Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[4-(Dimethylamino)benzylidene-amino]benzonitrile

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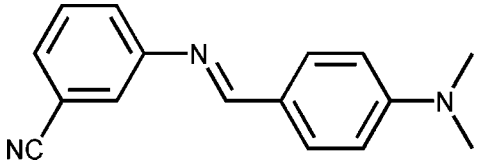
Received 19 March 2009; accepted 29 March 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.110; data-to-parameter ratio = 14.7.

The molecule of the title Schiff base, $C_{16}H_{15}N_3$, is non-planar and displays a *trans* configuration with respect to the C=N double bond. The two benzene rings make a dihedral angle of 49.24 (3)°.

Related literature

For general background on Schiff base coordination complexes, see: Garnovskii *et al.* (1993). For a related structure, see: Gong & Xu (2008)



Experimental

Crystal data

$C_{16}H_{15}N_3$
M_r = 249.31
Monoclinic, $P2_1/c$
a = 6.0924 (6) Å
b = 29.127 (3) Å
c = 7.3768 (7) Å
β = 92.924 (1)°
V = 1307.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.961, T_{max} = 1.000
(expected range = 0.947–0.985)
7018 measured reflections
2559 independent reflections
2241 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.110
S = 1.05
2559 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2436).

References

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Gong, X.-X. & Xu, H.-J. (2008). *Acta Cryst.* E**64**, o1188.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o945 [doi:10.1107/S1600536809011568]

3-[4-(Dimethylamino)benzylideneamino]benzonitrile

Hai-Jun Xu, Qin-Ying Tan, Li-Jing Cui and Kun Qian

S1. Comment

Schiff base compounds have attracted great attention and been extensively investigated in terms of their crystallography and coordination chemistry (Garnovskii *et al.*, 1993). As a continuation of our studies on Schiff-base compounds, we here report the synthesis and crystal structure of the title compound (I).

The molecule displays a *trans* configuration with respect to the C=N double bond (Fig. 1). The values of the C—C, C=C, C—N and C=N bond distances in (I) are similar to the corresponding bond lengths in 4-(2-Hydroxybenzylidene-amino)benzonitrile(Gong & Xu, 2008). The molecule is nonplanar and the dihedral angle between the planes of the two benzene rings is 49.24 (0.03) °.

S2. Experimental

All chemicals were obtained from commercial sources and directly used without further purification. 3-aminobenzonitrile (1.18 g, 10 mmol) and 4-(dimethylamino)benzaldehyde (1.49 g, 10 mmol) were dissolved in ethanol (20 ml). The mixture was heated to reflux for 6 h, then cooled to room temperature overnight and large amounts of a yellow precipitate were formed. Yellow crystals were obtained by recrystallization from ethanol(yield:2.04,82%). ^{1}H-NMR($CDCl_3$, 300 MHz): δ3.10 (s, 6 H), 6.73–6.76(d, 2 H), 7.45–7.50 (m, 4 H), 7.84–7.87 (d, 2 H), 8.27 (s, 1 H). Esi-MS: calcd for $C_{16}H_{15}N_3$ *m*/*z* 249.31, found 250.18[*M*+1]. For the X-ray diffraction analysis, suitable single crystals of compound (I) were obtained after two weeks by slow evaporation from an ethanol solution.

S3. Refinement

All H atoms attached to C were positioned geometrically and treated as riding, with C—H = 0.93 (aromatic), 0.93 (methine) or 0.96 Å (methyl) with U_{iso}(H) = 1.2Ueq(C).

