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4-[(*E*)-Phenyldiazenyl]-2-[(*E*)-phenyliminomethyl]phenol

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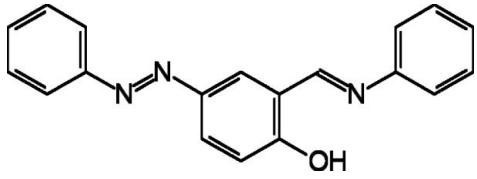
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.062; wR factor = 0.164; data-to-parameter ratio = 22.8.

The title azo–azomethine dye, $C_{19}H_{15}N_3O$, was synthesized by the reaction of 2-hydroxy-5-[(*E*)-phenyldiazenyl]benzaldehyde with aniline. With respect to the azo double bond, the two attached benzene rings display a *trans* configuration with a C—N=N—C torsion angle of 178.5 (3)°. The structure is stabilized by intramolecular O—H···N and intermolecular C—H···O hydrogen bonds.

Related literature

For related literature, see: Dal *et al.* (2007); Gordon & Gregory (1983); Jarrahpour *et al.* (2004); Karadayı *et al.* (2006*a*,*b*); Nedeltcheva *et al.* (2005); Yang *et al.* (2007); Zhang *et al.* (2007); Zollinger (1987).



Experimental

Crystal data

$C_{19}H_{15}N_3O$
M_r = 301.34
Monoclinic, $P2_1/c$
a = 10.336 (5) Å
b = 12.585 (5) Å
c = 12.384 (5) Å
β = 100.497 (5)°
V = 1583.9 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.2 × 0.2 × 0.2 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.791, T_{max} = 1
(expected range 0.983–0.984)
46323 measured reflections
4847 independent reflections
2551 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.164
S = 1.05
4847 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H9···N1	0.82	1.85	2.579 (2)	148
C7—H7···O1^{i}	0.995 (19)	2.50 (2)	3.448 (3)	158.4 (14)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: AT2350).

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supplementary materials

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4-[(*E*)-Phenyldiazenyl]-2-[(*E*)-phenyliminomethyl]phenol

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Comment

The application of aromatic azo dyes and Schiff bases in science and technology is well known and well documented (Gordon & Gregory, 1983; Zollinger, 1987; Nedeltcheva *et al.*, 2005). Synthetic dyes are widely used in a number of industries such as textile, leather, cosmetics, food and paper printing. Both Schiff bases and azo compounds are important structures in the medicinal and pharmaceutical fields and it has been suggested that the azomethine linkage might be responsible for the biological activities displayed by Schiff bases (Jarrahpour *et al.*, 2004). A good knowledge of the structure of dyes is the key to understand its properties and reactivity. Because of the importance of azo-azomethine compounds and in continuance of our interest in syntheses of azo and azomethine compounds we report herein the synthesis and structure of, (I), 4-[(*E*)-phenyldiazenyl]-2-[(*E*)-(phenylimino)methyl]phenol.

