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2-[4-(Dimethylamino)benzylideneimino]-phenol

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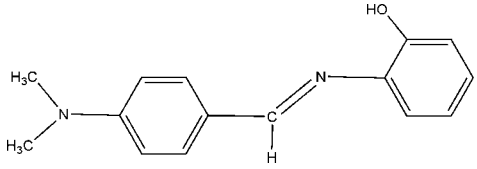
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.139; data-to-parameter ratio = 13.9.

The title compound, $C_{15}H_{16}N_2O$, has been synthesized and characterized by X-ray diffraction and FT–IR spectroscopic analysis. The dihedral angle between the aromatic ring planes is 11.17 (2)°. The molecule exhibits an intramolecular O—H···N hydrogen bond.

Related literature

For general background, see: Lindoy *et al.* (1976); Yamada (1999).



Experimental

Crystal data

$C_{15}H_{16}N_2O$
M_r = 240.30
Monoclinic, $P2_1/n$
a = 6.3549 (17) Å
b = 9.598 (3) Å
c = 21.211 (6) Å
β = 96.765 (4)°
V = 1284.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.46 × 0.43 × 0.28 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.978
6513 measured reflections
2262 independent reflections
1269 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
S = 1.01
2262 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	2.15	2.631 (3)	118

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: HG2356).

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supplementary materials

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2-[4-(Dimethylamino)benzylideneimino]phenol

Q. Wang and D.-Q. Wang

Comment

Schiff bases are used extensively as ligands in the field of coordination chemistry due to their applications in the preparation of dyes, liquid crystals and powerful corrosion inhibitors. Further more, they are used in the mechanism of many biochemical processes (Lindoy *et al.*, 1976; Yamada, 1999). We report here the synthesis and crystal structure of the title Schiff base compound, (I).

The molecular structure of (I) is shown in Fig.1. This compound contains two aromatic rings linked through an imino group. An E configuration with respect to the C═N bond is shown by the molecule, with a C—N═C—C torsion angle of 178.19 (3)°, the two six-membered aromatic rings C_1–C_6 and C_8–C_{13} form a dihedral angle of 11.17 (2)°. The bond length C7═N1 is 1.274 (3)Å in agreement with double-bond character, whereas bonds C1—N1, O1—C2, N2—C11, N2—C14 and N2—C15 are typical single bonds (Table 1).

Experimental

p-dimethylamino benzaldehyde (5 mmol, 745.9 mg) in absolute ethanol (15 ml) was added dropwise to an absolute ethanol solution (15 ml) of *o*-aminophenol (5 mmol, 545.7 mg). The mixture was heated under reflux with stirring for 6 h and then filtered. The resulting clear solution was kept at room temperature for one week, after which large yellow block-shaped crystals of the title compound suitable for X-ray diffraction analysis were obtained.

Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C—H = 0.96 Å (methylene) or 0.93 Å (aromatic), 0.93 Å (methenyl), O—H = 0.82 Å (hydroxyl) and U_{iso}(H) =1.2U_{eq}(C).

Figures

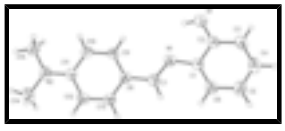

Fig. 1. The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

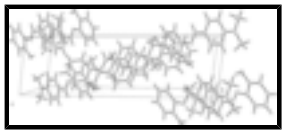

Fig. 2. The crystal packing of the title complex, viewed approximately along the *a* axis.