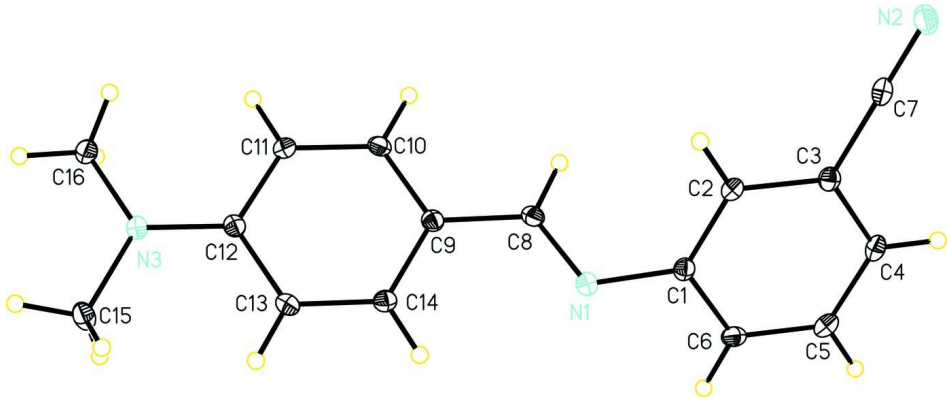

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

3-[4-(Dimethylamino)benzylideneamino]benzonitrile

Crystal data

$C_{16}H_{15}N_3$
$M_r = 249.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.0924\ (6)$ Å
$b = 29.127\ (3)$ Å
$c = 7.3768\ (7)$ Å
$\beta = 92.924\ (1)°$
$V = 1307.3\ (2)$ Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.267$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2559 reflections
$\theta = 2.8–26.0°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.961$, $T_{max} = 1.000$
7018 measured reflections
2559 independent reflections
2241 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.8°$
$h = -7\rightarrow7$
$k = -35\rightarrow25$
$l = -9\rightarrow8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.110$
$S = 1.05$
2559 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.1755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.61108 (15)	0.27979 (3)	0.59956 (13)	0.0190 (2)
N2	0.28428 (16)	0.47022 (3)	0.70360 (14)	0.0263 (3)
N3	0.14557 (15)	0.08098 (3)	0.61116 (13)	0.0189 (2)
C1	0.65373 (17)	0.32723 (4)	0.58571 (14)	0.0171 (2)
C2	0.50894 (17)	0.36071 (4)	0.64200 (14)	0.0169 (2)
H2A	0.3790	0.3523	0.6941	0.020*
C3	0.56051 (17)	0.40708 (4)	0.61955 (14)	0.0175 (3)
C4	0.75672 (18)	0.42049 (4)	0.54437 (14)	0.0190 (3)
H4A	0.7889	0.4514	0.5285	0.023*
C5	0.90207 (18)	0.38678 (4)	0.49403 (15)	0.0207 (3)
H5A	1.0341	0.3951	0.4452	0.025*
C6	0.85265 (17)	0.34081 (4)	0.51572 (15)	0.0197 (3)
H6A	0.9532	0.3186	0.4833	0.024*
C7	0.40682 (18)	0.44200 (4)	0.66975 (15)	0.0198 (3)
C8	0.42252 (17)	0.26531 (4)	0.53867 (14)	0.0174 (3)
H8A	0.3245	0.2863	0.4847	0.021*
C9	0.35526 (17)	0.21769 (4)	0.55017 (14)	0.0171 (3)
C10	0.14627 (17)	0.20363 (4)	0.48467 (15)	0.0188 (3)
H10A	0.0515	0.2251	0.4298	0.023*
C11	0.07713 (17)	0.15861 (4)	0.49941 (15)	0.0187 (3)
H11A	−0.0617	0.1502	0.4526	0.022*
C12	0.21502 (17)	0.12527 (4)	0.58471 (14)	0.0162 (2)
C13	0.42785 (17)	0.13953 (4)	0.64815 (14)	0.0176 (3)
H13A	0.5238	0.1182	0.7028	0.021*
C14	0.49460 (17)	0.18430 (4)	0.63022 (14)	0.0175 (2)
H14A	0.6355	0.1926	0.6722	0.021*
C15	0.30017 (19)	0.04552 (4)	0.67163 (16)	0.0229 (3)
H15A	0.3783	0.0553	0.7812	0.034*
H15B	0.4027	0.0401	0.5793	0.034*
H15C	0.2218	0.0177	0.6943	0.034*
C16	−0.06638 (18)	0.06583 (4)	0.53393 (16)	0.0222 (3)
H16A	−0.1766	0.0881	0.5599	0.033*
H16B	−0.1035	0.0368	0.5860	0.033*
H16C	−0.0590	0.0626	0.4049	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0189 (5)	0.0166 (5)	0.0216 (5)	0.0000 (4)	0.0009 (4)	0.0003 (4)
N2	0.0295 (5)	0.0194 (5)	0.0304 (6)	−0.0017 (4)	0.0058 (4)	−0.0035 (4)
N3	0.0188 (5)	0.0154 (5)	0.0224 (5)	−0.0007 (4)	0.0011 (4)	0.0008 (4)
C1	0.0179 (5)	0.0166 (5)	0.0162 (5)	−0.0016 (4)	−0.0034 (4)	0.0017 (4)
C2	0.0150 (5)	0.0187 (6)	0.0170 (5)	−0.0024 (4)	0.0005 (4)	0.0002 (4)
C3	0.0190 (5)	0.0182 (6)	0.0151 (5)	−0.0014 (4)	−0.0010 (4)	−0.0016 (4)
C4	0.0211 (5)	0.0184 (6)	0.0172 (5)	−0.0060 (4)	−0.0022 (4)	0.0005 (4)
C5	0.0161 (5)	0.0262 (6)	0.0196 (6)	−0.0049 (5)	0.0002 (4)	0.0005 (5)
C6	0.0149 (5)	0.0231 (6)	0.0209 (5)	0.0023 (4)	−0.0010 (4)	−0.0014 (4)
C7	0.0225 (6)	0.0170 (6)	0.0199 (5)	−0.0056 (5)	0.0009 (4)	−0.0009 (4)
C8	0.0165 (5)	0.0171 (6)	0.0187 (5)	0.0033 (4)	0.0027 (4)	0.0015 (4)
C9	0.0171 (5)	0.0170 (5)	0.0174 (6)	0.0012 (4)	0.0039 (4)	0.0001 (4)
C10	0.0164 (5)	0.0180 (6)	0.0221 (6)	0.0042 (4)	0.0013 (4)	0.0018 (4)
C11	0.0147 (5)	0.0196 (6)	0.0219 (6)	−0.0004 (4)	0.0014 (4)	−0.0001 (4)
C12	0.0181 (5)	0.0162 (5)	0.0148 (5)	0.0015 (4)	0.0046 (4)	−0.0003 (4)
C13	0.0186 (5)	0.0176 (5)	0.0167 (5)	0.0041 (4)	0.0013 (4)	0.0013 (4)
C14	0.0162 (5)	0.0189 (5)	0.0175 (5)	0.0008 (4)	0.0012 (4)	−0.0007 (4)
C15	0.0292 (6)	0.0158 (6)	0.0233 (6)	0.0000 (5)	−0.0039 (5)	0.0009 (4)
C16	0.0198 (6)	0.0184 (6)	0.0285 (6)	−0.0020 (4)	0.0035 (5)	−0.0007 (5)

