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(*E*)-2-Methyl-6-[(*p*-tolylimino)methyl]-phenol

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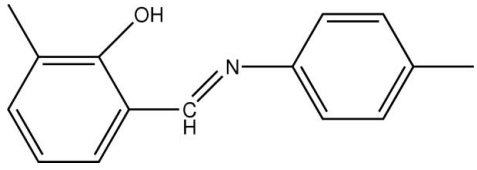
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.117; data-to-parameter ratio = 14.7.

The title compound, $C_{15}H_{15}NO$, adopts the enol–imine tautomeric form. There are two independent molecules in the asymmetric unit, with the two aromatic rings inclined at 14.94 (9) and 26.53 (5)°. The structure is stabilized by O—H···N intermolecular hydrogen bonds and C—H···π interactions.

Related literature

Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Hadjoudis *et al.*, 1987).

For related literature, see: Bernstein *et al.* (1995); Calligaris *et al.* (1972); Garnovski *et al.* (1993); Moustakali-Mavridis *et al.* (1978); Şahin *et al.* (2005).



Experimental

Crystal data

$C_{15}H_{15}NO$
M_r = 225.28
Triclinic, $P\overline{1}$
a = 7.9096 (6) Å
b = 11.2766 (8) Å
c = 14.1886 (10) Å
α = 77.291 (6)°
β = 85.053 (6)°
γ = 89.609 (6)°
V = 1229.83 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
0.50 × 0.35 × 0.24 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: none
20909 measured reflections
4830 independent reflections
2943 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 0.92
4830 reflections
328 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C1*A*–C6*A*, C1*B*–C6*B*, C9*A*–C14*A* and C9*B*–C14*B* rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C11*B*—H11*B*···O1*B*^{i}	0.93	2.60	3.302 (2)	133
O1*A*—H1*A*···N1*A*	1.04 (2)	1.68 (2)	2.6205 (17)	148.8 (19)
O1*B*—H1*B*···N1*B*	0.98 (2)	1.69 (3)	2.5915 (18)	150 (2)
C15*A*—H15*A*···*Cg*1^{ii}	0.96	2.86	3.647 (2)	140
C15*B*—H15*D*···*Cg*2^{iii}	0.96	2.84	3.731 (2)	154
C3*B*—H3*B*···*Cg*3^{ii}	0.93	3.11	3.8833 (19)	141
C7*A*—H7*B*···*Cg*4	0.96	2.86	3.791 (2)	163

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2013).

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supplementary materials

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(*E*)-2-Methyl-6-[(*p*-tolylimino)methyl]phenol

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Comment

Schiff have been extensively used as ligands in the field of coordination chemistry(Calligaris *et al.*, 1972; Garnovski *et al.*, 1993). Schiff base compounds can be classified by their photochromic and termochronic characteristics (Cohen *et al.*, 1964; Moustakali-Mavridis *et al.*, 1978;Hadjoudis *et al.*,1987). Based on studies of some thermochromic and Schiff base compounds, it has been proposed that molecules exhibiting monochromism are planar, while those exhibiting photochromic are non-planar(Moustakali-Mavridis *et al.*,1978). In this study, we report the structure of the title compound, (I). The asymmetric unit of (I) contains two independent molecules, A and B (Fig.1). Selected bond lengths and angles are given in Table 1. There is a good agreement between the bond lengths and angles of molecules A and B. The C6A—O1A, C8A=N1A, C6B—O1B and C8B=N1B bond lenghts confirm the enol-imin form of (I). These distances agree with the corresponding distance in (*E*)-2-methoxy-6- [(2-trifluoromethylphenylimino)methyl]phenol [1.346 (4) Å and 1.270 (5) Å; Şahin *et al.*, 2005], which also adopts the enol-imine form. The dihedral angle between the two benzene rings is 14.94 (5)° in molecule A and 26.53 (5)° in molecule B. Intramolecular O—H···N hydrogen bonds generate S(6) ring motifs (Bernstein *et al.*,1995)(Fig.1). In addition, molecules B are linked by C—H···O intermolecular hydrogen bonds in the crystal structure of (I). There are also C15A—H15A···*Cg*1^{ii}, C15B—H15D···*Cg*2^{iii} (*Cg*1 and *Cg*2 are centroid of the C1A—C6A and C1B—C6B rings, respectively) C3B—H3B···*Cg*3^{ii} and C7A—H7B···*Cg*4(*Cg*3 and *Cg*4 are centroid of the C9A—C14A and C9B—C14B rings, respectively) interactions (Fig. 2, Table 2).