The *ORTEP-3* (Farrugia, 1997) diagram of the molecule of (I) is illustrated in Fig.1. The crystal structure of the title compound which contains three benzene rings, an azo- (—N ═N—) and azomethine (—CH ═N—) groups. Individually each six-membered rings of benzene in the molecule is nearly planar with showing small distortions. The C5, C8, and C17 atoms deviate from the each benzene best plane by −0.009 (2), 0.0070 (2), and −0.0046 (2) Å. All bond lenghts and angles in (C14—C19), (C8—C13), and (C1—C6) benzene rings have normal values and; the average C—C bond lengths within these rings are 1.382 (3), 1.394 (2) and 1.372 (3) Å. The A/B, A/C and B/C dihedral angles between the planes of benzene rings, respectively, A(C14/C19), B(C8/C13, O1) and C(C1/C6) are 22.8 (5), 56.3 (5) and 39.8 (5)° which imply that aromatic rings rotate oppositely along the N2 ═N3 and N1—C7 axes. The whole molecule is not planar and the D/E diheadral angle between the planes of azo and azomethine groups [D(C14/N3/N2/C12) and E(C8/C7/N1/C6)] is 13.7 (2); the maximum deviations from the mean plane are −0.010 (2) and −0.028 (2) Å for atoms C12 and C7, respectively. With respect to the azo double bond, two benzene rings displays *trans* configuration and the torsion angle C12—N2—N3—C14 is 178.5 (3)°. This angle is reported in literature as −175.83° (Yang *et al.*, 2007) and 179.80 (17)° (Karadayı *et al.*, 2006*a*). The bond distance of azo linkage between N2 ═N3 [1.238 (2) Å] shows a small difference from the N═N distance found various compounds containing azobenzene group [1.255 (2) (Yang *et al.*, 2007)], 1.250 (2) (Karadayı *et al.*, 2006*b*), 1.257 (4) Å (Zhang *et al.*, 2007)]. The N2—C12 and N3—C14 bond lengths are 1.428 (2) and 1.432 (2) Å and also comparable with values in the literaure.

In azomethine group, a strong O—H···N intra-molecular hydrogen bond is observed (Fig.1) [N1···O1; 2.579 Å, N1···H9—O1; 147.93°] (Table 1) and this type hydrogen bond causes to reversible proton transfer between the amino N atom and the hydroxyl O atom. Similar interaction was found and showed good agreement with the values in the enol-imine tautomer structure (Dal *et al.*, 2007). In addition C9—O1 and N1—C7 bonds of 1.343 (2) and 1.283 (4) Å confirm single- and double-bond characters. The crystal packing (Fig. 2) is stabilized by C—H···O intermolecular hydrogen-bonding interaction in the unit cell.

Experimental

The azo-azomethine dye was prepared according to the known condensation method. The freshly destilled aniline (0.043 g, 50 mmol) and 0.1037 g (0.46 mmol) of 2-hydroxy-5-[(*E*)-phenyldiazenyl]benzaldehyde was dissolved in 75 ml absolute ethyl alcohol with a few drops of glacial acetic acid as a catalyst. The solution was refluxed for 5 h and then left at room temperature. After cooling, the azo-azomethine dye was obtained as orange microcrystals. The microcrystals were filtered off, washed with 20 ml of cold absolute ethyl alcohol and then dried. The dye was recrystallized from ethyl alcohol to produce crystals of suitable quality for X-ray diffraction analysis. Yield: 0.12 g (85%). m. p.: 410–411 K. Analysis calculated for $C_{19}H_{15}N_3O$: C 75.73, H 5.02, N 13.94%. Found: C 75.64, H 5.09, N 13.86%. IR(cm^{-1}, KBr): 3420 (Ar—OH), 3049 (Ar—C—H), 1620 (—CH═N—), 1346 (—N═ N—). ^{1}H NMR (DMSO-d$_6$, p.p.m.); 13.87 (s, 1H, —OH), 9.17 (s, 1H, —CH═ N—), 8.32–8.30 (d, Ar—H), 8.04–7.99 (dd, Ar—H), 7.88–7.85 (d, Ar—H), 7.62–7.57 (m, Ar—H).

Refinement

The H atom on C7 was located in difference maps and its coordinates and U_{iso} value was refined freely. In the final stage of refinement, the other H atoms were located in geometrically idealized positions (C—H = 0.93 and O—H = 0.82 Å) and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Figures

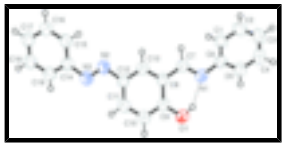

Fig. 1. Molecular structure of the title compound with atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

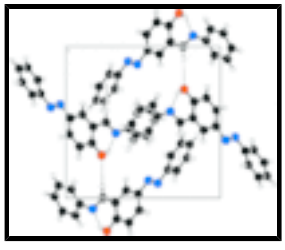

Fig. 2. The crystal packing of the title compound down the *a* axis.