2-[4-(Dimethylamino)benzylideneimino]phenol

Crystal data

$C_{15}H_{16}N_2O$	F_{000} = 512
M_r = 240.30	D_x = 1.242 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1366 reflections
a = 6.3549 (17) Å	θ = 2.3–22.8º
b = 9.598 (3) Å	μ = 0.08 mm^{-1}
c = 21.211 (6) Å	T = 298 (2) K
β = 96.765 (4)º	Block, yellow
V = 1284.7 (6) Å^3	0.46 × 0.43 × 0.28 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	2262 independent reflections
Radiation source: fine-focus sealed tube	1269 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→7
T_{min} = 0.965, T_{max} = 0.978	k = −11→11
6513 measured reflections	l = −24→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.139	$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.1997P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
2262 reflections	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
163 parameters	$\Delta\rho_{min}$ = −0.14 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}
N1	0.9004 (3)	1.00454 (18)	0.12707 (8)	0.0537 (5)
N2	1.1112 (3)	0.5763 (2)	−0.09216 (9)	0.0658 (6)
O1	0.5504 (2)	1.1421 (2)	0.14064 (8)	0.0830 (6)
H1	0.5841	1.0870	0.1141	0.125*
C1	0.9087 (3)	1.0960 (2)	0.17941 (10)	0.0512 (5)
C2	0.7186 (4)	1.1638 (2)	0.18561 (10)	0.0580 (6)
C3	0.7002 (4)	1.2532 (3)	0.23541 (12)	0.0700 (7)
H3	0.5718	1.2972	0.2391	0.084*
C4	0.8718 (5)	1.2771 (3)	0.27941 (12)	0.0727 (7)
H4	0.8601	1.3381	0.3129	0.087*
C5	1.0610 (4)	1.2116 (3)	0.27443 (12)	0.0752 (7)
H5	1.1770	1.2281	0.3045	0.090*
C6	1.0791 (4)	1.1213 (2)	0.22487 (11)	0.0670 (7)
H6	1.2075	1.0769	0.2219	0.080*
C7	1.0693 (4)	0.9545 (2)	0.10922 (10)	0.0557 (6)
H7	1.1979	0.9823	0.1311	0.067*
C8	1.0753 (3)	0.8578 (2)	0.05760 (9)	0.0500 (5)
C9	0.8952 (3)	0.8138 (2)	0.01932 (10)	0.0580 (6)
H9	0.7637	0.8478	0.0271	0.070*
C10	0.9054 (4)	0.7219 (2)	−0.02952 (11)	0.0609 (6)
H10	0.7810	0.6951	−0.0541	0.073*
C11	1.0993 (3)	0.6671 (2)	−0.04338 (9)	0.0520 (6)
C12	1.2811 (4)	0.7123 (2)	−0.00509 (11)	0.0635 (6)
H12	1.4132	0.6791	−0.0127	0.076*
C13	1.2672 (3)	0.8047 (3)	0.04335 (10)	0.0625 (6)
H13	1.3911	0.8331	0.0677	0.075*
C14	1.3081 (4)	0.5123 (3)	−0.10345 (12)	0.0839 (8)
H14A	1.2847	0.4527	−0.1399	0.126*
H14B	1.3624	0.4583	−0.0670	0.126*
H14C	1.4087	0.5833	−0.1109	0.126*
C15	0.9224 (4)	0.5312 (3)	−0.13154 (12)	0.0860 (8)
H15A	0.9609	0.4685	−0.1636	0.129*
H15B	0.8510	0.6107	−0.1515	0.129*