Experimental

The compound (*E*)-2-[(4-acetylphenylimino)methyl]-6-methylphenol was prepared by reflux a mixture of a solution containing 3-methylsalicylaldehyde (0.1 ml 0.82 mmol) in 20 ml e thanol and a solution containing 4-acetylaniline (0.11 g 0.82 mmol) in 20 ml e thanol. The reaction mixture was stirred for 1 h under reflux. The crystals of (*E*)-2-[(4-acetylphenylimino)methyl]- 6-methylphenol suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield % 34; m.p. 375–377 K).

Refinement

The H1A and H1B atoms were located in a difference map and refined freely (distances given in Table 2). All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

Figures

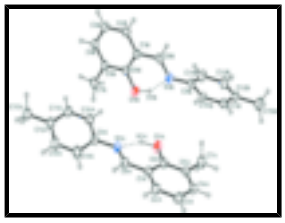


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability.

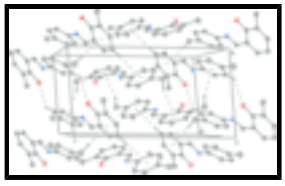


Fig. 2. A persvective view of the molecular packing of compound (I). Dashed lines indicate hydrogen bonds and C—H···π interactions. H atoms not involved in these interaction have been omitted for clarity.

(*E*)-2-Methyl-6-[(*p*-tolylimino)methyl]phenol

Crystal data

$C_{15}H_{15}NO$	$Z = 4$
$M_r = 225.28$	$F_{000} = 480$
Triclinic, $P\overline{1}$	$D_x = 1.217$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.9096$ (6) Å	Cell parameters from 18783 reflections
$b = 11.2766$ (8) Å	$\theta = 1.9$–29.6º
$c = 14.1886$ (10) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 77.291$ (6)º	$T = 296$ (2) K
$\beta = 85.053$ (6)º	Prism, yellow
$\gamma = 89.609$ (6)º	0.50 × 0.35 × 0.24 mm
$V = 1229.83$ (15) Å^3	

Data collection

Stoe IPDS II diffractometer	4830 independent reflections
Radiation source: fine-focus sealed tube	2943 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.053$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 296(2)$ K	$\theta_{min} = 1.9$º
rotation method scans	$h = -9\rightarrow9$
Absorption correction: none	$k = -13\rightarrow13$
20909 measured reflections	$l = -16\rightarrow17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.117$

$S = 0.92$

4830 reflections

328 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.16$ e Å^{-3}

$\Delta\rho_{min} = -0.12$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.019 (3)

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}
C1A	0.23665 (19)	0.27721 (13)	0.37918 (12)	0.0536 (4)
C2A	0.1707 (2)	0.16279 (14)	0.42648 (13)	0.0666 (4)
H2A	0.1335	0.1486	0.4920	0.080*
C3A	0.1602 (2)	0.07141 (15)	0.37789 (14)	0.0690 (5)
H3A	0.1160	−0.0043	0.4100	0.083*
C4A	0.2155 (2)	0.09258 (14)	0.28086 (13)	0.0613 (4)
H4A	0.2070	0.0302	0.2482	0.074*
C5A	0.28329 (19)	0.20322 (13)	0.23049 (12)	0.0561 (4)
C6A	0.29307 (18)	0.29602 (13)	0.28111 (12)	0.0535 (4)
C7A	0.3477 (3)	0.22438 (17)	0.12603 (14)	0.0818 (6)
H7A	0.3388	0.1503	0.1039	0.123*
H7B	0.4643	0.2505	0.1185	0.123*
H7C	0.2814	0.2860	0.0885	0.123*
C8A	0.2476 (2)	0.37106 (14)	0.43388 (13)	0.0574 (4)
H8A	0.204 (2)	0.3466 (15)	0.5044 (14)	0.072 (5)*
C9A	0.31094 (19)	0.56827 (13)	0.45024 (11)	0.0531 (4)
C10A	0.4080 (2)	0.67033 (14)	0.41056 (12)	0.0621 (4)
H10A	0.4684	0.6768	0.3504	0.074*
C11A	0.4170 (2)	0.76353 (15)	0.45894 (14)	0.0678 (5)
H11A	0.4837	0.8317	0.4304	0.081*