4-[(*E*)-Phenyldiazenyl]-2-[(*E*)-phenyliminomethyl]phenol

Crystal data

$C_{19}H_{15}N_3O$	F_{000} = 632
M_r = 301.34	D_x = 1.264 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6602 reflections
a = 10.336 (5) Å	θ = 2.3–30.5°
b = 12.585 (5) Å	μ = 0.08 mm^{-1}

c = 12.384 (5) Å	T = 293 (2) K
β = 100.497 (5)º	Needle, orange
V = 1583.9 (12) Å^3	0.2 × 0.2 × 0.2 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	R_{int} = 0.085
dtprofit.ref scans	θ_{max} = 30.6º
Absorption correction: multi-scan (Blessing, 1995)	θ_{min} = 2.3º
T_{min} = 0.791, T_{max} = 1	h = −14→14
46323 measured reflections	k = −17→17
4847 independent reflections	l = −17→17
2551 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.1046P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.062	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.164	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
4847 reflections	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
213 parameters	Extinction coefficient: 0.0125 (18)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.48073 (14)	−0.23333 (10)	0.71712 (9)	0.0751 (4)
H9	0.5287	−0.2752	0.6924	0.113*
H7	0.5447 (17)	−0.2617 (13)	0.4220 (16)	0.072 (5)*
N2	0.24465 (14)	0.03594 (11)	0.38273 (11)	0.0621 (4)
N3	0.15665 (14)	0.09609 (11)	0.40169 (12)	0.0641 (4)
N1	0.59285 (13)	−0.32426 (10)	0.57180 (11)	0.0575 (4)
C12	0.30030 (17)	−0.03066 (13)	0.47264 (13)	0.0574 (4)
C8	0.44771 (16)	−0.17781 (12)	0.52874 (13)	0.0540 (4)
C9	0.42251 (17)	−0.16835 (13)	0.63667 (13)	0.0591 (4)