H15C	0.8300	0.4844	−0.1058	0.129*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0543 (11)	0.0496 (11)	0.0585 (11)	0.0007 (9)	0.0128 (9)	0.0030 (9)
N2	0.0701 (14)	0.0662 (13)	0.0615 (12)	−0.0016 (11)	0.0094 (10)	−0.0093 (10)
O1	0.0568 (10)	0.0961 (14)	0.0948 (12)	0.0075 (9)	0.0035 (9)	−0.0183 (11)
C1	0.0568 (14)	0.0442 (13)	0.0537 (13)	−0.0019 (11)	0.0117 (11)	0.0057 (11)
C2	0.0537 (14)	0.0566 (15)	0.0647 (14)	0.0018 (12)	0.0115 (12)	0.0041 (12)
C3	0.0754 (18)	0.0633 (16)	0.0746 (17)	0.0154 (13)	0.0231 (14)	0.0005 (14)
C4	0.096 (2)	0.0613 (16)	0.0610 (15)	0.0118 (15)	0.0115 (15)	−0.0034 (13)
C5	0.0838 (19)	0.0736 (18)	0.0655 (15)	0.0110 (15)	−0.0027 (13)	−0.0087 (14)
C6	0.0650 (16)	0.0674 (16)	0.0679 (15)	0.0146 (13)	0.0048 (13)	−0.0032 (14)
C7	0.0554 (14)	0.0541 (14)	0.0573 (13)	−0.0036 (11)	0.0057 (11)	0.0020 (11)
C8	0.0502 (13)	0.0497 (13)	0.0511 (12)	−0.0016 (10)	0.0095 (10)	0.0028 (10)
C9	0.0462 (13)	0.0590 (15)	0.0704 (15)	−0.0002 (11)	0.0134 (11)	−0.0011 (12)
C10	0.0503 (14)	0.0664 (16)	0.0657 (14)	−0.0083 (12)	0.0057 (11)	−0.0051 (12)
C11	0.0576 (14)	0.0486 (13)	0.0504 (12)	−0.0009 (11)	0.0082 (11)	0.0060 (11)
C12	0.0547 (14)	0.0754 (17)	0.0601 (14)	0.0137 (12)	0.0053 (11)	−0.0025 (13)
C13	0.0491 (14)	0.0762 (17)	0.0605 (14)	0.0024 (12)	−0.0007 (11)	−0.0061 (13)
C14	0.097 (2)	0.0773 (19)	0.0790 (17)	0.0201 (16)	0.0160 (15)	−0.0149 (15)
C15	0.092 (2)	0.090 (2)	0.0771 (17)	−0.0174 (16)	0.0113 (15)	−0.0220 (16)

Geometric parameters (Å, °)

N1—C7	1.274 (3)	C7—H7	0.9300
N1—C1	1.411 (2)	C8—C13	1.387 (3)
N2—C11	1.362 (3)	C8—C9	1.389 (3)
N2—C14	1.439 (3)	C9—C10	1.368 (3)
N2—C15	1.445 (3)	C9—H9	0.9300
O1—C2	1.362 (3)	C10—C11	1.403 (3)
O1—H1	0.8200	C10—H10	0.9300
C1—C6	1.384 (3)	C11—C12	1.400 (3)
C1—C2	1.392 (3)	C12—C13	1.368 (3)
C2—C3	1.377 (3)	C12—H12	0.9300
C3—C4	1.369 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—H14A	0.9600
C4—C5	1.372 (3)	C14—H14B	0.9600
C4—H4	0.9300	C14—H14C	0.9600
C5—C6	1.377 (3)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C6—H6	0.9300	C15—H15C	0.9600
C7—C8	1.439 (3)		
C7—N1—C1	120.93 (19)	C9—C8—C7	123.2 (2)
C11—N2—C14	121.8 (2)	C10—C9—C8	122.0 (2)
C11—N2—C15	120.9 (2)	C10—C9—H9	119.0
C14—N2—C15	117.1 (2)	C8—C9—H9	119.0