C12A	0.3306 (2)	0.75839 (14)	0.54776 (13)	0.0609 (4)
C13A	0.2324 (3)	0.65632 (17)	0.58553 (15)	0.0841 (6)
H13A	0.1707	0.6505	0.6453	0.101*
C14A	0.2213 (3)	0.56250 (16)	0.53879 (14)	0.0813 (6)
H14A	0.1531	0.4950	0.5670	0.098*
C15A	0.3405 (3)	0.85941 (17)	0.60073 (16)	0.0792 (5)
H15A	0.4558	0.8877	0.5956	0.119*
H15B	0.3020	0.8299	0.6678	0.119*
H15C	0.2701	0.9251	0.5726	0.119*
N1A	0.30543 (16)	0.47736 (11)	0.39523 (10)	0.0554 (3)
O1A	0.35994 (17)	0.40415 (10)	0.23241 (9)	0.0744 (4)
H1A	0.364 (3)	0.457 (2)	0.2836 (17)	0.110 (7)*
C1B	0.88929 (18)	0.65606 (13)	0.21026 (11)	0.0519 (4)
C2B	1.01065 (19)	0.68057 (14)	0.26863 (12)	0.0583 (4)
H2B	1.1005	0.6275	0.2816	0.070*
C3B	1.0002 (2)	0.78185 (15)	0.30757 (13)	0.0644 (4)
H3B	1.0816	0.7972	0.3471	0.077*
C4B	0.8667 (2)	0.86086 (14)	0.28724 (12)	0.0626 (4)
H4B	0.8607	0.9298	0.3132	0.075*
C5B	0.74271 (19)	0.84109 (14)	0.23002 (12)	0.0572 (4)
C6B	0.75455 (18)	0.73671 (14)	0.19187 (11)	0.0551 (4)
C7B	0.5984 (2)	0.92663 (17)	0.20821 (15)	0.0763 (5)
H7E	0.6112	0.9944	0.2379	0.114*
H7F	0.4932	0.8850	0.2335	0.114*
H7D	0.5984	0.9553	0.1393	0.114*
C8B	0.9041 (2)	0.54888 (14)	0.16924 (12)	0.0569 (4)
H8B	0.999 (2)	0.4956 (15)	0.1862 (12)	0.068 (5)*
C9B	0.80495 (19)	0.41573 (14)	0.07874 (12)	0.0558 (4)
C10B	0.72686 (19)	0.41690 (15)	−0.00490 (12)	0.0602 (4)
H10B	0.6719	0.4865	−0.0347	0.072*
C11B	0.7298 (2)	0.31583 (16)	−0.04446 (13)	0.0639 (4)
H11B	0.6786	0.3190	−0.1015	0.077*
C12B	0.8071 (2)	0.20989 (16)	−0.00153 (13)	0.0639 (4)
C13B	0.8825 (2)	0.20895 (16)	0.08259 (14)	0.0740 (5)
H13B	0.9350	0.1386	0.1131	0.089*
C14B	0.8819 (2)	0.31007 (15)	0.12260 (14)	0.0705 (5)
H14B	0.9338	0.3070	0.1795	0.085*
C15B	0.8069 (3)	0.09968 (18)	−0.04533 (16)	0.0880 (6)
H15D	0.8968	0.1075	−0.0964	0.132*
H15E	0.7000	0.0933	−0.0712	0.132*
H15F	0.8239	0.0281	0.0037	0.132*
N1B	0.79365 (16)	0.52231 (12)	0.11649 (10)	0.0603 (3)
O1B	0.63181 (15)	0.71702 (13)	0.13661 (10)	0.0774 (4)
H1B	0.662 (3)	0.641 (2)	0.1163 (17)	0.118 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1A	0.0567 (8)	0.0498 (8)	0.0552 (10)	−0.0006 (6)	−0.0050 (7)	−0.0137 (7)
C2A	0.0800 (11)	0.0582 (9)	0.0602 (11)	−0.0147 (8)	0.0033 (8)	−0.0130 (8)
C3A	0.0798 (11)	0.0549 (9)	0.0721 (12)	−0.0175 (8)	0.0011 (9)	−0.0159 (9)
C4A	0.0639 (9)	0.0546 (9)	0.0709 (12)	−0.0030 (7)	−0.0075 (8)	−0.0247 (8)