C6	0.67019 (16)	−0.40859 (12)	0.53999 (13)	0.0546 (4)
C14	0.10512 (17)	0.16376 (13)	0.31110 (13)	0.0578 (4)
C7	0.53349 (17)	−0.25941 (13)	0.50009 (15)	0.0580 (4)
C13	0.38619 (16)	−0.10726 (13)	0.44932 (13)	0.0585 (4)
H13	0.4036	−0.112	0.3784	0.07*
C10	0.33650 (19)	−0.09080 (15)	0.66034 (15)	0.0717 (5)
H10	0.3199	−0.0844	0.7314	0.086*
C15	0.16560 (17)	0.18035 (13)	0.22070 (14)	0.0619 (4)
H15	0.2437	0.1456	0.2158	0.074*
C16	0.1088 (2)	0.24865 (14)	0.13864 (15)	0.0690 (5)
H16	0.1482	0.2592	0.0777	0.083*
C5	0.78119 (18)	−0.43801 (14)	0.61248 (15)	0.0673 (5)
H5	0.804	−0.4028	0.6793	0.081*
C19	−0.00986 (19)	0.21633 (15)	0.31761 (16)	0.0727 (5)
H19	−0.0503	0.2058	0.378	0.087*
C17	−0.0057 (2)	0.30123 (15)	0.14625 (16)	0.0764 (6)
H17	−0.0428	0.3482	0.0912	0.092*
C18	−0.0652 (2)	0.28446 (17)	0.23504 (16)	0.0819 (6)
H18	−0.1434	0.3193	0.2395	0.098*
C1	0.63438 (18)	−0.46354 (14)	0.44241 (14)	0.0656 (5)
H1	0.558	−0.4451	0.3939	0.079*
C11	0.27546 (19)	−0.02315 (14)	0.57930 (15)	0.0689 (5)
H11	0.2172	0.028	0.5959	0.083*
C2	0.7120 (2)	−0.54561 (15)	0.41722 (17)	0.0779 (6)
H2	0.6884	−0.5822	0.3513	0.093*
C4	0.8591 (2)	−0.51975 (16)	0.58651 (18)	0.0843 (6)
H4	0.9354	−0.5386	0.6349	0.101*
C3	0.8235 (2)	−0.57321 (16)	0.48888 (19)	0.0859 (6)
H3	0.8757	−0.6286	0.4715	0.103*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0919 (10)	0.0822 (8)	0.0507 (7)	0.0245 (7)	0.0117 (6)	0.0054 (6)
N2	0.0631 (9)	0.0604 (8)	0.0607 (9)	0.0068 (7)	0.0062 (7)	−0.0030 (7)
N3	0.0637 (9)	0.0631 (9)	0.0639 (9)	0.0064 (7)	0.0068 (7)	−0.0030 (7)
N1	0.0596 (8)	0.0574 (8)	0.0543 (8)	0.0055 (6)	0.0074 (6)	0.0010 (6)
C12	0.0594 (10)	0.0562 (9)	0.0548 (10)	0.0016 (8)	0.0056 (8)	0.0003 (8)
C8	0.0560 (10)	0.0548 (9)	0.0501 (9)	0.0016 (7)	0.0064 (7)	−0.0006 (7)
C9	0.0643 (11)	0.0614 (10)	0.0499 (9)	0.0051 (8)	0.0060 (7)	0.0007 (8)
C6	0.0589 (10)	0.0520 (9)	0.0545 (10)	0.0013 (7)	0.0145 (8)	0.0064 (7)
C14	0.0599 (10)	0.0553 (9)	0.0551 (9)	0.0030 (8)	0.0020 (8)	−0.0037 (8)
C7	0.0608 (10)	0.0625 (10)	0.0505 (10)	0.0023 (8)	0.0098 (8)	0.0026 (8)
C13	0.0612 (10)	0.0612 (9)	0.0529 (9)	0.0022 (8)	0.0097 (8)	0.0006 (8)
C10	0.0829 (13)	0.0783 (12)	0.0555 (11)	0.0147 (10)	0.0167 (9)	−0.0039 (9)
C15	0.0624 (11)	0.0575 (10)	0.0656 (11)	0.0052 (8)	0.0111 (9)	−0.0040 (8)
C16	0.0831 (14)	0.0648 (10)	0.0586 (11)	0.0055 (10)	0.0117 (9)	0.0025 (8)
C5	0.0746 (12)	0.0638 (10)	0.0613 (11)	0.0087 (9)	0.0064 (9)	0.0050 (8)

C19	0.0706 (12)	0.0864 (13)	0.0614 (11)	0.0166 (10)	0.0130 (9)	−0.0034 (10)
C17	0.0888 (15)	0.0722 (12)	0.0627 (12)	0.0194 (11)	−0.0005 (10)	0.0009 (9)
C18	0.0765 (14)	0.0959 (15)	0.0697 (13)	0.0331 (11)	0.0033 (10)	−0.0036 (11)
C1	0.0684 (12)	0.0651 (10)	0.0632 (11)	−0.0006 (9)	0.0117 (9)	−0.0053 (9)
C11	0.0698 (12)	0.0688 (11)	0.0680 (12)	0.0149 (9)	0.0122 (9)	−0.0049 (9)
C2	0.0968 (15)	0.0688 (11)	0.0720 (13)	0.0029 (11)	0.0258 (11)	−0.0122 (10)
C4	0.0888 (15)	0.0783 (13)	0.0836 (15)	0.0273 (11)	0.0096 (12)	0.0133 (11)
C3	0.1000 (17)	0.0712 (12)	0.0902 (16)	0.0264 (12)	0.0274 (13)	0.0045 (12)

Geometric parameters (Å, °)