C2—O1—H1	109.5	C9—C10—C11	121.5 (2)
C6—C1—C2	117.9 (2)	C9—C10—H10	119.3
C6—C1—N1	127.7 (2)	C11—C10—H10	119.3
C2—C1—N1	114.4 (2)	N2—C11—C12	121.6 (2)
O1—C2—C3	120.1 (2)	N2—C11—C10	121.9 (2)
O1—C2—C1	118.7 (2)	C12—C11—C10	116.6 (2)
C3—C2—C1	121.2 (2)	C13—C12—C11	121.0 (2)
C4—C3—C2	119.6 (2)	C13—C12—H12	119.5
C4—C3—H3	120.2	C11—C12—H12	119.5
C2—C3—H3	120.2	C12—C13—C8	122.5 (2)
C3—C4—C5	120.4 (2)	C12—C13—H13	118.7
C3—C4—H4	119.8	C8—C13—H13	118.7
C5—C4—H4	119.8	N2—C14—H14A	109.5
C4—C5—C6	120.0 (2)	N2—C14—H14B	109.5
C4—C5—H5	120.0	H14A—C14—H14B	109.5
C6—C5—H5	120.0	N2—C14—H14C	109.5
C5—C6—C1	120.9 (2)	H14A—C14—H14C	109.5
C5—C6—H6	119.5	H14B—C14—H14C	109.5
C1—C6—H6	119.5	N2—C15—H15A	109.5
N1—C7—C8	124.6 (2)	N2—C15—H15B	109.5
N1—C7—H7	117.7	H15A—C15—H15B	109.5
C8—C7—H7	117.7	N2—C15—H15C	109.5
C13—C8—C9	116.5 (2)	H15A—C15—H15C	109.5
C13—C8—C7	120.3 (2)	H15B—C15—H15C	109.5
C7—N1—C1—C6	−14.3 (3)	N1—C7—C8—C9	3.4 (3)
C7—N1—C1—C2	167.72 (19)	C13—C8—C9—C10	0.6 (3)
C6—C1—C2—O1	178.8 (2)	C7—C8—C9—C10	179.9 (2)
N1—C1—C2—O1	−3.0 (3)	C8—C9—C10—C11	0.1 (3)
C6—C1—C2—C3	−0.1 (3)	C14—N2—C11—C12	5.7 (3)
N1—C1—C2—C3	178.10 (18)	C15—N2—C11—C12	−179.6 (2)
O1—C2—C3—C4	−178.3 (2)	C14—N2—C11—C10	−175.4 (2)
C1—C2—C3—C4	0.6 (3)	C15—N2—C11—C10	−0.7 (3)
C2—C3—C4—C5	−0.6 (4)	C9—C10—C11—N2	−179.6 (2)
C3—C4—C5—C6	0.1 (4)	C9—C10—C11—C12	−0.6 (3)
C4—C5—C6—C1	0.4 (4)	N2—C11—C12—C13	179.3 (2)
C2—C1—C6—C5	−0.4 (3)	C10—C11—C12—C13	0.3 (3)
N1—C1—C6—C5	−178.3 (2)	C11—C12—C13—C8	0.4 (4)
C1—N1—C7—C8	178.19 (18)	C9—C8—C13—C12	−0.9 (3)
N1—C7—C8—C13	−177.4 (2)	C7—C8—C13—C12	179.8 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	2.15	2.631 (3)	118

Fig. 1

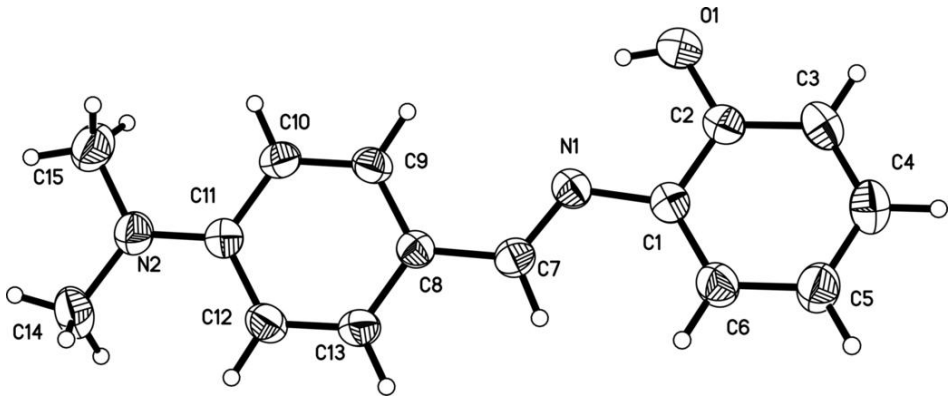

Fig. 2