C5A	0.0575 (9)	0.0537 (9)	0.0593 (10)	0.0030 (7)	−0.0041 (7)	−0.0176 (8)
C6A	0.0571 (8)	0.0459 (8)	0.0570 (10)	0.0006 (6)	−0.0057 (7)	−0.0102 (7)
C7A	0.1063 (14)	0.0729 (12)	0.0681 (12)	−0.0071 (10)	0.0107 (11)	−0.0265 (10)
C8A	0.0642 (9)	0.0526 (9)	0.0561 (10)	−0.0011 (7)	−0.0040 (8)	−0.0138 (8)
C9A	0.0583 (8)	0.0486 (8)	0.0540 (9)	0.0023 (6)	−0.0066 (7)	−0.0138 (7)
C10A	0.0710 (10)	0.0567 (9)	0.0586 (10)	−0.0059 (7)	0.0010 (8)	−0.0152 (8)
C11A	0.0745 (11)	0.0559 (9)	0.0756 (12)	−0.0104 (8)	−0.0042 (9)	−0.0207 (9)
C12A	0.0667 (10)	0.0550 (9)	0.0664 (11)	0.0091 (7)	−0.0132 (8)	−0.0225 (8)
C13A	0.1088 (15)	0.0715 (12)	0.0738 (13)	−0.0092 (10)	0.0212 (11)	−0.0311 (10)
C14A	0.1053 (14)	0.0608 (10)	0.0773 (13)	−0.0187 (9)	0.0244 (11)	−0.0259 (10)
C15A	0.0890 (13)	0.0702 (11)	0.0892 (14)	0.0066 (9)	−0.0150 (11)	−0.0383 (10)
N1A	0.0633 (7)	0.0469 (7)	0.0579 (8)	0.0019 (6)	−0.0063 (6)	−0.0151 (6)
O1A	0.1094 (9)	0.0509 (6)	0.0598 (8)	−0.0139 (6)	0.0066 (7)	−0.0102 (6)
C1B	0.0517 (8)	0.0535 (8)	0.0515 (9)	−0.0038 (6)	−0.0004 (7)	−0.0153 (7)
C2B	0.0574 (9)	0.0585 (9)	0.0603 (10)	0.0020 (7)	−0.0091 (7)	−0.0144 (8)
C3B	0.0691 (10)	0.0664 (10)	0.0633 (11)	−0.0034 (8)	−0.0137 (8)	−0.0228 (9)
C4B	0.0735 (10)	0.0576 (9)	0.0607 (11)	−0.0046 (8)	−0.0017 (8)	−0.0226 (8)
C5B	0.0612 (9)	0.0566 (9)	0.0540 (10)	0.0006 (7)	0.0021 (7)	−0.0153 (8)
C6B	0.0532 (8)	0.0625 (9)	0.0520 (9)	−0.0019 (7)	−0.0049 (7)	−0.0176 (7)
C7B	0.0802 (12)	0.0700 (11)	0.0821 (13)	0.0162 (9)	−0.0087 (10)	−0.0239 (10)
C8B	0.0552 (9)	0.0572 (9)	0.0593 (10)	−0.0019 (7)	−0.0011 (8)	−0.0164 (8)
C9B	0.0564 (9)	0.0572 (9)	0.0568 (10)	−0.0027 (7)	−0.0014 (7)	−0.0202 (8)
C10B	0.0569 (9)	0.0644 (10)	0.0625 (10)	−0.0008 (7)	−0.0064 (8)	−0.0202 (8)
C11B	0.0588 (9)	0.0774 (11)	0.0599 (11)	−0.0080 (8)	−0.0039 (8)	−0.0250 (9)
C12B	0.0655 (10)	0.0656 (10)	0.0651 (11)	−0.0088 (8)	0.0028 (8)	−0.0272 (9)
C13B	0.0917 (13)	0.0607 (10)	0.0751 (13)	0.0084 (9)	−0.0179 (10)	−0.0229 (9)
C14B	0.0852 (12)	0.0668 (11)	0.0666 (12)	0.0042 (9)	−0.0203 (9)	−0.0250 (9)
C15B	0.1060 (15)	0.0790 (13)	0.0894 (15)	−0.0067 (11)	−0.0049 (12)	−0.0421 (12)
N1B	0.0623 (8)	0.0612 (8)	0.0623 (9)	−0.0011 (6)	−0.0049 (7)	−0.0244 (7)
O1B	0.0668 (7)	0.0895 (9)	0.0906 (10)	0.0160 (6)	−0.0281 (7)	−0.0436 (8)