O1—C9	1.3436 (19)	C10—H10	0.93
O1—H9	0.82	C15—C16	1.378 (2)
N2—N3	1.2382 (19)	C15—H15	0.93
N2—C12	1.428 (2)	C16—C17	1.374 (3)
N3—C14	1.432 (2)	C16—H16	0.93
N1—C7	1.278 (2)	C5—C4	1.380 (3)
N1—C6	1.427 (2)	C5—H5	0.93
C12—C13	1.376 (2)	C19—C18	1.377 (3)
C12—C11	1.394 (2)	C19—H19	0.93
C8—C13	1.390 (2)	C17—C18	1.371 (3)
C8—C9	1.412 (2)	C17—H17	0.93
C8—C7	1.443 (2)	C18—H18	0.93
C9—C10	1.387 (2)	C1—C2	1.378 (3)
C6—C5	1.373 (2)	C1—H1	0.93
C6—C1	1.383 (2)	C11—H11	0.93
C14—C19	1.375 (2)	C2—C3	1.365 (3)
C14—C15	1.394 (2)	C2—H2	0.93
C7—H7	0.996 (18)	C4—C3	1.374 (3)
C13—H13	0.93	C4—H4	0.93
C10—C11	1.378 (2)	C3—H3	0.93
C9—O1—H9	109.5	C17—C16—C15	120.44 (18)
N3—N2—C12	114.61 (14)	C17—C16—H16	119.8
N2—N3—C14	113.36 (14)	C15—C16—H16	119.8
C7—N1—C6	120.37 (14)	C6—C5—C4	120.15 (18)
C13—C12—C11	118.92 (16)	C6—C5—H5	119.9
C13—C12—N2	115.53 (15)	C4—C5—H5	119.9
C11—C12—N2	125.55 (16)	C14—C19—C18	120.18 (18)
C13—C8—C9	118.44 (15)	C14—C19—H19	119.9
C13—C8—C7	120.20 (15)	C18—C19—H19	119.9
C9—C8—C7	121.35 (15)	C18—C17—C16	119.93 (18)
O1—C9—C10	119.29 (15)	C18—C17—H17	120
O1—C9—C8	121.03 (15)	C16—C17—H17	120
C10—C9—C8	119.67 (15)	C17—C18—C19	120.35 (19)
C5—C6—C1	119.70 (16)	C17—C18—H18	119.8
C5—C6—N1	117.63 (15)	C19—C18—H18	119.8
C1—C6—N1	122.62 (15)	C2—C1—C6	119.90 (18)
C19—C14—C15	119.59 (16)	C2—C1—H1	120
C19—C14—N3	116.26 (16)	C6—C1—H1	120.1

