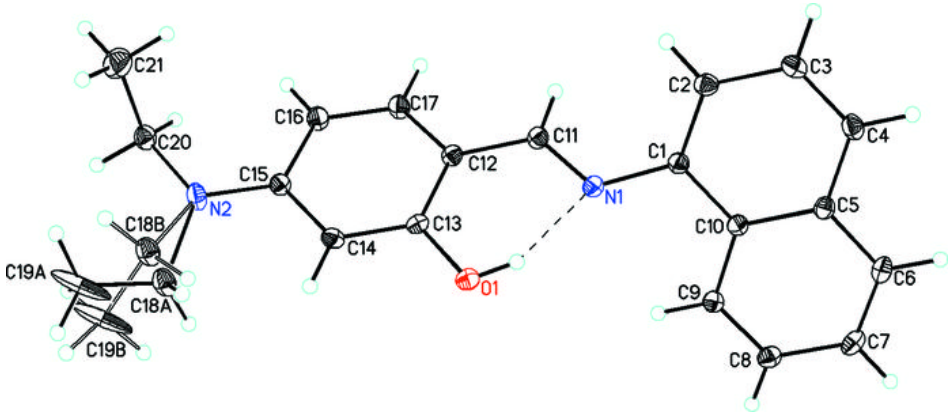
C21
C20
N2
C15
C16
C17
C12
C11
N1
C1
C2
C3
C4
C5
C10
C6
C9
C8
C7
C13
C14
O1
C18B
C19A
C18A
C19B

Fig. 2

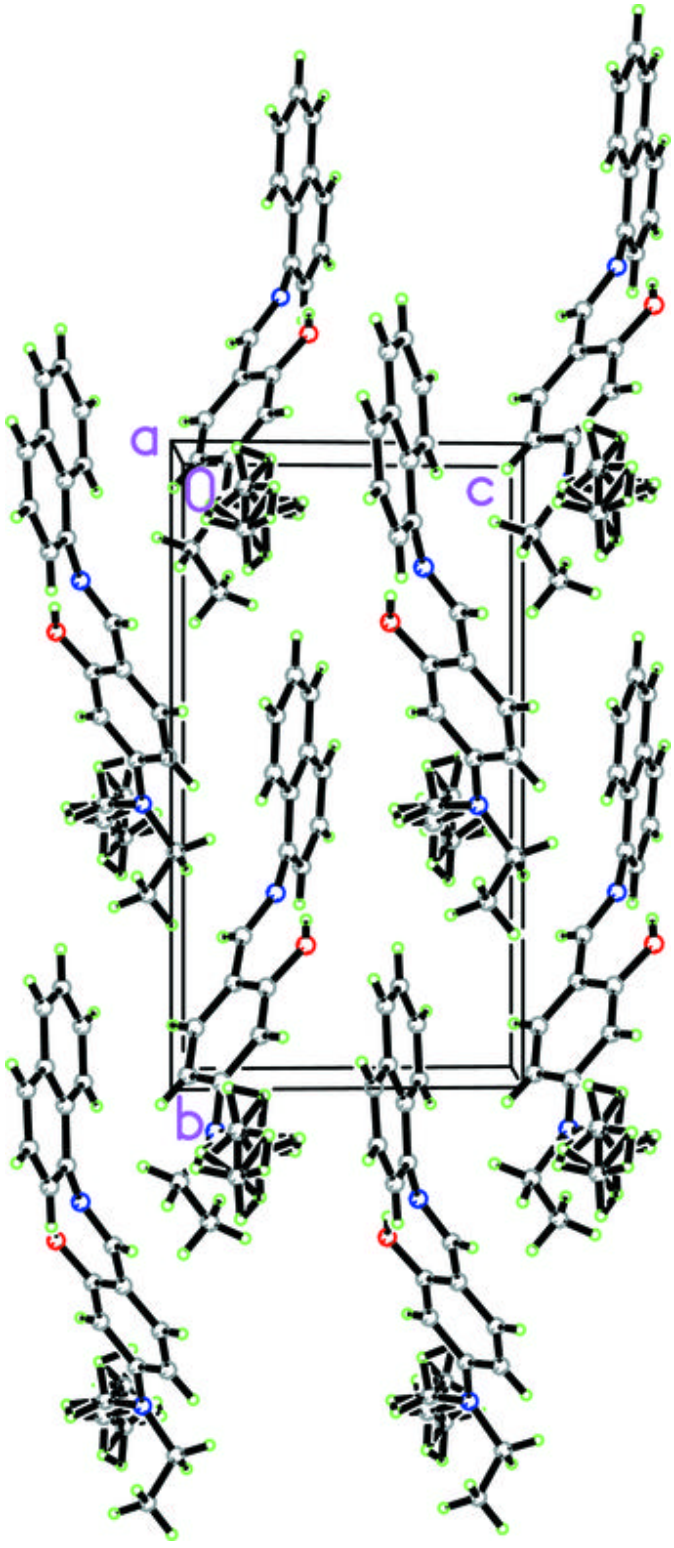

Fig. 3

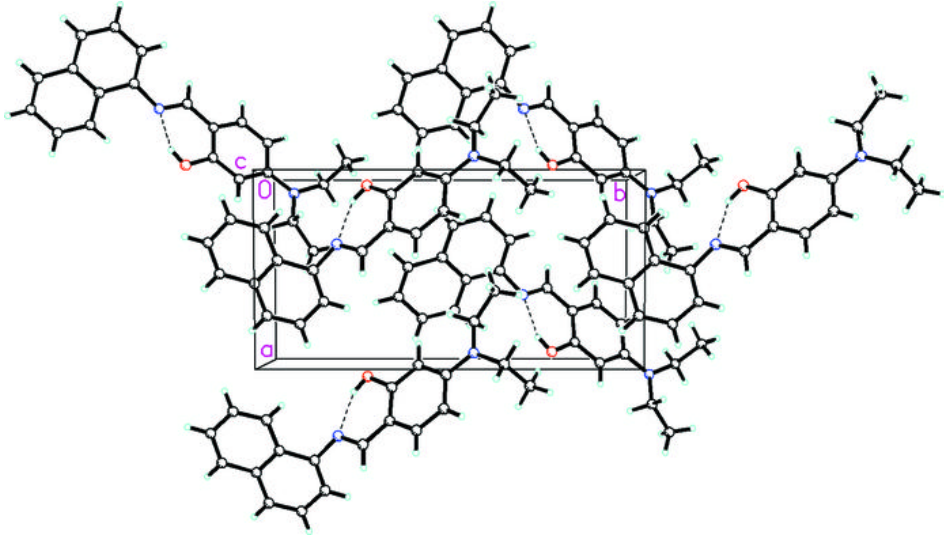

Fig. 4