Geometric parameters (Å, °)

C1A—C6A	1.395 (2)	C1B—C2B	1.387 (2)
C1A—C2A	1.398 (2)	C1B—C6B	1.400 (2)
C1A—C8A	1.451 (2)	C1B—C8B	1.452 (2)
C2A—C3A	1.367 (2)	C2B—C3B	1.373 (2)
C2A—H2A	0.9300	C2B—H2B	0.9300
C3A—C4A	1.377 (2)	C3B—C4B	1.385 (2)
C3A—H3A	0.9300	C3B—H3B	0.9300
C4A—C5A	1.380 (2)	C4B—C5B	1.375 (2)
C4A—H4A	0.9300	C4B—H4B	0.9300
C5A—C6A	1.399 (2)	C5B—C6B	1.399 (2)
C5A—C7A	1.493 (2)	C5B—C7B	1.498 (2)
C6A—O1A	1.3488 (18)	C6B—O1B	1.3480 (18)

C7A—H7A	0.9600	C7B—H7E	0.9600
C7A—H7B	0.9600	C7B—H7F	0.9600
C7A—H7C	0.9600	C7B—H7D	0.9600
C8A—N1A	1.274 (2)	C8B—N1B	1.276 (2)
C8A—H8A	1.008 (18)	C8B—H8B	0.970 (17)
C9A—C10A	1.372 (2)	C9B—C14B	1.381 (2)
C9A—C14A	1.377 (2)	C9B—C10B	1.382 (2)
C9A—N1A	1.4215 (18)	C9B—N1B	1.4188 (19)
C10A—C11A	1.381 (2)	C10B—C11B	1.376 (2)
C10A—H10A	0.9300	C10B—H10B	0.9300
C11A—C12A	1.370 (2)	C11B—C12B	1.380 (2)
C11A—H11A	0.9300	C11B—H11B	0.9300
C12A—C13A	1.373 (3)	C12B—C13B	1.378 (2)
C12A—C15A	1.502 (2)	C12B—C15B	1.507 (2)
C13A—C14A	1.374 (2)	C13B—C14B	1.381 (2)
C13A—H13A	0.9300	C13B—H13B	0.9300
C14A—H14A	0.9300	C14B—H14B	0.9300
C15A—H15A	0.9600	C15B—H15D	0.9600
C15A—H15B	0.9600	C15B—H15E	0.9600
C15A—H15C	0.9600	C15B—H15F	0.9600
O1A—H1A	1.04 (2)	O1B—H1B	0.98 (2)