Geometric parameters (Å, º)

N1—C8	1.2833 (14)	C8—H8A	0.9300
N1—C1	1.4105 (14)	C9—C10	1.3998 (15)
N2—C7	1.1466 (15)	C9—C14	1.4013 (15)
N3—C12	1.3746 (14)	C10—C11	1.3834 (16)
N3—C15	1.4526 (14)	C10—H10A	0.9300
N3—C16	1.4531 (14)	C11—C12	1.4109 (15)
C1—C2	1.3924 (15)	C11—H11A	0.9300
C1—C6	1.3984 (15)	C12—C13	1.4181 (15)
C2—C3	1.3986 (15)	C13—C14	1.3743 (15)
C2—H2A	0.9300	C13—H13A	0.9300
C3—C4	1.3988 (15)	C14—H14A	0.9300
C3—C7	1.4434 (16)	C15—H15A	0.9600
C4—C5	1.3854 (16)	C15—H15B	0.9600
C4—H4A	0.9300	C15—H15C	0.9600
C5—C6	1.3836 (16)	C16—H16A	0.9600
C5—H5A	0.9300	C16—H16B	0.9600
C6—H6A	0.9300	C16—H16C	0.9600
C8—C9	1.4501 (15)		
C8—N1—C1	117.49 (9)	C14—C9—C8	121.43 (10)
C12—N3—C15	120.76 (9)	C11—C10—C9	121.69 (10)
C12—N3—C16	120.20 (9)	C11—C10—H10A	119.2
C15—N3—C16	116.99 (9)	C9—C10—H10A	119.2

C2—C1—C6	119.09 (10)	C10—C11—C12	120.71 (10)
C2—C1—N1	122.86 (10)	C10—C11—H11A	119.6
C6—C1—N1	118.04 (10)	C12—C11—H11A	119.6
C1—C2—C3	119.44 (10)	N3—C12—C11	121.91 (9)
C1—C2—H2A	120.3	N3—C12—C13	120.73 (10)
C3—C2—H2A	120.3	C11—C12—C13	117.33 (10)
C2—C3—C4	121.21 (10)	C14—C13—C12	121.08 (10)
C2—C3—C7	119.83 (10)	C14—C13—H13A	119.5
C4—C3—C7	118.94 (10)	C12—C13—H13A	119.5
C5—C4—C3	118.64 (10)	C13—C14—C9	121.54 (10)
C5—C4—H4A	120.7	C13—C14—H14A	119.2
C3—C4—H4A	120.7	C9—C14—H14A	119.2
C6—C5—C4	120.59 (10)	N3—C15—H15A	109.5
C6—C5—H5A	119.7	N3—C15—H15B	109.5
C4—C5—H5A	119.7	H15A—C15—H15B	109.5
C5—C6—C1	120.95 (10)	N3—C15—H15C	109.5
C5—C6—H6A	119.5	H15A—C15—H15C	109.5
C1—C6—H6A	119.5	H15B—C15—H15C	109.5
N2—C7—C3	177.67 (13)	N3—C16—H16A	109.5
N1—C8—C9	123.00 (10)	N3—C16—H16B	109.5
N1—C8—H8A	118.5	H16A—C16—H16B	109.5
C9—C8—H8A	118.5	N3—C16—H16C	109.5
C10—C9—C14	117.61 (10)	H16A—C16—H16C	109.5
C10—C9—C8	120.95 (10)	H16B—C16—H16C	109.5