C15—C14—N3	124.14 (16)	C10—C11—C12	120.61 (17)
N1—C7—C8	121.50 (16)	C10—C11—H11	119.7
N1—C7—H7	122.0 (10)	C12—C11—H11	119.7
C8—C7—H7	116.5 (10)	C3—C2—C1	120.06 (19)
C12—C13—C8	121.89 (15)	C3—C2—H2	120
C12—C13—H13	119.1	C1—C2—H2	120
C8—C13—H13	119.1	C3—C4—C5	119.8 (2)
C11—C10—C9	120.45 (17)	C3—C4—H4	120.1
C11—C10—H10	119.8	C5—C4—H4	120.1
C9—C10—H10	119.8	C2—C3—C4	120.42 (19)
C16—C15—C14	119.50 (17)	C2—C3—H3	119.8
C16—C15—H15	120.2	C4—C3—H3	119.8
C14—C15—H15	120.2		
C12—N2—N3—C14	178.48 (13)	C19—C14—C15—C16	−0.5 (3)
N3—N2—C12—C13	172.13 (14)	N3—C14—C15—C16	−178.89 (15)
N3—N2—C12—C11	−8.5 (3)	C14—C15—C16—C17	0.9 (3)
C13—C8—C9—O1	−179.01 (15)	C1—C6—C5—C4	2.2 (3)
C7—C8—C9—O1	1.9 (3)	N1—C6—C5—C4	179.39 (16)
C13—C8—C9—C10	0.9 (3)	C15—C14—C19—C18	0.4 (3)
C7—C8—C9—C10	−178.15 (17)	N3—C14—C19—C18	178.89 (16)
C7—N1—C6—C5	145.60 (17)	C15—C16—C17—C18	−1.1 (3)
C7—N1—C6—C1	−37.2 (2)	C16—C17—C18—C19	1.0 (3)
N2—N3—C14—C19	167.01 (15)	C14—C19—C18—C17	−0.6 (3)
N2—N3—C14—C15	−14.5 (2)	C5—C6—C1—C2	−1.7 (3)
C6—N1—C7—C8	175.83 (15)	N1—C6—C1—C2	−178.78 (16)
C13—C8—C7—N1	178.92 (15)	C9—C10—C11—C12	−0.8 (3)
C9—C8—C7—N1	−2.0 (3)	C13—C12—C11—C10	0.4 (3)
C11—C12—C13—C8	0.6 (3)	N2—C12—C11—C10	−178.94 (17)
N2—C12—C13—C8	−179.95 (15)	C6—C1—C2—C3	0.5 (3)
C9—C8—C13—C12	−1.3 (2)	C6—C5—C4—C3	−1.5 (3)
C7—C8—C13—C12	177.79 (15)	C1—C2—C3—C4	0.1 (3)
O1—C9—C10—C11	−179.98 (17)	C5—C4—C3—C2	0.3 (3)
C8—C9—C10—C11	0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H9···N1	0.82	1.85	2.579 (2)	148
C7—H7···O1^{i}	0.995 (19)	2.50 (2)	3.448 (3)	158.4 (14)

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

Fig. 1

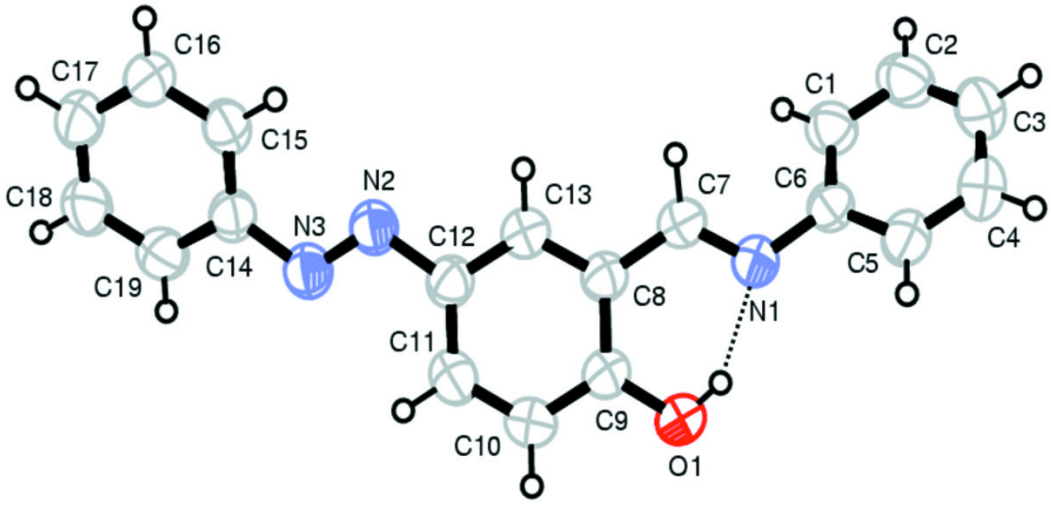
C16
C17
C15
C18
N2
N3
C12
C13
C7
C6
C1
C2
C3
C4
C5
C14
C19
C8
N1
C11
C9
C10
O1

Fig. 2