C6A—C1A—C2A	118.49 (14)	C2B—C1B—C6B	118.65 (13)
C6A—C1A—C8A	122.34 (14)	C2B—C1B—C8B	119.97 (14)
C2A—C1A—C8A	119.15 (15)	C6B—C1B—C8B	121.38 (14)
C3A—C2A—C1A	121.01 (16)	C3B—C2B—C1B	121.06 (15)
C3A—C2A—H2A	119.5	C3B—C2B—H2B	119.5
C1A—C2A—H2A	119.5	C1B—C2B—H2B	119.5
C2A—C3A—C4A	119.37 (15)	C2B—C3B—C4B	119.07 (15)
C2A—C3A—H3A	120.3	C2B—C3B—H3B	120.5
C4A—C3A—H3A	120.3	C4B—C3B—H3B	120.5
C3A—C4A—C5A	122.27 (14)	C5B—C4B—C3B	122.39 (15)
C3A—C4A—H4A	118.9	C5B—C4B—H4B	118.8
C5A—C4A—H4A	118.9	C3B—C4B—H4B	118.8
C4A—C5A—C6A	117.74 (15)	C4B—C5B—C6B	117.69 (14)
C4A—C5A—C7A	121.96 (14)	C4B—C5B—C7B	122.27 (14)
C6A—C5A—C7A	120.28 (14)	C6B—C5B—C7B	120.04 (15)
O1A—C6A—C1A	120.87 (13)	O1B—C6B—C5B	117.50 (14)
O1A—C6A—C5A	118.03 (14)	O1B—C6B—C1B	121.37 (14)
C1A—C6A—C5A	121.10 (14)	C5B—C6B—C1B	121.13 (14)
C5A—C7A—H7A	109.5	C5B—C7B—H7E	109.5
C5A—C7A—H7B	109.5	C5B—C7B—H7F	109.5
H7A—C7A—H7B	109.5	H7E—C7B—H7F	109.5
C5A—C7A—H7C	109.5	C5B—C7B—H7D	109.5
H7A—C7A—H7C	109.5	H7E—C7B—H7D	109.5
H7B—C7A—H7C	109.5	H7F—C7B—H7D	109.5
N1A—C8A—C1A	122.40 (16)	N1B—C8B—C1B	121.77 (15)
N1A—C8A—H8A	122.4 (9)	N1B—C8B—H8B	120.9 (10)
C1A—C8A—H8A	115.2 (9)	C1B—C8B—H8B	117.3 (10)
C10A—C9A—C14A	118.05 (14)	C14B—C9B—C10B	118.41 (14)

C10A—C9A—N1A	117.47 (14)	C14B—C9B—N1B	124.15 (15)
C14A—C9A—N1A	124.44 (14)	C10B—C9B—N1B	117.37 (14)
C9A—C10A—C11A	120.77 (16)	C11B—C10B—C9B	120.49 (16)
C9A—C10A—H10A	119.6	C11B—C10B—H10B	119.8
C11A—C10A—H10A	119.6	C9B—C10B—H10B	119.8
C12A—C11A—C10A	121.90 (16)	C10B—C11B—C12B	121.61 (16)
C12A—C11A—H11A	119.1	C10B—C11B—H11B	119.2
C10A—C11A—H11A	119.1	C12B—C11B—H11B	119.2
C11A—C12A—C13A	116.41 (15)	C13B—C12B—C11B	117.51 (15)
C11A—C12A—C15A	122.06 (16)	C13B—C12B—C15B	121.71 (17)
C13A—C12A—C15A	121.53 (17)	C11B—C12B—C15B	120.78 (17)
C12A—C13A—C14A	122.75 (17)	C12B—C13B—C14B	121.51 (17)
C12A—C13A—H13A	118.6	C12B—C13B—H13B	119.2
C14A—C13A—H13A	118.6	C14B—C13B—H13B	119.2
C13A—C14A—C9A	120.11 (17)	C13B—C14B—C9B	120.45 (16)
C13A—C14A—H14A	119.9	C13B—C14B—H14B	119.8
C9A—C14A—H14A	119.9	C9B—C14B—H14B	119.8
C12A—C15A—H15A	109.5	C12B—C15B—H15D	109.5
C12A—C15A—H15B	109.5	C12B—C15B—H15E	109.5
H15A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
C12A—C15A—H15C	109.5	C12B—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15D—C15B—H15F	109.5
H15B—C15A—H15C	109.5	H15E—C15B—H15F	109.5
C8A—N1A—C9A	121.10 (14)	C8B—N1B—C9B	121.94 (14)
C6A—O1A—H1A	105.8 (12)	C6B—O1B—H1B	105.7 (13)
C6A—C1A—C2A—C3A	−0.5 (2)	C6B—C1B—C2B—C3B	−0.2 (2)
C8A—C1A—C2A—C3A	−179.19 (16)	C8B—C1B—C2B—C3B	179.44 (15)
C1A—C2A—C3A—C4A	0.0 (3)	C1B—C2B—C3B—C4B	−0.5 (2)
C2A—C3A—C4A—C5A	0.6 (3)	C2B—C3B—C4B—C5B	0.6 (3)
C3A—C4A—C5A—C6A	−0.7 (2)	C3B—C4B—C5B—C6B	0.1 (2)
C3A—C4A—C5A—C7A	178.17 (17)	C3B—C4B—C5B—C7B	179.95 (16)
C2A—C1A—C6A—O1A	−179.06 (14)	C4B—C5B—C6B—O1B	179.35 (15)
C8A—C1A—C6A—O1A	−0.5 (2)	C7B—C5B—C6B—O1B	−0.6 (2)
C2A—C1A—C6A—C5A	0.4 (2)	C4B—C5B—C6B—C1B	−0.9 (2)
C8A—C1A—C6A—C5A	179.04 (14)	C7B—C5B—C6B—C1B	179.25 (15)
C4A—C5A—C6A—O1A	179.67 (14)	C2B—C1B—C6B—O1B	−179.26 (15)
C7A—C5A—C6A—O1A	0.8 (2)	C8B—C1B—C6B—O1B	1.1 (2)
C4A—C5A—C6A—C1A	0.2 (2)	C2B—C1B—C6B—C5B	1.0 (2)
C7A—C5A—C6A—C1A	−178.71 (16)	C8B—C1B—C6B—C5B	−178.73 (14)
C6A—C1A—C8A—N1A	1.8 (2)	C2B—C1B—C8B—N1B	178.88 (15)
C2A—C1A—C8A—N1A	−179.63 (16)	C6B—C1B—C8B—N1B	−1.4 (2)
C14A—C9A—C10A—C11A	0.9 (3)	C14B—C9B—C10B—C11B	−1.6 (2)
N1A—C9A—C10A—C11A	178.81 (15)	N1B—C9B—C10B—C11B	−178.71 (13)
C9A—C10A—C11A—C12A	0.0 (3)	C9B—C10B—C11B—C12B	1.3 (2)
C10A—C11A—C12A—C13A	−1.0 (3)	C10B—C11B—C12B—C13B	−0.4 (2)
C10A—C11A—C12A—C15A	179.83 (16)	C10B—C11B—C12B—C15B	179.19 (16)
C11A—C12A—C13A—C14A	0.9 (3)	C11B—C12B—C13B—C14B	−0.3 (3)
C15A—C12A—C13A—C14A	−179.85 (19)	C15B—C12B—C13B—C14B	−179.83 (18)
C12A—C13A—C14A—C9A	0.0 (3)	C12B—C13B—C14B—C9B	0.0 (3)

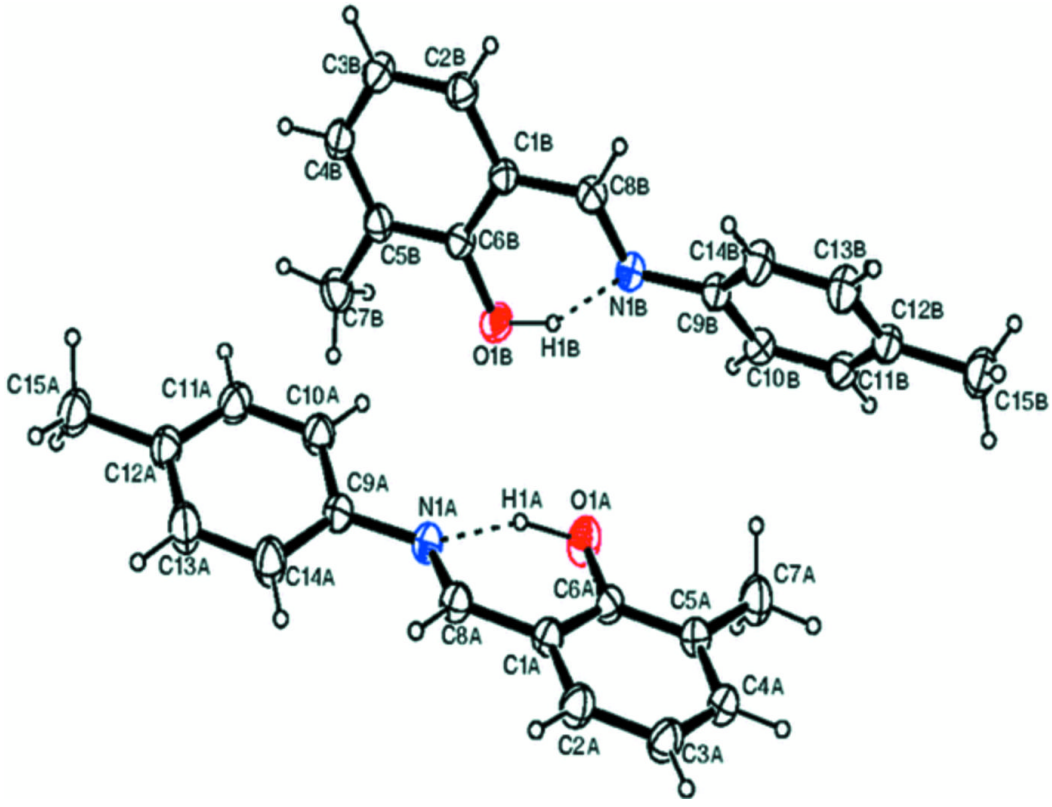
C10A—C9A—C14A—C13A	−0.9 (3)	C10B—C9B—C14B—C13B	0.9 (3)
N1A—C9A—C14A—C13A	−178.67 (18)	N1B—C9B—C14B—C13B	177.86 (16)
C1A—C8A—N1A—C9A	178.55 (13)	C1B—C8B—N1B—C9B	−178.03 (14)
C10A—C9A—N1A—C8A	165.81 (15)	C14B—C9B—N1B—C8B	28.3 (2)
C14A—C9A—N1A—C8A	−16.5 (2)	C10B—C9B—N1B—C8B	−154.72 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11B—H11B···O1B^{i}	0.93	2.60	3.302 (2)	133
O1A—H1A···N1A	1.04 (2)	1.68 (2)	2.6205 (17)	148.8 (19)
O1B—H1B···N1B	0.98 (2)	1.69 (3)	2.5915 (18)	150 (2)
C15A—H15A···Cg1^{ii}	0.96	2.86	3.647 (2)	140
C15B—H15D···Cg2^{iii}	0.96	2.84	3.731 (2)	154
C3B—H3B···Cg3^{ii}	0.93	3.11	3.8833 (19)	141
C7A—H7B···Cg4	0.96	2.86	3.791 (2)	163

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

Fig. 1


C3B
C2B
C1B
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C5B
C6B
C14B
C13B
C7B
N1B
C9B
C12B
O1B
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C12A
C9A
N1A
H1A
O1A
C13A
C14A
C6A
C5A
C7A
C8A
C1A
C4A
C2A
C3A

Fig. 2